
py-pde Documentation

Release unknown

David Zwicker

Apr 04, 2024

CONTENTS

1	Getting started	3
1.1	When (not) to use the package	3
1.2	Installation	3
1.2.1	Install using pip	3
1.2.2	Install using conda	4
1.2.3	Install from source	4
	Required prerequisites	4
	Optional packages	4
	Downloading <i>py-pde</i>	5
1.3	Package overview	5
2	Examples	7
2.1	Plotting a vector field	7
2.2	Solving Laplace's equation in 2d	8
2.3	Plotting a scalar field in cylindrical coordinates	9
2.4	Solving Poisson's equation in 1d	10
2.5	Simple diffusion equation	11
2.6	Kuramoto-Sivashinsky - Using <i>PDE</i> class	12
2.7	Spherically symmetric PDE	13
2.8	Diffusion on a Cartesian grid	15
2.9	Stochastic simulation	16
2.10	Time-dependent boundary conditions	17
2.11	Setting boundary conditions	18
2.12	1D problem - Using <i>PDE</i> class	19
2.13	Heterogeneous boundary conditions	20
2.14	Brusselator - Using the <i>PDE</i> class	22
2.15	Writing and reading trajectory data	23
2.16	Diffusion equation with spatial dependence	24
2.17	Using simulation trackers	25
2.18	Schrödinger's Equation	26
2.19	Kuramoto-Sivashinsky - Using custom class	28
2.20	Custom Class for coupled PDEs	29
2.21	1D problem - Using custom class	31
2.22	Visualizing a scalar field	32
2.23	Kuramoto-Sivashinsky - Compiled methods	33
2.24	Solver comparison	35
2.25	Custom PDE class: SIR model	37
2.26	Brusselator - Using custom class	39
3	User manual	41

3.1	Mathematical basics	41
3.1.1	Curvilinear coordinates	41
	Polar coordinates	41
	Spherical coordinates	41
	Cylindrical coordinates	42
3.1.2	Spatial discretization	42
3.1.3	Temporal evolution	43
3.2	Basic usage	43
3.2.1	Defining the geometry	43
3.2.2	Initializing a field	43
3.2.3	Specifying the PDE	44
3.2.4	Running the simulation	44
3.2.5	Analyzing the results	44
3.3	Advanced usage	45
3.3.1	Boundary conditions	45
3.3.2	Expressions	46
3.3.3	Custom PDE classes	47
3.3.4	Low-level operators	48
	Differential operators	48
	Field integration	49
	Field interpolation	49
	Inner products	49
3.3.5	Numba-accelerated PDEs	50
3.3.6	Configuration parameters	51
3.4	Performance	52
3.4.1	Measuring performance	52
3.4.2	Improving performance	53
3.4.3	Multiprocessing using MPI	54
3.5	Contributing code	55
3.5.1	Structure of the package	55
3.5.2	Extending functionality	55
3.5.3	Design choices	55
3.5.4	Coding style	55
3.5.5	Running unit tests	56
3.6	Citing the package	56
3.7	Code of Conduct	57
3.7.1	Our Pledge	57
3.7.2	Our Standards	57
3.7.3	Our Responsibilities	57
3.7.4	Scope	57
3.7.5	Enforcement	58
3.7.6	Attribution	58
4	Reference manual	59
4.1	pde.fields package	59
4.1.1	pde.fields.base module	60
4.1.2	pde.fields.collection module	74
4.1.3	pde.fields.scalar module	80
4.1.4	pde.fields.tensorial module	85
4.1.5	pde.fields.vectorial module	89
4.2	pde.grids package	94
4.2.1	pde.grids.boundaries package	95
	Boundary conditions	95
	Boundaries overview	96

	pde.grids.boundaries.axes module	97
	pde.grids.boundaries.axis module	99
	pde.grids.boundaries.local module	102
4.2.2	pde.grids.coordinates package	127
	pde.grids.coordinates.base module	127
	pde.grids.coordinates.bipolar module	130
	pde.grids.coordinates.bispherical module	130
	pde.grids.coordinates.cartesian module	131
	pde.grids.coordinates.cylindrical module	131
	pde.grids.coordinates.polar module	132
	pde.grids.coordinates.spherical module	132
4.2.3	pde.grids.operators package	133
	pde.grids.operators.cartesian module	133
	pde.grids.operators.common module	135
	pde.grids.operators.cylindrical_sym module	136
	pde.grids.operators.polar_sym module	139
	pde.grids.operators.spherical_sym module	141
4.2.4	pde.grids.base module	144
4.2.5	pde.grids.cartesian module	157
4.2.6	pde.grids.cylindrical module	161
4.2.7	pde.grids.spherical module	165
4.3	pde.pdes package	170
4.3.1	pde.pdes.allen_cahn module	170
4.3.2	pde.pdes.base module	171
4.3.3	pde.pdes.cahn_hilliard module	175
4.3.4	pde.pdes.diffusion module	176
4.3.5	pde.pdes.kpz_interface module	177
4.3.6	pde.pdes.kuramoto_sivashinsky module	178
4.3.7	pde.pdes.laplace module	180
4.3.8	pde.pdes.pde module	181
4.3.9	pde.pdes.swift_hohenberg module	183
4.3.10	pde.pdes.wave module	184
4.4	pde.solvers package	185
4.4.1	pde.solvers.adams_bashforth module	188
4.4.2	pde.solvers.base module	188
4.4.3	pde.solvers.controller module	190
4.4.4	pde.solvers.crank_nicolson module	192
4.4.5	pde.solvers.explicit module	192
4.4.6	pde.solvers.explicit_mpi module	193
4.4.7	pde.solvers.implicit module	194
4.4.8	pde.solvers.scipy module	195
4.5	pde.storage package	195
4.5.1	pde.storage.base module	196
4.5.2	pde.storage.file module	201
4.5.3	pde.storage.memory module	202
4.5.4	pde.storage.movie module	204
4.6	pde.tools package	207
4.6.1	pde.tools.cache module	207
4.6.2	pde.tools.config module	213
4.6.3	pde.tools.cuboid module	214
4.6.4	pde.tools.docstrings module	217
4.6.5	pde.tools.expressions module	217
4.6.6	pde.tools.ffmpeg module	223
4.6.7	pde.tools.math module	225

4.6.8	pde.tools.misc module	226
4.6.9	pde.tools.mpi module	229
4.6.10	pde.tools.numba module	231
4.6.11	pde.tools.output module	233
4.6.12	pde.tools.parameters module	234
4.6.13	pde.tools.parse_duration module	237
4.6.14	pde.tools.plotting module	237
4.6.15	pde.tools.spectral module	242
4.6.16	pde.tools.typing module	243
4.7	pde.trackers package	243
4.7.1	pde.trackers.base module	244
4.7.2	pde.trackers.interactive module	247
4.7.3	pde.trackers.interrupts module	249
4.7.4	pde.trackers.trackers module	253
4.8	pde.visualization package	262
4.8.1	pde.visualization.movies module	262
4.8.2	pde.visualization.plotting module	264
Python Module Index		271
Index		273

The *py-pde* python package provides methods and classes useful for solving partial differential equations (PDEs) of the form

$$\partial_t u(\boldsymbol{x}, t) = \mathcal{D}[u(\boldsymbol{x}, t)] + \eta(u, \boldsymbol{x}, t) ,$$

where \mathcal{D} is a (non-linear) operator containing spatial derivatives that defines the time evolution of a (set of) physical fields u with possibly tensorial character, which depend on spatial coordinates \boldsymbol{x} and time t . The framework also supports stochastic differential equations in the Itô representation, where the noise is represented by η above.

The main audience for the package are researchers and students who want to investigate the behavior of a PDE and get an intuitive understanding of the role of the different terms and the boundary conditions. To support this, *py-pde* evaluates PDEs using the methods of lines with a finite-difference approximation of the differential operators. Consequently, the mathematical operator \mathcal{D} can be naturally translated to a function evaluating the evolution rate of the PDE.



Contents

GETTING STARTED

1.1 When (not) to use the package

py-pde provides a straight-forward way to simulate partial differential equations (PDEs) using a finite-difference scheme. Advantages of this approach include:

- Supports non-linear PDEs with complex boundary conditions.
- Direct specification of the evolution equations using a syntax that is similar to the underlying mathematical equations.
- Supports collections of multiple fields of vectorial or tensorial character.

However, there are of course also disadvantages to the approach taken by *py-pde*:

- Only suited for simple geometries (like rectangles, disks, or cylinders) with a fixed discretization.
- Optimized for PDEs that describe the time-evolution of a physical system. Neither time-independent systems nor integro-differential equation are fully supported.
- Finite-differences can lead to numerical instabilities.
- Provided generic solvers might not be most suitable choice for particular equations.

1.2 Installation

The *py-pde* package is developed for python 3.9 and has been tested up to version 3.12 under Linux, Windows, and macOS. Before you can start using the package, you need to install it using one of the following methods.

1.2.1 Install using pip

The package is available on [pypi](#), so you should be able to install it by running

```
pip install py-pde
```

In order to have all features of the package available, you might also want to install the following optional packages:

```
pip install h5py pandas pyfftw tqdm
```

Moreover, **ffmpeg** needs to be installed and for creating movies.

1.2.2 Install using conda

The *py-pde* package is also available on [conda](#) using the *conda-forge* channel. You can thus install it using

```
conda install -c conda-forge py-pde
```

This installation includes many dependencies to have most features of *py-pde*.

1.2.3 Install from source

Installing from source can be necessary if the pypi installation does not work or if the latest source code should be installed from github.

Required prerequisites

The code builds on other python packages, which need to be installed for *py-pde* to function properly. The required packages are listed in the table below:

Package	Minimal version	Usage
matplotlib	3.1	Visualizing results
numba	0.59	Just-in-time compilation to accelerate numerics
numpy	1.22	Handling numerical data
scipy	1.10	Miscellaneous scientific functions
sympy	1.9	Dealing with user-defined mathematical expressions
tqdm	4.66	Display progress bars during calculations

The simplest way to install these packages is to use the `requirements.txt` in the base folder:

```
pip install -r requirements.txt
```

Alternatively, these package can be installed via your operating system's package manager, e.g. using **macports**, **homebrew**, or **conda**. The package versions given above are minimal requirements, although this is not tested systematically. Generally, it should help to install the latest version of the package.

Optional packages

The following packages should be installed to use some miscellaneous features:

Package	Minimal version	Usage
ffmpeg-python	0.2	Reading and writing videos
h5py	2.10	Storing data in the hierarchical file format
ipywidgets	8	Jupyter notebook support
mpi4py	3	Parallel processing using MPI
napari	0.4.8	Displaying images interactively
numba-mpi	0.22	Parallel processing using MPI+numba
pandas	2	Handling tabular data
pyfftw	0.12	Faster Fourier transforms
rocket-fft	0.2.4	Numba-compiled fast Fourier transforms

For making movies, the `ffmpeg` should be available. Additional packages might be required for running the tests in the folder `tests` and to build the documentation in the folder `docs`. These packages are listed in the files `requirements.txt` in the respective folders.

Downloading *py-pde*

The package can be simply checked out from github.com/zwicker-group/py-pde. To import the package from any python session, it might be convenient to include the root folder of the package into the `PYTHONPATH` environment variable.

This documentation can be built by calling the `make html` in the `docs` folder. The final documentation will be available in `docs/build/html`. Note that a LaTeX documentation can be build using `make latexpdf`.

1.3 Package overview

The main aim of the *pde* package is to simulate partial differential equations in simple geometries. Here, the time evolution of a PDE is determined using the method of lines by explicitly discretizing space using fixed grids. The differential operators are implemented using the *finite difference method*. For simplicity, we consider only regular, orthogonal grids, where each axis has a uniform discretization and all axes are (locally) orthogonal. Currently, we support simulations on *CartesianGrid*, *PolarSymGrid*, *SphericalSymGrid*, and *CylindricalSymGrid*, with and without periodic boundaries where applicable.

Fields are defined by specifying values at the grid points using the classes *ScalarField*, *VectorField*, and *Tensor2Field*. These classes provide methods for applying differential operators to the fields, e.g., the result of applying the Laplacian to a scalar field is returned by calling the method `laplace()`, which returns another instance of *ScalarField*, whereas `gradient()` returns a *VectorField*. Combining these functions with ordinary arithmetics on fields allows to represent the right hand side of many partial differential equations that appear in physics. Importantly, the differential operators work with flexible boundary conditions.

The PDEs to solve are represented as a separate class inheriting from *PDEBase*. One example defined in this package is the diffusion equation implemented as *DiffusionPDE*, but more specific situations need to be implemented by the user. Most notably, PDEs can be specified by their expression using the convenient *PDE* class.

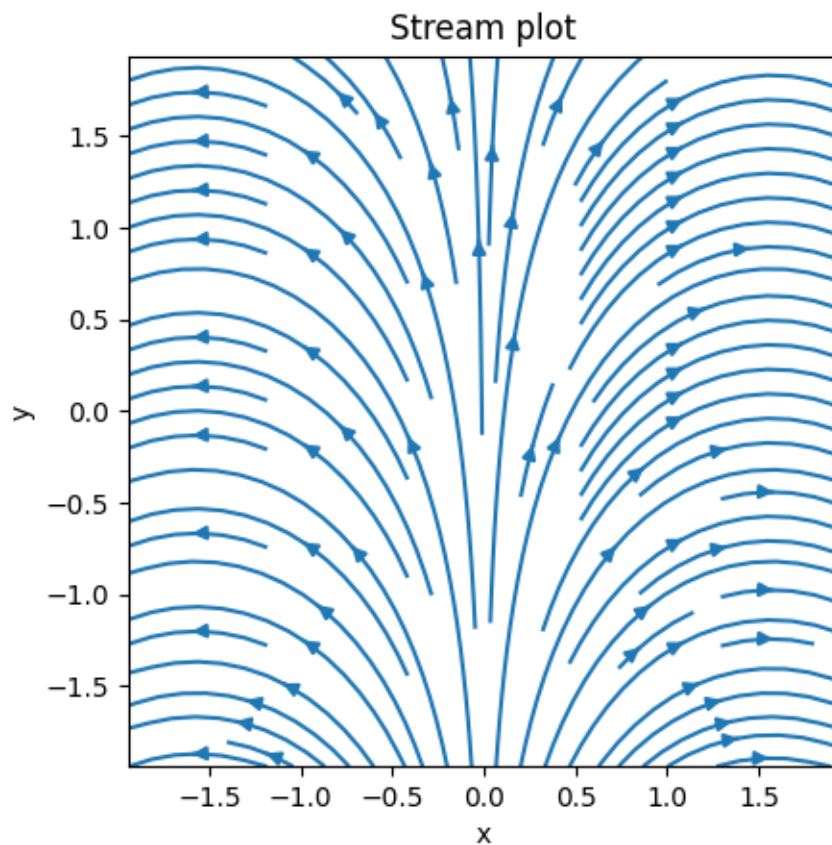
The PDEs are solved using solver classes, where a simple explicit solver is implemented by *ExplicitSolver*, but more advanced implementations can be done. To obtain more details during the simulation, trackers can be attached to the solver instance, which analyze intermediate states periodically. Typical trackers include *ProgressTracker* (display simulation progress), *PlotTracker* (display images of the simulation), and *SteadyStateTracker* (aborting simulation when a stationary state is reached). Others can be found in the *trackers* module. Moreover, we provide *MemoryStorage* and *FileStorage*, which can be used as trackers to store the intermediate state to memory and to a file, respectively.

EXAMPLES

These are example scripts using the *py-pde* package, which illustrates some of the most important features of the package.

2.1 Plotting a vector field

This example shows how to initialize and visualize the vector field $\mathbf{u} = (\sin(x), \cos(x))$.



```
from pde import CartesianGrid, VectorField  
grid = CartesianGrid([[-2, 2], [-2, 2]], 32)
```

(continues on next page)

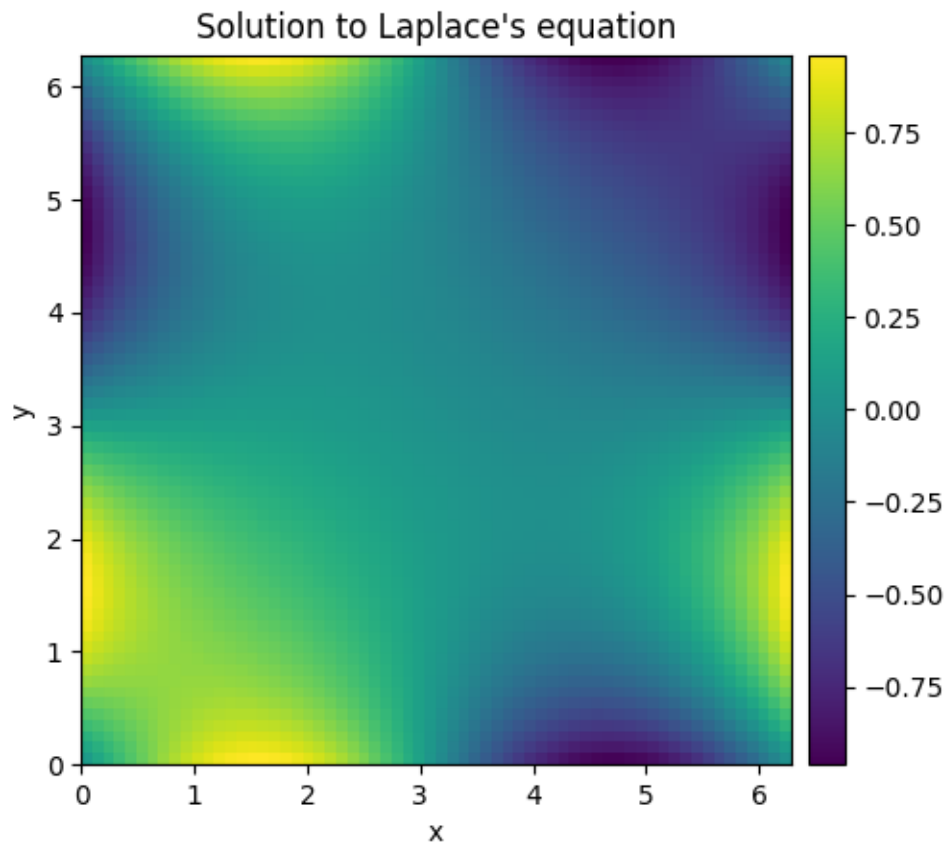
(continued from previous page)

```
field = VectorField.from_expression(grid, ["sin(x)", "cos(x)"])
field.plot(method="streamplot", title="Stream plot")
```

Total running time of the script: (0 minutes 0.508 seconds)

2.2 Solving Laplace's equation in 2d

This example shows how to solve a 2d Laplace equation with spatially varying boundary conditions.



```
import numpy as np

from pde import CartesianGrid, solve_laplace_equation

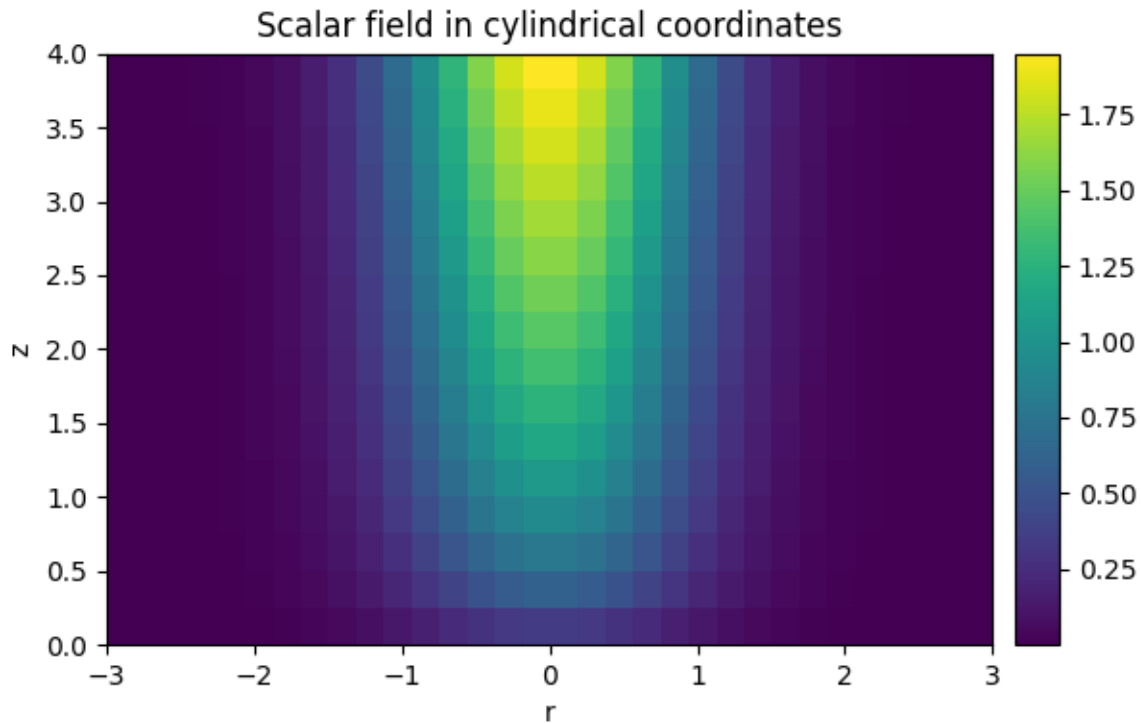
grid = CartesianGrid([0, 2 * np.pi] * 2, 64)
bcs = [{"value": "sin(y)"}, {"value": "sin(x)"}]

res = solve_laplace_equation(grid, bcs)
res.plot()
```

Total running time of the script: (0 minutes 0.650 seconds)

2.3 Plotting a scalar field in cylindrical coordinates

This example shows how to initialize and visualize the scalar field $u = \sqrt{z} \exp(-r^2)$ in cylindrical coordinates.



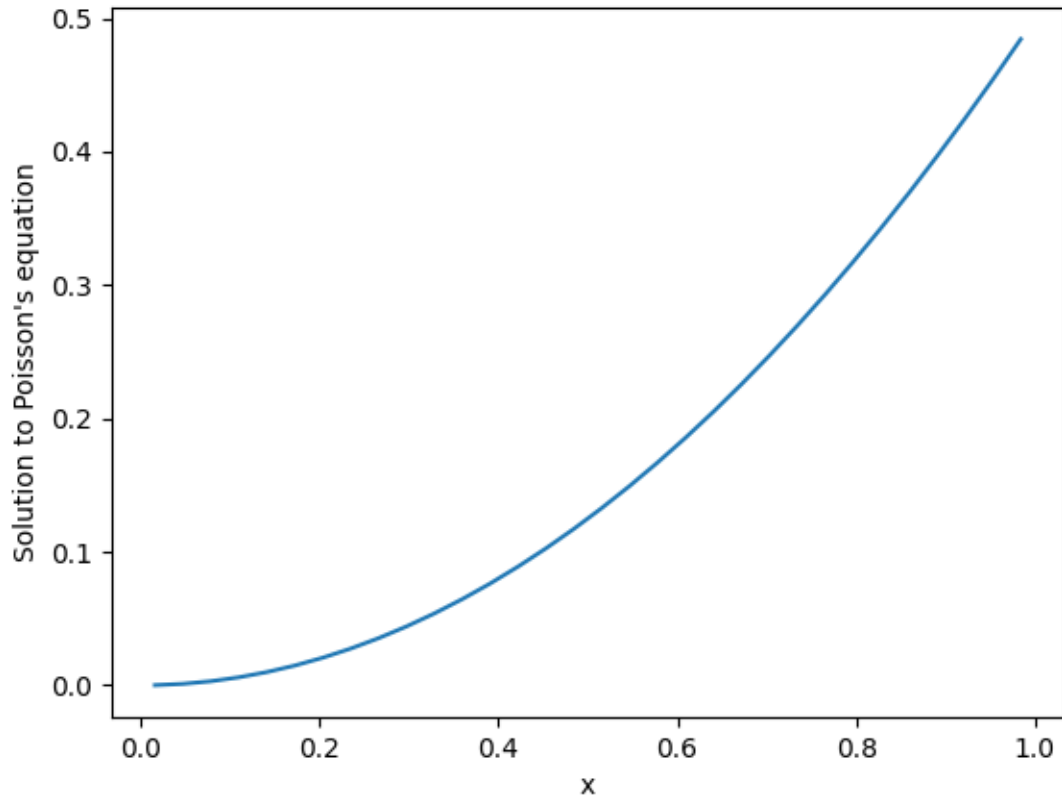
```
from pde import CylindricalSymGrid, ScalarField

grid = CylindricalSymGrid(radius=3, bounds_z=[0, 4], shape=16)
field = ScalarField.from_expression(grid, "sqrt(z) * exp(-r**2)")
field.plot(title="Scalar field in cylindrical coordinates")
```

Total running time of the script: (0 minutes 0.384 seconds)

2.4 Solving Poisson's equation in 1d

This example shows how to solve a 1d Poisson equation with boundary conditions.



```
from pde import CartesianGrid, ScalarField, solve_poisson_equation

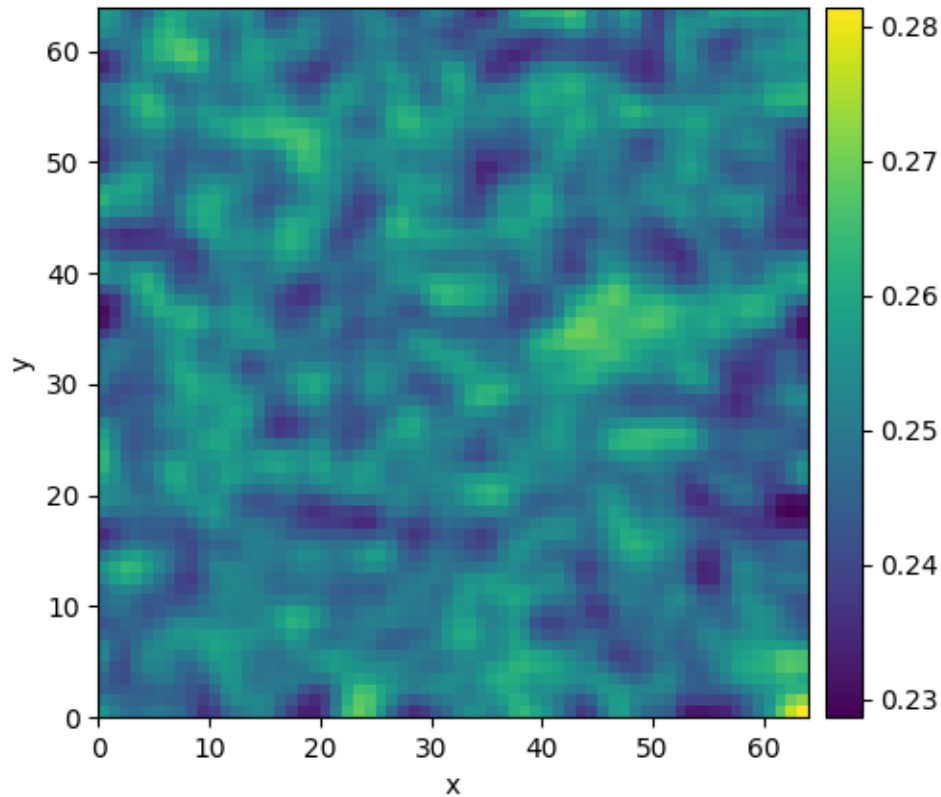
grid = CartesianGrid([[0, 1]], 32, periodic=False)
field = ScalarField(grid, 1)
result = solve_poisson_equation(field, bc=[{"value": 0}, {"derivative": 1}])

result.plot()
```

Total running time of the script: (0 minutes 0.100 seconds)

2.5 Simple diffusion equation

This example solves a simple diffusion equation in two dimensions.



```

0%|          | 0/10.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/10.0 [00:00<?, ?it/s]
0%|          | 0/10.0 [00:08<?, ?it/s]
0%|          | 0.004/10.0 [00:09<6:15:31, 2254.00s/it]
0%|          | 0.021/10.0 [00:09<1:11:24, 429.36s/it]
8%|█         | 0.76/10.0 [00:09<01:49, 11.88s/it]
72%|██████   | 7.167/10.0 [00:09<00:03, 1.28s/it]
72%|██████   | 7.167/10.0 [00:09<00:03, 1.28s/it]
100%|███████ | 10.0/10.0 [00:09<00:00, 1.09it/s]
100%|███████ | 10.0/10.0 [00:09<00:00, 1.09it/s]

```

```

from pde import DiffusionPDE, ScalarField, UnitGrid

grid = UnitGrid([64, 64]) # generate grid
state = ScalarField.random_uniform(grid, 0.2, 0.3) # generate initial condition

```

(continues on next page)

(continued from previous page)

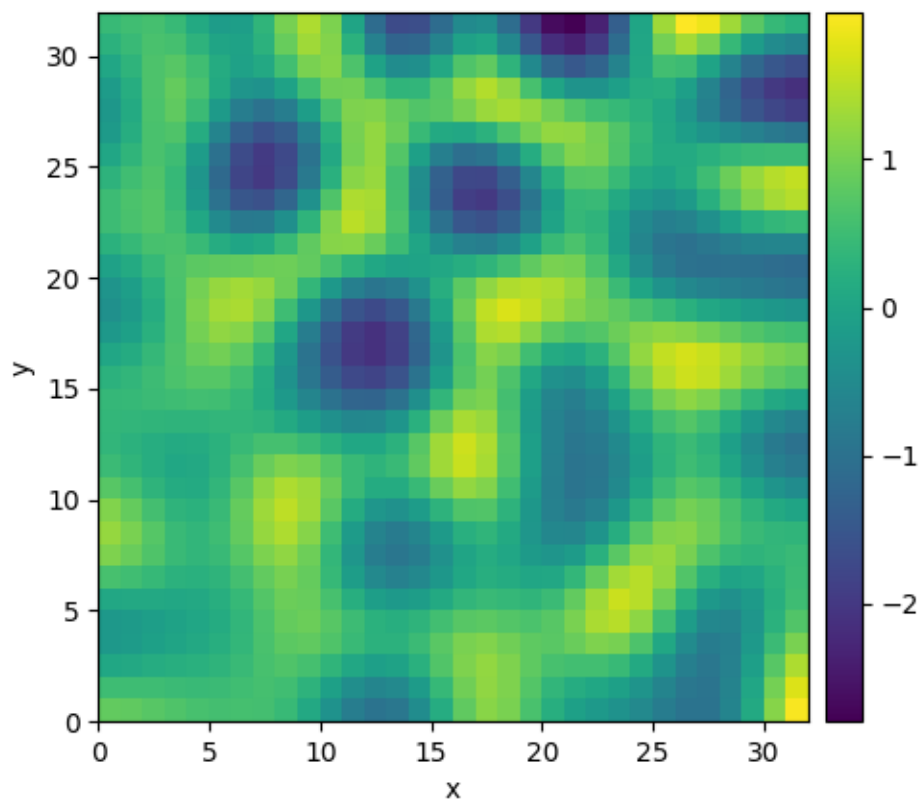
```
eq = DiffusionPDE(diffusivity=0.1) # define the pde
result = eq.solve(state, t_range=10)
result.plot()
```

Total running time of the script: (0 minutes 9.340 seconds)

2.6 Kuramoto-Sivashinsky - Using *PDE* class

This example implements a scalar PDE using the *PDE*. We here consider the Kuramoto–Sivashinsky equation, which for instance describes the dynamics of flame fronts:

$$\partial_t u = -\frac{1}{2}|\nabla u|^2 - \nabla^2 u - \nabla^4 u$$



```
0%|          | 0/10.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/10.0 [00:00<?, ?it/s]
0%|          | 0/10.0 [00:13<?, ?it/s]
0%|          | 0.01/10.0 [00:24<6:41:20, 2410.41s/it]
0%|          | 0.02/10.0 [00:24<3:20:28, 1205.22s/it]
1%|          | 0.12/10.0 [00:24<33:04, 200.87s/it]
59%|██████   | 5.91/10.0 [00:24<00:16, 4.08s/it]
```

(continues on next page)

(continued from previous page)

```

59% |██████████| 5.91/10.0 [00:24<00:16, 4.08s/it]
100% |██████████| 10.0/10.0 [00:24<00:00, 2.41s/it]
100% |██████████| 10.0/10.0 [00:24<00:00, 2.41s/it]

```

```

from pde import PDE, ScalarField, UnitGrid

grid = UnitGrid([32, 32]) # generate grid
state = ScalarField.random_uniform(grid) # generate initial condition

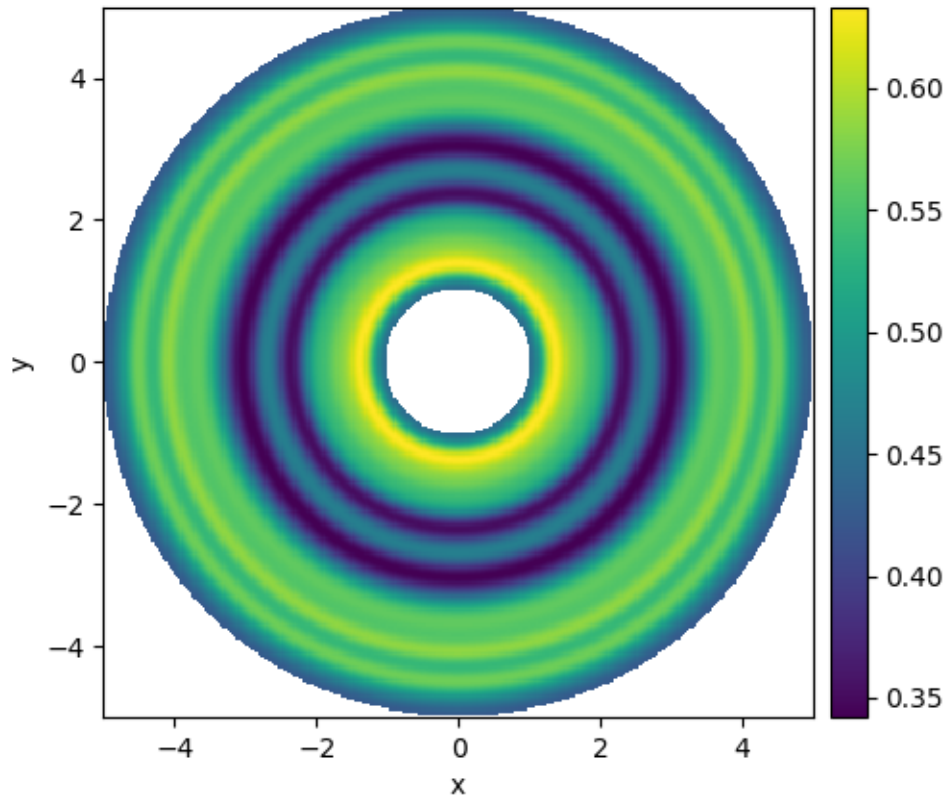
eq = PDE({"u": "-gradient_squared(u) / 2 - laplace(u + laplace(u))"}) # define the
↪pde
result = eq.solve(state, t_range=10, dt=0.01)
result.plot()

```

Total running time of the script: (0 minutes 24.288 seconds)

2.7 Spherically symmetric PDE

This example illustrates how to solve a PDE in a spherically symmetric geometry.



```

0%|          | 0/0.1 [00:00<?, ?it/s]
Initializing: 0%|          | 0/0.1 [00:00<?, ?it/s]
0%|          | 0/0.1 [00:01<?, ?it/s]
8%|█         | 0.008/0.1 [00:02<00:23, 252.25s/it]
44%|███      | 0.044/0.1 [00:02<00:02, 45.87s/it]
44%|███      | 0.044/0.1 [00:02<00:02, 45.88s/it]
100%|███████| 0.1/0.1 [00:02<00:00, 20.19s/it]
100%|███████| 0.1/0.1 [00:02<00:00, 20.19s/it]

```

```

from pde import DiffusionPDE, ScalarField, SphericalSymGrid

grid = SphericalSymGrid(radius=[1, 5], shape=128) # generate grid
state = ScalarField.random_uniform(grid) # generate initial condition

eq = DiffusionPDE(0.1) # define the PDE
result = eq.solve(state, t_range=0.1, dt=0.001)

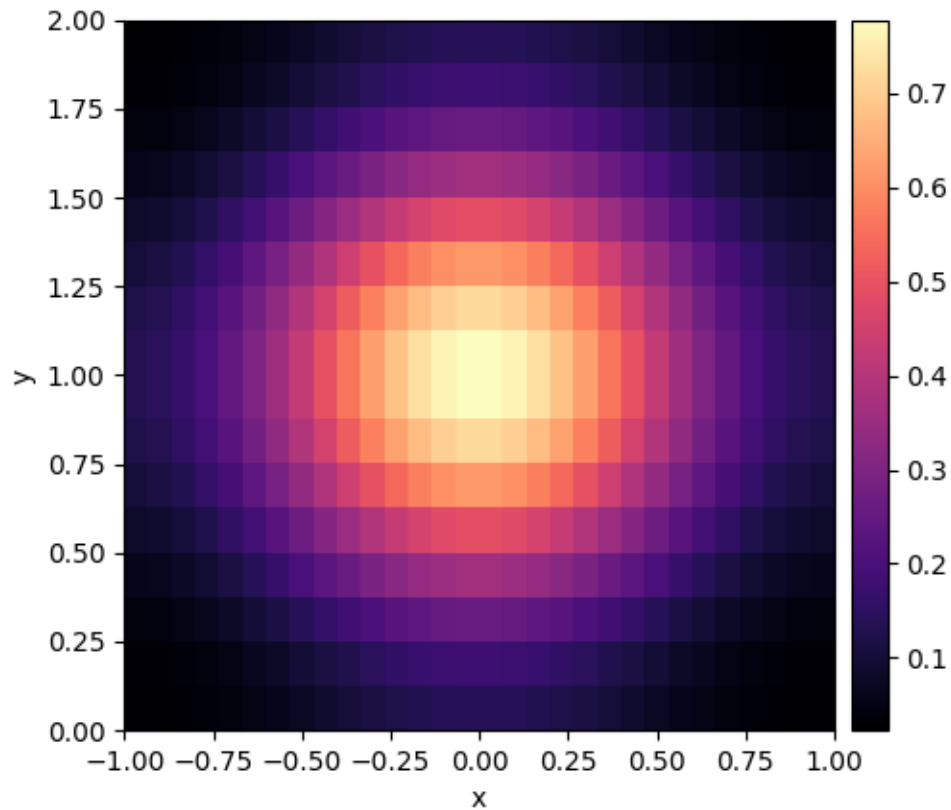
result.plot(kind="image")

```

Total running time of the script: (0 minutes 2.190 seconds)

2.8 Diffusion on a Cartesian grid

This example shows how to solve the diffusion equation on a Cartesian grid.



```

0%|          | 0/1.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/1.0 [00:00<?, ?it/s]
0%|          | 0/1.0 [00:03<?, ?it/s]
1%|          | 0.01/1.0 [00:03<06:35, 399.64s/it]
4%|          | 0.04/1.0 [00:03<01:35, 99.92s/it]
4%|          | 0.04/1.0 [00:03<01:35, 99.95s/it]
100%|██████████| 1.0/1.0 [00:03<00:00, 4.00s/it]
100%|██████████| 1.0/1.0 [00:03<00:00, 4.00s/it]

```

```

from pde import CartesianGrid, DiffusionPDE, ScalarField

grid = CartesianGrid([[-1, 1], [0, 2]], [30, 16]) # generate grid
state = ScalarField(grid) # generate initial condition
state.insert([0, 1], 1)

```

(continues on next page)

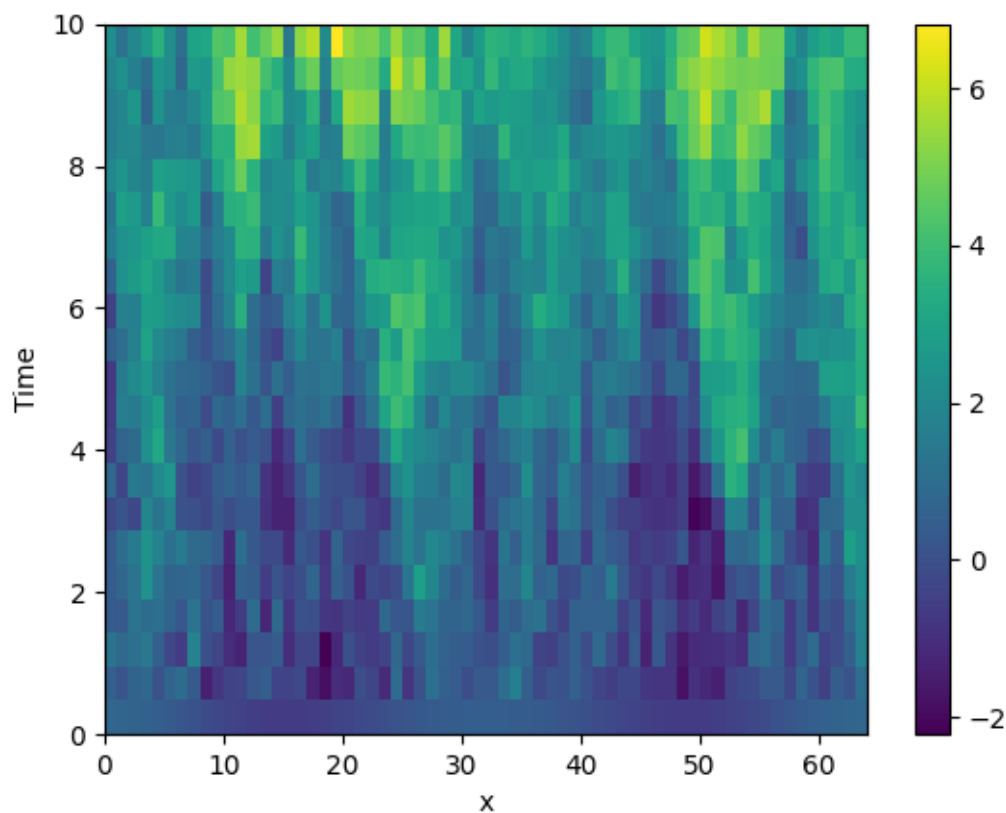
(continued from previous page)

```
eq = DiffusionPDE(0.1) # define the pde
result = eq.solve(state, t_range=1, dt=0.01)
result.plot(cmap="magma")
```

Total running time of the script: (0 minutes 4.148 seconds)

2.9 Stochastic simulation

This example illustrates how a stochastic simulation can be done.



```
from pde import KPZInterfacePDE, MemoryStorage, ScalarField, UnitGrid, plot_kymograph

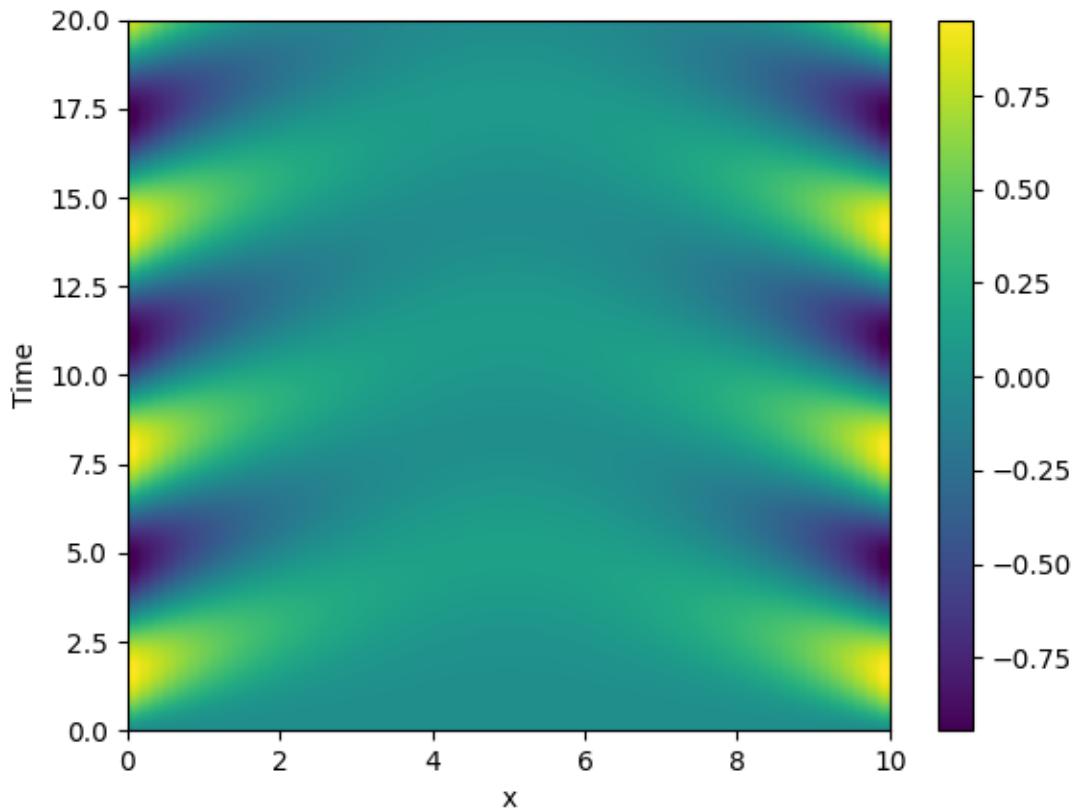
grid = UnitGrid([64]) # generate grid
state = ScalarField.random_harmonic(grid) # generate initial condition

eq = KPZInterfacePDE(noise=1) # define the SDE
storage = MemoryStorage()
eq.solve(state, t_range=10, dt=0.01, tracker=storage.tracker(0.5))
plot_kymograph(storage)
```

Total running time of the script: (0 minutes 4.754 seconds)

2.10 Time-dependent boundary conditions

This example solves a simple diffusion equation in one dimensions with time-dependent boundary conditions.



```
from pde import PDE, CartesianGrid, MemoryStorage, ScalarField, plot_kymograph

grid = CartesianGrid([[0, 10]], [64]) # generate grid
state = ScalarField(grid) # generate initial condition

eq = PDE({"c": "laplace(c)"}, bc={"value_expression": "sin(t)"})

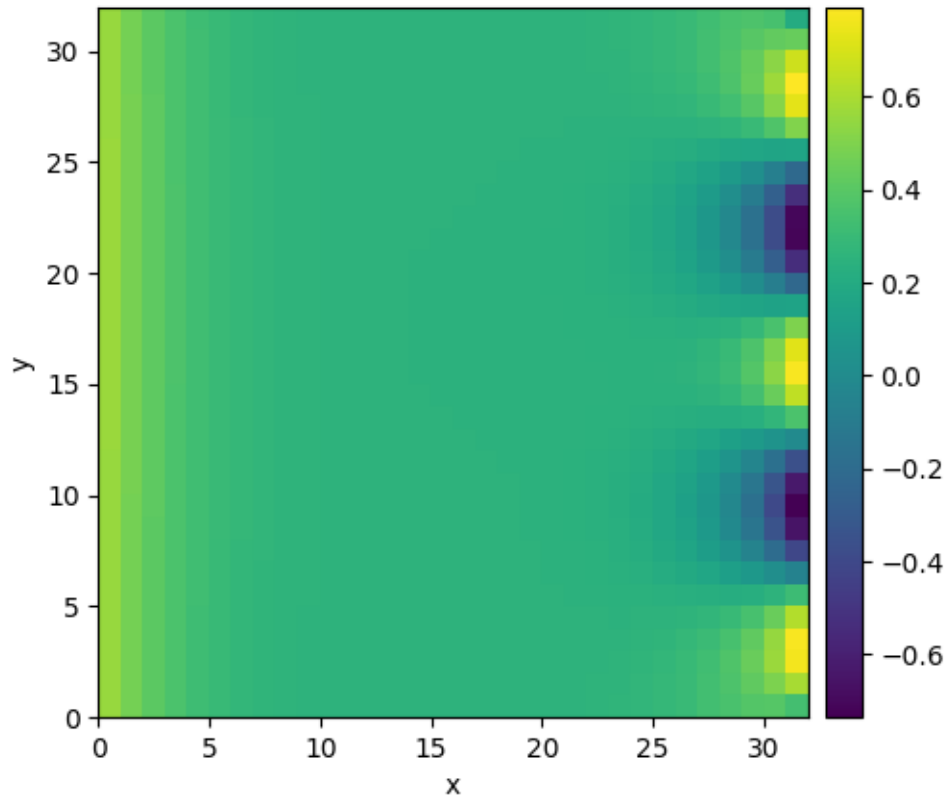
storage = MemoryStorage()
eq.solve(state, t_range=20, dt=1e-4, tracker=storage.tracker(0.1))

# plot the trajectory as a space-time plot
plot_kymograph(storage)
```

Total running time of the script: (0 minutes 8.168 seconds)

2.11 Setting boundary conditions

This example shows how different boundary conditions can be specified.



```

0%|          | 0/10.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/10.0 [00:00<?, ?it/s]
0%|          | 0/10.0 [00:04<?, ?it/s]
0%|          | 0.005/10.0 [00:04<2:23:00, 858.45s/it]
0%|          | 0.03/10.0 [00:04<23:46, 143.09s/it]
15%|█        | 1.49/10.0 [00:04<00:24, 2.88s/it]
15%|█        | 1.49/10.0 [00:04<00:24, 2.89s/it]
100%|███████| 10.0/10.0 [00:04<00:00, 2.32it/s]
100%|███████| 10.0/10.0 [00:04<00:00, 2.32it/s]

```

```

from pde import DiffusionPDE, ScalarField, UnitGrid

grid = UnitGrid([32, 32], periodic=[False, True]) # generate grid
state = ScalarField.random_uniform(grid, 0.2, 0.3) # generate initial condition

```

(continues on next page)

(continued from previous page)

```
# set boundary conditions `bc` for all axes
bc_x_left = {"derivative": 0.1}
bc_x_right = {"value": "sin(y / 2)"}
bc_x = [bc_x_left, bc_x_right]
bc_y = "periodic"
eq = DiffusionPDE(bc=[bc_x, bc_y])

result = eq.solve(state, t_range=10, dt=0.005)
result.plot()
```

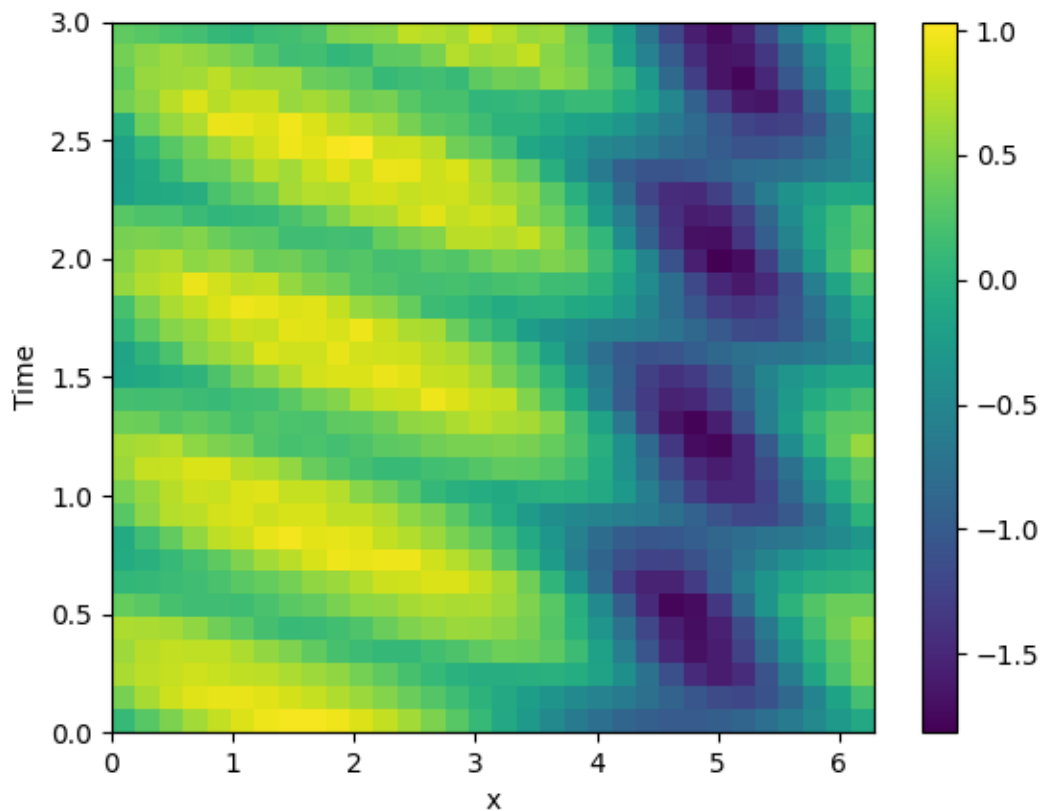
Total running time of the script: (0 minutes 4.455 seconds)

2.12 1D problem - Using *PDE* class

This example implements a PDE that is only defined in one dimension. Here, we chose the [Korteweg-de Vries equation](#), given by

$$\partial_t \phi = 6\phi \partial_x \phi - \partial_x^3 \phi$$

which we implement using the *PDE*.



```
from math import pi

from pde import PDE, CartesianGrid, MemoryStorage, ScalarField, plot_kymograph

# initialize the equation and the space
eq = PDE({"ψ": "6 * ψ * d_dx(ψ) - laplace(d_dx(ψ))"})
grid = CartesianGrid([[0, 2 * pi]], [32], periodic=True)
state = ScalarField.from_expression(grid, "sin(x)")

# solve the equation and store the trajectory
storage = MemoryStorage()
eq.solve(state, t_range=3, solver="scipy", tracker=storage.tracker(0.1))

# plot the trajectory as a space-time plot
plot_kymograph(storage)
```

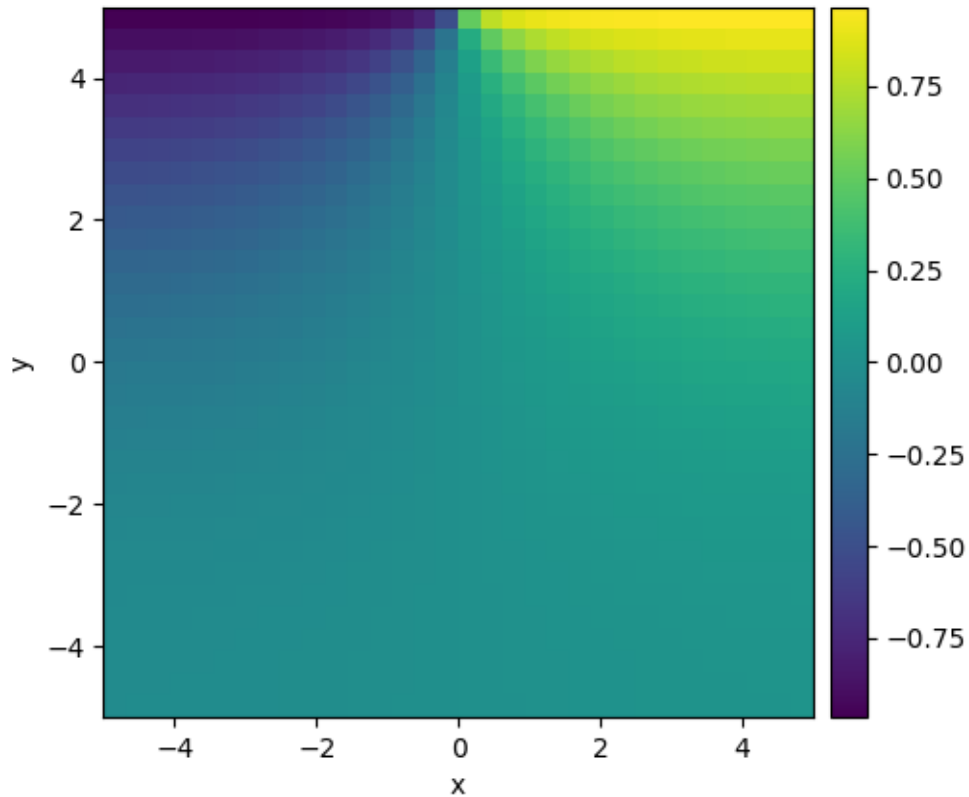
Total running time of the script: (0 minutes 7.844 seconds)

2.13 Heterogeneous boundary conditions

This example implements a spatially coupled SIR model with the following dynamics for the density of susceptible, infected, and recovered individuals:

$$\begin{aligned}\partial_t s &= D \nabla^2 s - \beta i s \\ \partial_t i &= D \nabla^2 i + \beta i s - \gamma i \\ \partial_t r &= D \nabla^2 r + \gamma i\end{aligned}$$

Here, D is the diffusivity, β the infection rate, and γ the recovery rate.



```

0%|          | 0/10.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/10.0 [00:00<?, ?it/s]
0%|          | 0/10.0 [00:00<?, ?it/s]
3%|█         | 0.27/10.0 [00:00<00:06, 1.46it/s]
9%|██        | 0.9/10.0 [00:00<00:02, 4.08it/s]
42%|██████   | 4.23/10.0 [00:00<00:00, 10.28it/s]
42%|██████   | 4.23/10.0 [00:00<00:01, 5.71it/s]
100%|██████████| 10.0/10.0 [00:00<00:00, 13.49it/s]
100%|██████████| 10.0/10.0 [00:00<00:00, 13.48it/s]

```

```

import numpy as np

from pde import CartesianGrid, DiffusionPDE, ScalarField

# define grid and an initial state
grid = CartesianGrid([[-5, 5], [-5, 5]], 32)
field = ScalarField(grid)

```

```

# define the boundary conditions, which here are calculated from a function

```

(continues on next page)

(continued from previous page)

```
def bc_value(adjacent_value, dx, x, y, t):
    """return boundary value"""
    return np.sign(x)

bc_x = "derivative"
bc_y = ["derivative", {"value_expression": bc_value}]

# define and solve a simple diffusion equation
eq = DiffusionPDE(bc=[bc_x, bc_y])
res = eq.solve(field, t_range=10, dt=0.01, backend="numpy")
res.plot()
```

Total running time of the script: (0 minutes 0.875 seconds)

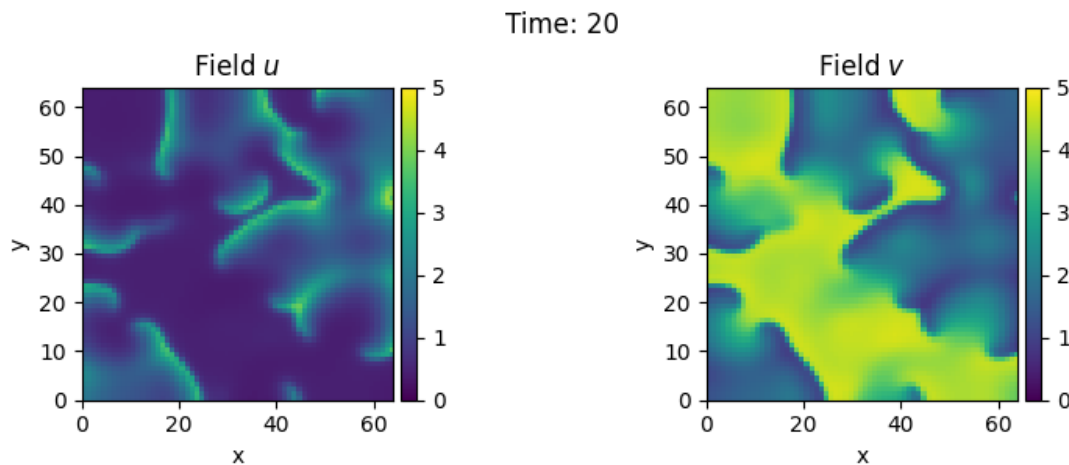
2.14 Brusselator - Using the *PDE* class

This example uses the *PDE* class to implement the *Brusselator* with spatial coupling,

$$\begin{aligned}\partial_t u &= D_0 \nabla^2 u + a - (1 + b)u + vu^2 \\ \partial_t v &= D_1 \nabla^2 v + bu - vu^2\end{aligned}$$

Here, D_0 and D_1 are the respective diffusivity and the parameters a and b are related to reaction rates.

Note that the same result can also be achieved with a *full implementation of a custom class*, which allows for more flexibility at the cost of code complexity.



```
from pde import PDE, FieldCollection, PlotTracker, ScalarField, UnitGrid

# define the PDE
a, b = 1, 3
d0, d1 = 1, 0.1
eq = PDE(
    {
        "u": f"{d0} * laplace(u) + {a} - ({b} + 1) * u + u**2 * v",
        "v": f"{d1} * laplace(v) + {b} * u - u**2 * v",
    }
)
```

(continues on next page)

(continued from previous page)

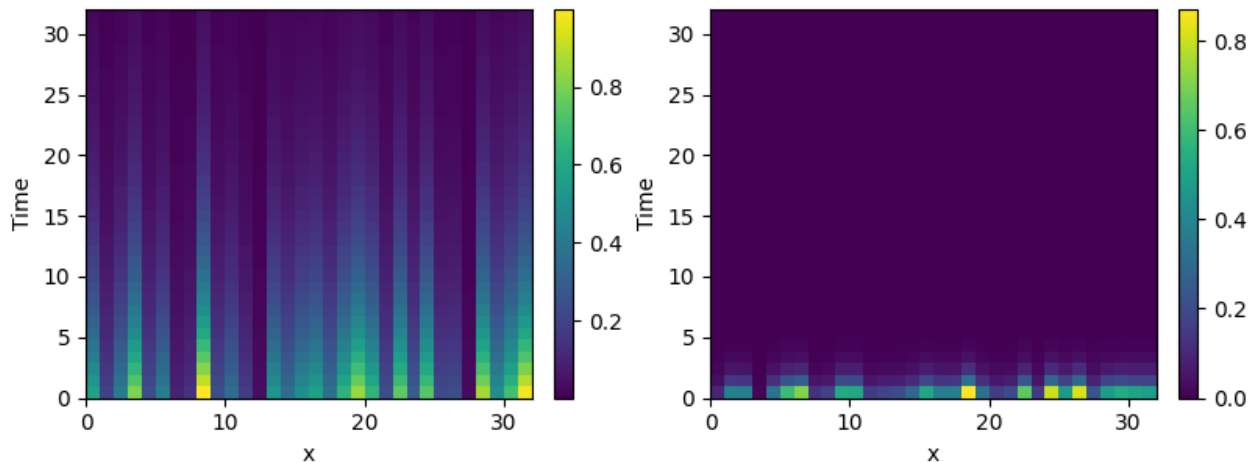
```
# initialize state
grid = UnitGrid([64, 64])
u = ScalarField(grid, a, label="Field $u$")
v = b / a + 0.1 * ScalarField.random_normal(grid, label="Field $v$")
state = FieldCollection([u, v])

# simulate the pde
tracker = PlotTracker(interrupts=1, plot_args={"vmin": 0, "vmax": 5})
sol = eq.solve(state, t_range=20, dt=1e-3, tracker=tracker)
```

Total running time of the script: (0 minutes 26.170 seconds)

2.15 Writing and reading trajectory data

This example illustrates how to store intermediate data to a file for later post-processing. The storage frequency is an argument to the tracker.



```
from tempfile import NamedTemporaryFile

import pde

# define grid, state and pde
grid = pde.UnitGrid([32])
state = pde.FieldCollection(
    [pde.ScalarField.random_uniform(grid), pde.VectorField.random_uniform(grid)]
)
eq = pde.PDE({"s": "-0.1 * s", "v": "-v"})

# get a temporary file to write data to
path = NamedTemporaryFile(suffix=".hdf5")

# run a simulation and write the results
writer = pde.FileStorage(path.name, write_mode="truncate")
eq.solve(state, t_range=32, dt=0.01, tracker=writer.tracker(1))

# read the simulation back in again
```

(continues on next page)

(continued from previous page)

```
reader = pde.FileStorage(path.name, write_mode="read_only")
pde.plot_kymographs(reader)
```

Total running time of the script: (0 minutes 4.871 seconds)

2.16 Diffusion equation with spatial dependence

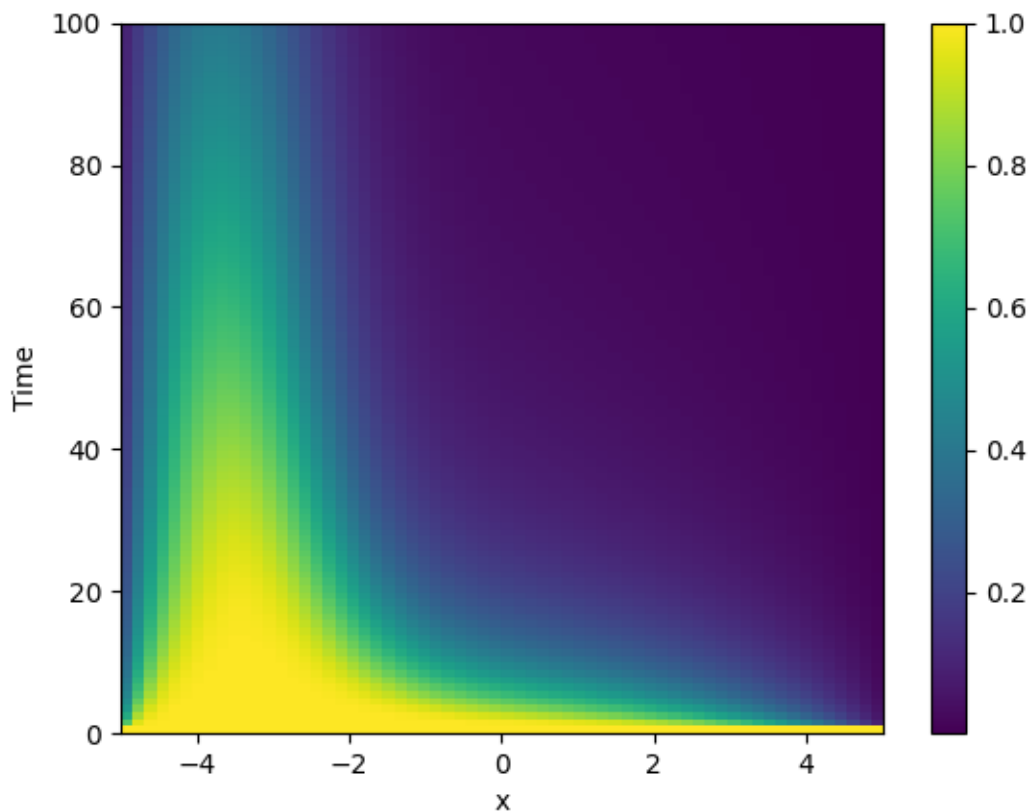
This example solve the [Diffusion equation](#) with a heterogeneous diffusivity:

$$\partial_t c = \nabla(D(r)\nabla c)$$

using the [PDE](#) class. In particular, we consider $D(x) = 1.01 + \tanh(x)$, which gives a low diffusivity on the left side of the domain.

Note that the naive implementation, `PDE({"c": "divergence((1.01 + tanh(x)) * gradient(c))"})`, has numerical instabilities. This is because two finite difference approximations are nested. To arrive at a more stable numerical scheme, it is advisable to expand the divergence,

$$\partial_t c = D\nabla^2 c + \nabla D \cdot \nabla c$$



```

from pde import PDE, CartesianGrid, MemoryStorage, ScalarField, plot_kymograph

# Expanded definition of the PDE
diffusivity = "1.01 + tanh(x)"
term_1 = f"({diffusivity}) * laplace(c)"
term_2 = f"dot(gradient({diffusivity}), gradient(c))"
eq = PDE({"c": f"{term_1} + {term_2}"}, bc={"value": 0})

grid = CartesianGrid([[-5, 5]], 64) # generate grid
field = ScalarField(grid, 1) # generate initial condition

storage = MemoryStorage() # store intermediate information of the simulation
res = eq.solve(field, 100, dt=1e-3, tracker=storage.tracker(1)) # solve the PDE

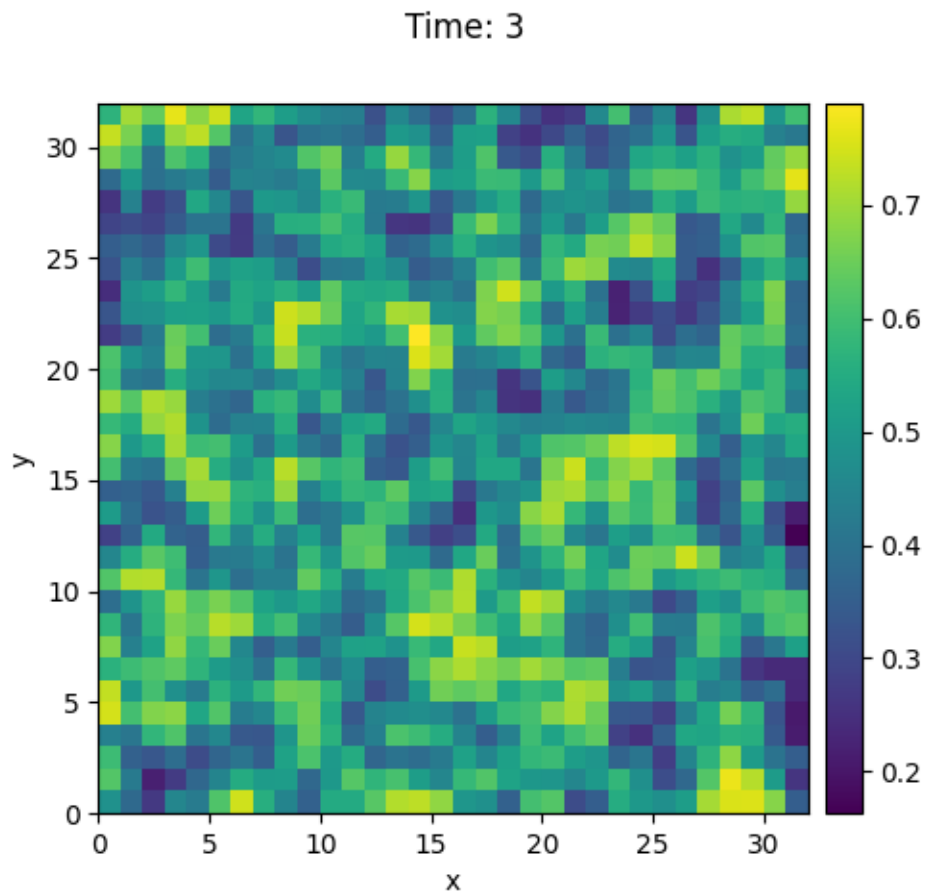
plot_kymograph(storage) # visualize the result in a space-time plot

```

Total running time of the script: (0 minutes 11.536 seconds)

2.17 Using simulation trackers

This example illustrates how trackers can be used to analyze simulations.



```

0%|          | 0/3.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/3.0 [00:00<?, ?it/s]
0%|          | 0/3.0 [00:04<?, ?it/s]
3%|█         | 0.1/3.0 [00:04<02:06, 43.57s/it]
7%|██        | 0.2/3.0 [00:04<01:01, 21.79s/it]
27%|██████   | 0.8/3.0 [00:04<00:11,  5.45s/it]
27%|██████   | 0.8/3.0 [00:04<00:12,  5.65s/it]
100%|██████████| 3.0/3.0 [00:04<00:00,  1.51s/it]
100%|██████████| 3.0/3.0 [00:04<00:00,  1.51s/it]
513.4306826593169
513.4306826593169
513.430682659317
513.4306826593169

```

```

import pde

grid = pde.UnitGrid([32, 32]) # generate grid
state = pde.ScalarField.random_uniform(grid) # generate initial condition

storage = pde.MemoryStorage()

trackers = [
    "progress", # show progress bar during simulation
    "steady_state", # abort when steady state is reached
    storage.tracker(interrupts=1), # store data every simulation time unit
    pde.PlotTracker(show=True), # show images during simulation
    # print some output every 5 real seconds:
    pde.PrintTracker(interrupts=pde.RealtimeInterrupts(duration=5)),
]

eq = pde.DiffusionPDE(0.1) # define the PDE
eq.solve(state, 3, dt=0.1, tracker=trackers)

for field in storage:
    print(field.integral)

```

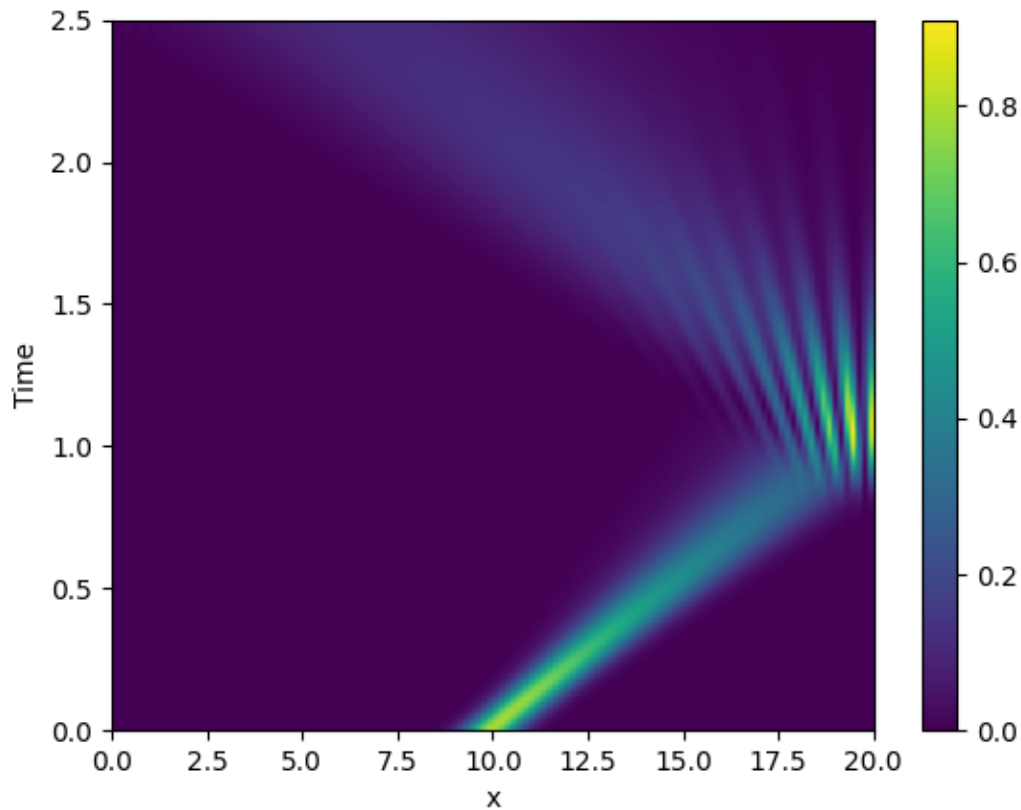
Total running time of the script: (0 minutes 4.568 seconds)

2.18 Schrödinger's Equation

This example implements a complex PDE using the *PDE*. We here chose the *Schrödinger equation* without a spatial potential in non-dimensional form:

$$i\partial_t\psi = -\nabla^2\psi$$

Note that the example imposes Neumann conditions at the wall, so the wave packet is expected to reflect off the wall.



```

from math import sqrt

from pde import PDE, CartesianGrid, MemoryStorage, ScalarField, plot_kymograph

grid = CartesianGrid([[0, 20]], 128, periodic=False) # generate grid

# create a (normalized) wave packet with a certain form as an initial condition
initial_state = ScalarField.from_expression(grid, "exp(I * 5 * x) * exp(-(x - 10)**2)
↪")
initial_state /= sqrt(initial_state.to_scalar("norm_squared").integral.real)

eq = PDE({"ψ": f"I * laplace(ψ)"}) # define the pde

# solve the pde and store intermediate data
storage = MemoryStorage()
eq.solve(initial_state, t_range=2.5, dt=1e-5, tracker=[storage.tracker(0.02)])

# visualize the results as a space-time plot
plot_kymograph(storage, scalar="norm_squared")

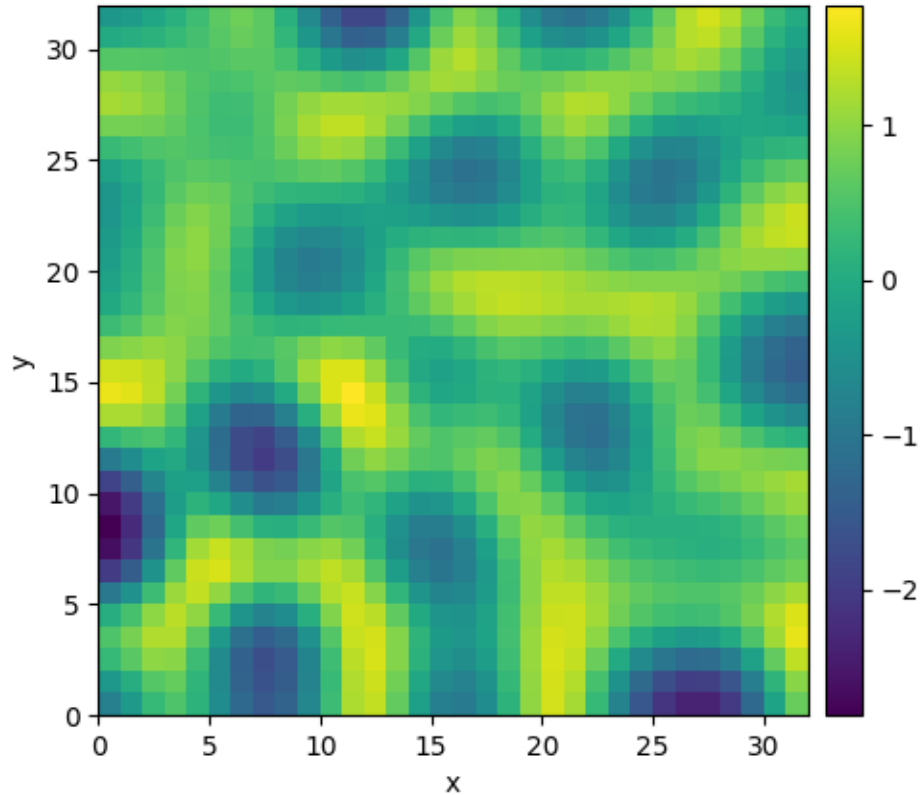
```

Total running time of the script: (0 minutes 5.974 seconds)

2.19 Kuramoto-Sivashinsky - Using custom class

This example implements a scalar PDE using a custom class. We here consider the Kuramoto–Sivashinsky equation, which for instance describes the dynamics of flame fronts:

$$\partial_t u = -\frac{1}{2}|\nabla u|^2 - \nabla^2 u - \nabla^4 u$$



```

0%|          | 0/10.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/10.0 [00:00<?, ?it/s]
0%|          | 0/10.0 [00:00<?, ?it/s]
3%|█         | 0.27/10.0 [00:00<00:11, 1.20s/it]
8%|██        | 0.75/10.0 [00:00<00:04, 2.03it/s]
30%|██████   | 3.0/10.0 [00:00<00:01, 5.22it/s]
80%|██████████| 7.98/10.0 [00:01<00:00, 7.72it/s]
80%|██████████| 7.98/10.0 [00:01<00:00, 6.54it/s]
100%|██████████| 10.0/10.0 [00:01<00:00, 8.19it/s]
100%|██████████| 10.0/10.0 [00:01<00:00, 8.19it/s]

```

```

from pde import PDEBase, ScalarField, UnitGrid

class KuramotoSivashinskyPDE(PDEBase):
    """Implementation of the normalized Kuramoto-Sivashinsky equation"""

    def evolution_rate(self, state, t=0):
        """implement the python version of the evolution equation"""
        state_lap = state.laplace(bc="auto_periodic_neumann")
        state_lap2 = state_lap.laplace(bc="auto_periodic_neumann")
        state_grad = state.gradient(bc="auto_periodic_neumann")
        return -state_grad.to_scalar("squared_sum") / 2 - state_lap - state_lap2

grid = UnitGrid([32, 32]) # generate grid
state = ScalarField.random_uniform(grid) # generate initial condition

eq = KuramotoSivashinskyPDE() # define the pde
result = eq.solve(state, t_range=10, dt=0.01)
result.plot()

```

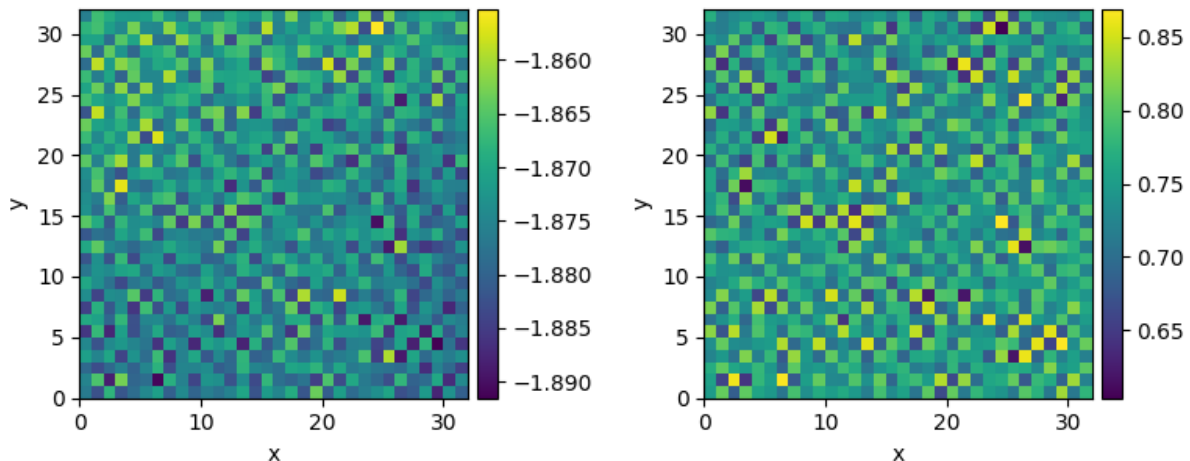
Total running time of the script: (0 minutes 1.355 seconds)

2.20 Custom Class for coupled PDEs

This example shows how to solve a set of coupled PDEs, the spatially coupled [FitzHugh–Nagumo model](#), which is a simple model for the excitable dynamics of coupled Neurons:

$$\begin{aligned}\partial_t u &= \nabla^2 u + u(u - \alpha)(1 - u) + w \\ \partial_t w &= \epsilon u\end{aligned}$$

Here, α denotes the external stimulus and ϵ defines the recovery time scale. We implement this as a custom PDE class below.



```

0%|          | 0/100.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/100.0 [00:00<?, ?it/s]
0%|          | 0/100.0 [00:00<?, ?it/s]
0%|          | 0.27/100.0 [00:00<01:10, 1.41it/s]

```

(continues on next page)

(continued from previous page)

1%	0.87/100.0	[00:00<00:26, 3.79it/s]
4%	3.94/100.0	[00:00<00:10, 9.41it/s]
11%	11.01/100.0	[00:00<00:07, 12.45it/s]
21%	21.37/100.0	[00:01<00:06, 12.86it/s]
33%	33.13/100.0	[00:02<00:04, 13.66it/s]
47%	46.58/100.0	[00:03<00:03, 13.81it/s]
60%	60.4/100.0	[00:04<00:02, 14.01it/s]
75%	74.65/100.0	[00:05<00:01, 14.09it/s]
89%	89.0/100.0	[00:06<00:00, 14.18it/s]
89%	89.0/100.0	[00:07<00:00, 12.68it/s]
100%	100.0/100.0	[00:07<00:00, 14.24it/s]
100%	100.0/100.0	[00:07<00:00, 14.24it/s]

```

from pde import FieldCollection, PDEBase, UnitGrid

class FitzhughNagumoPDE(PDEBase):
    """FitzHugh-Nagumo model with diffusive coupling"""

    def __init__(self, stimulus=0.5, tau=10, a=0, b=0, bc="auto_periodic_neumann"):
        super().__init__()
        self.bc = bc
        self.stimulus = stimulus
        self.tau = tau
        self.a = a
        self.b = b

    def evolution_rate(self, state, t=0):
        v, w = state  # membrane potential and recovery variable

        v_t = v.laplace(bc=self.bc) + v - v**3 / 3 - w + self.stimulus
        w_t = (v + self.a - self.b * w) / self.tau

        return FieldCollection([v_t, w_t])

grid = UnitGrid([32, 32])
state = FieldCollection.scalar_random_uniform(2, grid)

eq = FitzhughNagumoPDE()
result = eq.solve(state, t_range=100, dt=0.01)
result.plot()

```

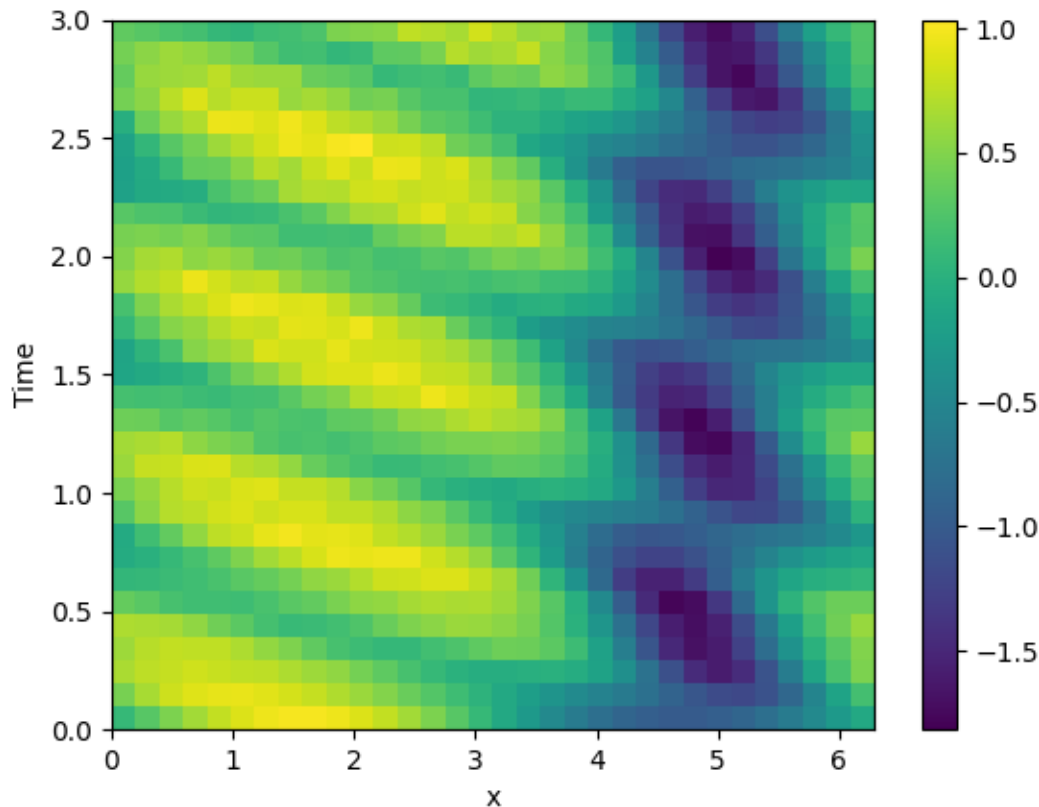
Total running time of the script: (0 minutes 7.322 seconds)

2.21 1D problem - Using custom class

This example implements a PDE that is only defined in one dimension. Here, we chose the [Korteweg-de Vries equation](#), given by

$$\partial_t \phi = 6\phi \partial_x \phi - \partial_x^3 \phi$$

which we implement using a custom PDE class below.



```
from math import pi

from pde import CartesianGrid, MemoryStorage, PDEBase, ScalarField, plot_kymograph

class KortewegDeVriesPDE(PDEBase):
    """Korteweg-de Vries equation"""

    def evolution_rate(self, state, t=0):
        """implement the python version of the evolution equation"""
        assert state.grid.dim == 1 # ensure the state is one-dimensional
        grad_x = state.gradient("auto_periodic_neumann")[0]
        return 6 * state * grad_x - grad_x.laplace("auto_periodic_neumann")

# initialize the equation and the space
```

(continues on next page)

(continued from previous page)

```

grid = CartesianGrid([[0, 2 * pi]], [32], periodic=True)
state = ScalarField.from_expression(grid, "sin(x)")

# solve the equation and store the trajectory
storage = MemoryStorage()
eq = KortewegDeVriesPDE()
eq.solve(state, t_range=3, solver="scipy", tracker=storage.tracker(0.1))

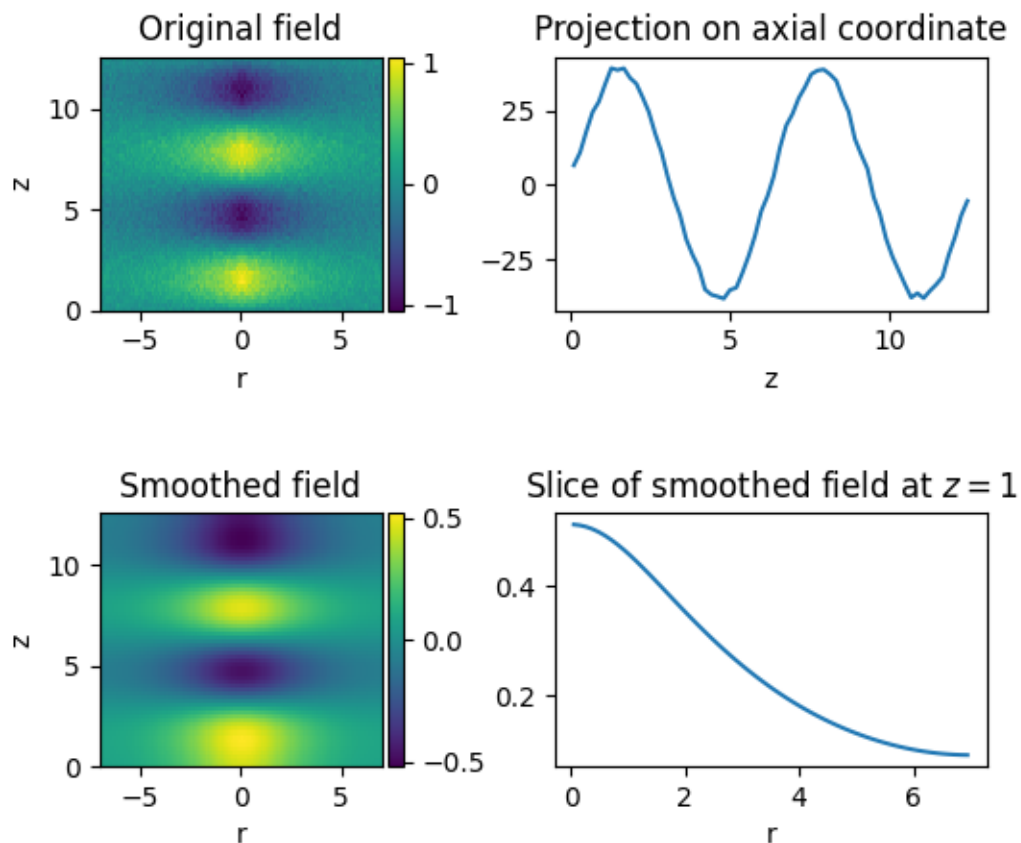
# plot the trajectory as a space-time plot
plot_kymograph(storage)

```

Total running time of the script: (0 minutes 2.201 seconds)

2.22 Visualizing a scalar field

This example displays methods for visualizing scalar fields.



```

import matplotlib.pyplot as plt
import numpy as np

from pde import CylindricalSymGrid, ScalarField

```

(continues on next page)

(continued from previous page)

```

# create a scalar field with some noise
grid = CylindricalSymGrid(7, [0, 4 * np.pi], 64)
data = ScalarField.from_expression(grid, "sin(z) * exp(-r / 3)")
data += 0.05 * ScalarField.random_normal(grid)

# manipulate the field
smoothed = data.smooth() # Gaussian smoothing to get rid of the noise
projected = data.project("r") # integrate along the radial direction
sliced = smoothed.slice({"z": 1}) # slice the smoothed data

# create four plots of the field and the modifications
fig, axes = plt.subplots(nrows=2, ncols=2)
data.plot(ax=axes[0, 0], title="Original field")
smoothed.plot(ax=axes[1, 0], title="Smoothed field")
projected.plot(ax=axes[0, 1], title="Projection on axial coordinate")
sliced.plot(ax=axes[1, 1], title="Slice of smoothed field at $z=1$")
plt.subplots_adjust(hspace=0.8)
plt.show()

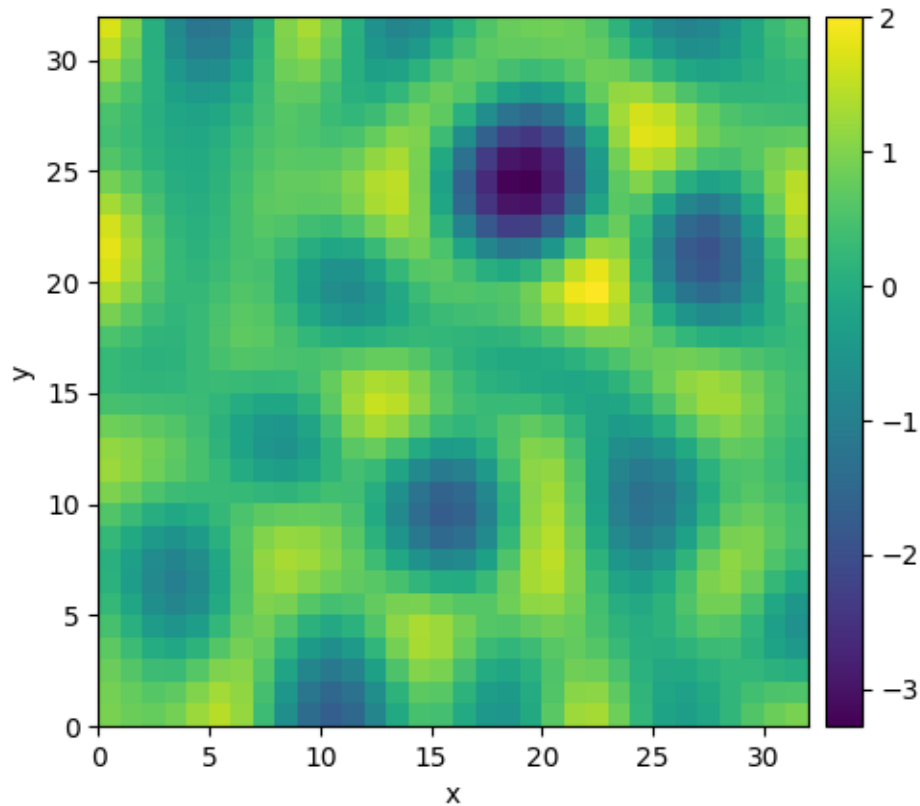
```

Total running time of the script: (0 minutes 0.296 seconds)

2.23 Kuramoto-Sivashinsky - Compiled methods

This example implements a scalar PDE using a custom class with a numba-compiled method for accelerated calculations. We here consider the [Kuramoto–Sivashinsky equation](#), which for instance describes the dynamics of flame fronts:

$$\partial_t u = -\frac{1}{2}|\nabla u|^2 - \nabla^2 u - \nabla^4 u$$



```

0%|          | 0/10.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/10.0 [00:00<?, ?it/s]
0%|          | 0/10.0 [00:09<?, ?it/s]
0%|          | 0.01/10.0 [00:10<2:57:20, 1065.12s/it]
0%|          | 0.02/10.0 [00:10<1:28:35, 532.58s/it]
2%|█         | 0.2/10.0 [00:10<08:41, 53.26s/it]
92%|██████████| 9.19/10.0 [00:10<00:00, 1.16s/it]
92%|██████████| 9.19/10.0 [00:10<00:00, 1.16s/it]
100%|██████████| 10.0/10.0 [00:10<00:00, 1.07s/it]
100%|██████████| 10.0/10.0 [00:10<00:00, 1.07s/it]

```

```

import numba as nb

from pde import PDEBase, ScalarField, UnitGrid

class KuramotoSivashinskyPDE(PDEBase):
    """Implementation of the normalized Kuramoto-Sivashinsky equation"""

    def __init__(self, bc="auto_periodic_neumann"):

```

(continues on next page)

(continued from previous page)

```

super().__init__()
self.bc = bc

def evolution_rate(self, state, t=0):
    """implement the python version of the evolution equation"""
    state_lap = state.laplace(bc=self.bc)
    state_lap2 = state_lap.laplace(bc=self.bc)
    state_grad_sq = state.gradient_squared(bc=self.bc)
    return -state_grad_sq / 2 - state_lap - state_lap2

def _make_pde_rhs_numba(self, state):
    """numba-compiled implementation of the PDE"""
    gradient_squared = state.grid.make_operator("gradient_squared", bc=self.bc)
    laplace = state.grid.make_operator("laplace", bc=self.bc)

    @nb.njit
    def pde_rhs(data, t):
        return -0.5 * gradient_squared(data) - laplace(data + laplace(data))

    return pde_rhs

grid = UnitGrid([32, 32]) # generate grid
state = ScalarField.random_uniform(grid) # generate initial condition

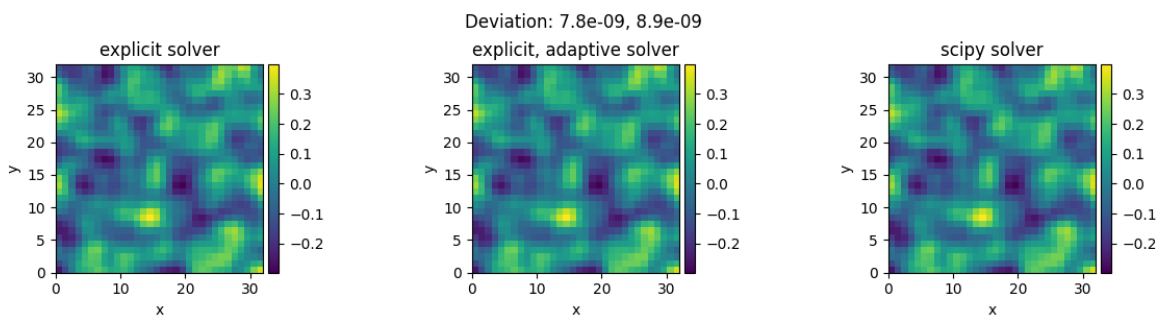
eq = KuramotoSivashinskyPDE() # define the pde
result = eq.solve(state, t_range=10, dt=0.01)
result.plot()

```

Total running time of the script: (0 minutes 10.811 seconds)

2.24 Solver comparison

This example shows how to set up solvers explicitly and how to extract diagnostic information.



```

Diagnostic information from first run:
{'controller': {'t_start': 0, 't_end': 1.0, 'profiler': {'solver': 0.
→05024239299999067, 'tracker': 4.056299999888324e-05, 'compilation': 4.
→170617233999991}, 'jit_count': {'make_stepper': 11, 'simulation': 0}, 'solver_start_
': '2024-04-04 06:59:04.939262', 'successful': True, 'stop_reason': 'Reached final_
→time', 'solver_duration': '0:00:00.050297', 't_final': 1.0, 'process_count': 1},
→'package_version': 'unknown', 'solver': {'class': 'ExplicitSolver', 'pde_class':
→'DiffusionPDE', 'dt': 0.001, 'steps': 1000, 'state_modifications': 0.0, 'stochastic

```

(continues on next page)

(continued from previous page)

```

→': False, 'scheme': 'euler', 'backend': 'numba'}}

Diagnostic information from second run:
{'controller': {'t_start': 0, 't_end': 1.0, 'profiler': {'solver': 0.
→17841695699999605, 'tracker': 4.13550000075702e-05, 'compilation': 1.
→08852466499999942}, 'jit_count': {'make_stepper': 2, 'simulation': 0}, 'solver_start
→': '2024-04-04 06:59:06.078613', 'successful': True, 'stop_reason': 'Reached final_
→time', 'solver_duration': '0:00:00.178473', 't_final': 1.0, 'process_count': 1},
→'package_version': 'unknown', 'solver': {'class': 'ExplicitSolver', 'pde_class':
→'DiffusionPDE', 'dt': 0.001, 'dt_adaptive': True, 'steps': 12, 'stochastic': False,
→'state_modifications': 0.0, 'dt_statistics': {'min': 0.001, 'max': 0.
→16657480937209937, 'mean': 0.08333333333333334, 'std': 0.05136475321124537, 'count
→': 12.0}, 'scheme': 'runge-kutta', 'backend': 'numba'}}

Diagnostic information from third run:
{'controller': {'t_start': 0, 't_end': 1.0, 'profiler': {'solver': 0.
→002736429000009366, 'tracker': 4.210099999113481e-05, 'compilation': 0.
→6017242369999849}, 'jit_count': {'make_stepper': 1, 'simulation': 0}, 'solver_start
→': '2024-04-04 06:59:08.186659', 'successful': True, 'stop_reason': 'Reached final_
→time', 'solver_duration': '0:00:00.002776', 't_final': 1.0, 'process_count': 1},
→'package_version': 'unknown', 'solver': {'class': 'ScipySolver', 'pde_class':
→'DiffusionPDE', 'dt': None, 'steps': 50, 'stochastic': False, 'backend': 'numba'}}

```

```

import pde

# initialize the grid, an initial condition, and the PDE
grid = pde.UnitGrid([32, 32])
field = pde.ScalarField.random_uniform(grid, -1, 1)
eq = pde.DiffusionPDE()

# try the explicit solver
solver1 = pde.ExplicitSolver(eq)
controller1 = pde.Controller(solver1, t_range=1, tracker=None)
sol1 = controller1.run(field, dt=1e-3)
sol1.label = "explicit solver"
print("Diagnostic information from first run:")
print(controller1.diagnostics)
print()

# try an explicit solver with adaptive time steps
solver2 = pde.ExplicitSolver(eq, scheme="runge-kutta", adaptive=True)
controller2 = pde.Controller(solver2, t_range=1, tracker=None)
sol2 = controller2.run(field, dt=1e-3)
sol2.label = "explicit, adaptive solver"
print("Diagnostic information from second run:")
print(controller2.diagnostics)
print()

# try the standard scipy solver
solver3 = pde.ScipySolver(eq)
controller3 = pde.Controller(solver3, t_range=1, tracker=None)

```

(continues on next page)

(continued from previous page)

```

sol3 = controller3.run(field)
sol3.label = "scipy solver"
print("Diagnostic information from third run:")
print(controller3.diagnostics)
print()

# plot both fields and give the deviation as the title
title = f"Deviation: {((sol1 - sol2)**2).average:.2g}, {((sol1 - sol3)**2).average:.2g}"
pde.FieldCollection([sol1, sol2, sol3]).plot(title=title)

```

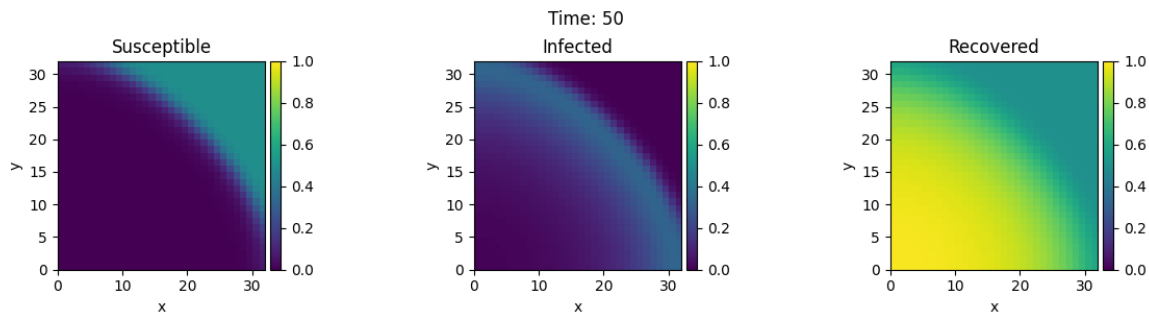
Total running time of the script: (0 minutes 7.886 seconds)

2.25 Custom PDE class: SIR model

This example implements a [spatially coupled SIR model](#) with the following dynamics for the density of susceptible, infected, and recovered individuals:

$$\begin{aligned}
 \partial_t s &= D \nabla^2 s - \beta i s \\
 \partial_t i &= D \nabla^2 i + \beta i s - \gamma i \\
 \partial_t r &= D \nabla^2 r + \gamma i
 \end{aligned}$$

Here, D is the diffusivity, β the infection rate, and γ the recovery rate.



```

0%|          | 0/50.0 [00:00<?, ?it/s]
Initializing: 0%|          | 0/50.0 [00:00<?, ?it/s]
0%|          | 0/50.0 [00:00<?, ?it/s]
0%|          | 0.02/50.0 [00:00<30:53, 37.09s/it]
0%|          | 0.05/50.0 [00:00<12:25, 14.92s/it]
1%|          | 0.47/50.0 [00:00<01:24, 1.70s/it]
5%|█         | 2.31/50.0 [00:01<00:21, 2.26it/s]
12%|██        | 6.21/50.0 [00:01<00:10, 4.16it/s]
24%|████       | 11.89/50.0 [00:02<00:07, 4.98it/s]
36%|██████      | 17.9/50.0 [00:03<00:05, 5.74it/s]
50%|████████     | 24.93/50.0 [00:04<00:04, 5.97it/s]
64%|██████████    | 31.76/50.0 [00:05<00:02, 6.10it/s]
77%|███████████   | 38.49/50.0 [00:06<00:01, 6.39it/s]
92%|████████████  | 45.93/50.0 [00:07<00:00, 6.44it/s]
92%|████████████  | 45.93/50.0 [00:07<00:00, 5.87it/s]
100%|█████████████| 50.0/50.0 [00:07<00:00, 6.39it/s]
100%|█████████████| 50.0/50.0 [00:07<00:00, 6.39it/s]

```

```

from pde import FieldCollection, PDEBase, PlotTracker, ScalarField, UnitGrid

class SIRPDE(PDEBase):
    """SIR-model with diffusive mobility"""

    def __init__(
        self, beta=0.3, gamma=0.9, diffusivity=0.1, bc="auto_periodic_neumann"
    ):
        super().__init__()
        self.beta = beta # transmission rate
        self.gamma = gamma # recovery rate
        self.diffusivity = diffusivity # spatial mobility
        self.bc = bc # boundary condition

    def get_state(self, s, i):
        """generate a suitable initial state"""
        norm = (s + i).data.max() # maximal density
        if norm > 1:
            s /= norm
            i /= norm
        s.label = "Susceptible"
        i.label = "Infected"

        # create recovered field
        r = ScalarField(s.grid, data=1 - s - i, label="Recovered")
        return FieldCollection([s, i, r])

    def evolution_rate(self, state, t=0):
        s, i, r = state
        diff = self.diffusivity
        ds_dt = diff * s.laplace(self.bc) - self.beta * i * s
        di_dt = diff * i.laplace(self.bc) + self.beta * i * s - self.gamma * i
        dr_dt = diff * r.laplace(self.bc) + self.gamma * i
        return FieldCollection([ds_dt, di_dt, dr_dt])

eq = SIRPDE(beta=2, gamma=0.1)

# initialize state
grid = UnitGrid([32, 32])
s = ScalarField(grid, 1)
i = ScalarField(grid, 0)
i.data[0, 0] = 1
state = eq.get_state(s, i)

# simulate the pde
tracker = PlotTracker(interrupts=10, plot_args={"vmin": 0, "vmax": 1})
sol = eq.solve(state, t_range=50, dt=1e-2, tracker=["progress", tracker])

```

Total running time of the script: (0 minutes 8.115 seconds)

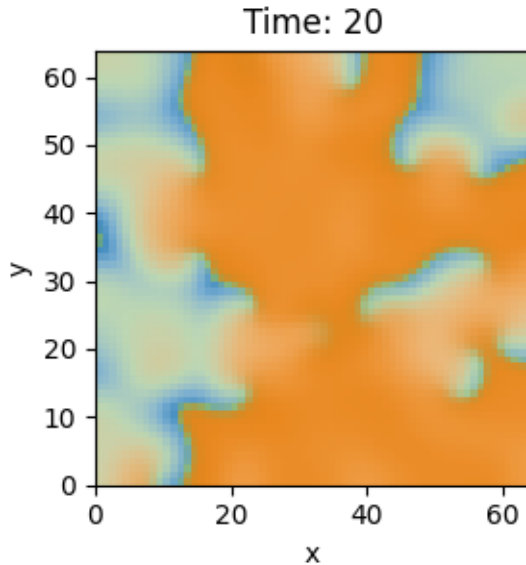
2.26 Brusselator - Using custom class

This example implements the [Brusselator](#) with spatial coupling,

$$\begin{aligned}\partial_t u &= D_0 \nabla^2 u + a - (1 + b)u + vu^2 \\ \partial_t v &= D_1 \nabla^2 v + bu - vu^2\end{aligned}$$

Here, D_0 and D_1 are the respective diffusivity and the parameters a and b are related to reaction rates.

Note that the PDE can also be implemented using the [PDE](#) class; see [the example](#). However, that implementation is less flexible and might be more difficult to extend later.



```
import numba as nb
import numpy as np

from pde import FieldCollection, PDEBase, PlotTracker, ScalarField, UnitGrid

class BrusselatorPDE(PDEBase):
    """Brusselator with diffusive mobility"""

    def __init__(self, a=1, b=3, diffusivity=[1, 0.1], bc="auto_periodic_neumann"):
        super().__init__()
        self.a = a
        self.b = b
        self.diffusivity = diffusivity # spatial mobility
        self.bc = bc # boundary condition

    def get_initial_state(self, grid):
        """prepare a useful initial state"""
        u = ScalarField(grid, self.a, label="Field $u$")
        v = self.b / self.a + 0.1 * ScalarField.random_normal(grid, label="Field $v$")
        return FieldCollection([u, v])

    def evolution_rate(self, state, t=0):
        """pure python implementation of the PDE"""
        u, v = state
```

(continues on next page)

(continued from previous page)

```

    rhs = state.copy()
    d0, d1 = self.diffusivity
    rhs[0] = d0 * u.laplace(self.bc) + self.a - (self.b + 1) * u + u**2 * v
    rhs[1] = d1 * v.laplace(self.bc) + self.b * u - u**2 * v
    return rhs

def _make_pde_rhs_numba(self, state):
    """numba-compiled implementation of the PDE"""
    d0, d1 = self.diffusivity
    a, b = self.a, self.b
    laplace = state.grid.make_operator("laplace", bc=self.bc)

    @nb.njit
    def pde_rhs(state_data, t):
        u = state_data[0]
        v = state_data[1]

        rate = np.empty_like(state_data)
        rate[0] = d0 * laplace(u) + a - (1 + b) * u + v * u**2
        rate[1] = d1 * laplace(v) + b * u - v * u**2
        return rate

    return pde_rhs

# initialize state
grid = UnitGrid([64, 64])
eq = BrusselatorPDE(diffusivity=[1, 0.1])
state = eq.get_initial_state(grid)

# simulate the pde
tracker = PlotTracker(interrupts=1, plot_args={"kind": "merged", "vmin": 0, "vmax": 5}
→)
sol = eq.solve(state, t_range=20, dt=1e-3, tracker=tracker)

```

Total running time of the script: (0 minutes 8.316 seconds)

3.1 Mathematical basics

To solve partial differential equations (PDEs), the *py-pde* package provides differential operators to express spatial derivatives. These operators are implemented using the [finite difference method](#) to support various boundary conditions. The time evolution of the PDE is then calculated using the method of lines by explicitly discretizing space using the grid classes. This reduces the PDEs to a set of ordinary differential equations, which can be solved using standard methods as described below.

3.1.1 Curvilinear coordinates

The package supports multiple curvilinear coordinate systems. They allow to exploit symmetries present in physical systems. Consequently, many grids implemented in *py-pde* inherently assume symmetry of the described fields. However, a drawback of curvilinear coordinates are the fact that the basis vectors now depend on position, which makes tensor fields less intuitive and complicates the expression of differential operators. To avoid confusion, we here specify the used coordinate systems explicitly:

Polar coordinates

Polar coordinates describe points by a radius r and an angle ϕ in a two-dimensional coordinates system. They are defined by the transformation

$$\begin{cases} x = r \cos(\phi) \\ y = r \sin(\phi) \end{cases} \quad \text{for } r \in [0, \infty] \text{ and } \phi \in [0, 2\pi)$$

The associated symmetric grid [PolarSymGrid](#) assumes that fields only depend on the radial coordinate r . Note that vector and tensor fields can still have components in the polar direction. In particular, vector fields still have two components: $\vec{v}(r) = v_r(r)\vec{e}_r + v_\phi(r)\vec{e}_\phi$.

Spherical coordinates

Spherical coordinates describe points by a radius r , an azimuthal angle θ , and a polar angle ϕ . The conversion to ordinary Cartesian coordinates reads

$$\begin{cases} x = r \sin(\theta) \cos(\phi) \\ y = r \sin(\theta) \sin(\phi) \\ z = r \cos(\theta) \end{cases} \quad \text{for } r \in [0, \infty], \theta \in [0, \pi], \text{ and } \phi \in [0, 2\pi)$$

The associated symmetric grid *SphericalSymGrid* assumes that fields only depend on the radial coordinate r . Note that vector and tensor fields can still have components in the two angular direction.

Warning: Not all results of differential operators on vectorial and tensorial fields can be expressed in terms of fields that only depend on the radial coordinate r . In particular, the gradient of a vector field can only be calculated if the azimuthal component of the vector field vanishes. Similarly, the divergence of a tensor field can only be taken in special situations.

Cylindrical coordinates

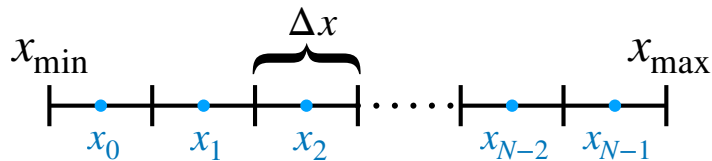
Cylindrical coordinates describe points by a radius r , an axial coordinate z , and a polar angle ϕ . The conversion to ordinary Cartesian coordinates reads

$$\begin{cases} x = r \cos(\phi) \\ y = r \sin(\phi) \\ z = z \end{cases} \quad \text{for } r \in [0, \infty], z \in \mathbb{R}, \text{ and } \phi \in [0, 2\pi)$$

The associated symmetric grid *CylindricalSymGrid* assumes that fields only depend on the coordinates r and z . Vector and tensor fields still specify all components in the three-dimensional space.

Warning: The order of components in the vector and tensor fields defined on cylindrical grids is different than in ordinary math. While it is common to use (r, ϕ, z) , we here use the order (r, z, ϕ) . It might thus be best to access components by name instead of index.

3.1.2 Spatial discretization



The finite differences scheme used by *py-pde* is currently restricted to orthogonal coordinate systems with uniform discretization. Because of the orthogonality, each axis of the grid can be discretized independently. For simplicity, we only consider uniform grids, where the support points are spaced equidistantly along a given axis, i.e., the discretization Δx is constant. If a given axis covers values in a range $[x_{\min}, x_{\max}]$, a discretization with N support points can then be thought of as covering the axis with N equal-sized boxes; see inset. Field values are then specified for each box, i.e., the support points lie at the centers of the box:

$$x_i = x_{\min} + \left(i + \frac{1}{2}\right) \Delta x \quad \text{for } i = 0, \dots, N-1$$

$$\Delta x = \frac{x_{\max} - x_{\min}}{N}$$

which is also indicated in the inset.

Differential operators are implemented using the usual second-order central differences. This requires the introducing of virtual support points at x_{-1} and x_N , which can be determined from the boundary conditions at $x = x_{\min}$ and $x = x_{\max}$, respectively. The field classes automate this transparently. However, if you need more control over boundary conditions, you can access the full underlying data using the `field._data_full`, which will have $N + 2$ entries along an axis

that has N support points. In this case, the first and last entries (`data_full[0]` and `data_full[N + 1]`) denote the lower and upper virtual point, respectively. The actual field data can be obtained using `data_full[1:-1]` or the `field.data` attribute for convenience. Note that functions evaluating differential operators generally expect the full data as input while they return only valid data.

3.1.3 Temporal evolution

Once the fields have been discretized, the PDE reduces to a set of coupled ordinary differential equations (ODEs), which can be solved using standard methods. This reduction is also known as the method of lines. The *py-pde* package implements the simple Euler scheme and a more advanced *Runge-Kutta scheme* in the *ExplicitSolver* class. For the simple implementations of these explicit methods, the user typically specifies a fixed time step, although adaptive methods, which adjust the time step automatically, are also often used and available in the package. One problem with explicit solvers is that they require small time steps to stably evolve some PDEs; such PDEs are then often called ‘stiff’. Stiff PDEs can sometimes be solved more efficiently by using implicit methods. This package provides a simple implementation of the *Backward Euler method* in the *ImplicitSolver* class. Finally, more advanced methods are available by wrapping the `scipy.integrate.solve_ivp()` in the *ScipySolver* class.

3.2 Basic usage

We here describe the typical workflow to solve a PDE using *py-pde*. Throughout this section, we assume that the package has been imported using `import pde`.

3.2.1 Defining the geometry

The state of the system is described in a discretized geometry, also known as a *grid*. The package focuses on simple geometries, which work well for the employed finite difference scheme. Grids are defined by instance of various classes that capture the symmetries of the underlying space. In particular, the package offers Cartesian grids of 1 to 3 dimensions via *CartesianGrid*, as well as curvilinear coordinate for spherically symmetric systems in two dimension (*PolarSymGrid*) and three dimensions (*SphericalSymGrid*), as well as the special class *CylindricalSymGrid* for a cylindrical geometry which is symmetric in the angle.

All grids allow to set the size of the underlying geometry and the number of support points along each axis, which determines the spatial resolution. Moreover, most grids support periodic boundary conditions. For example, a rectangular grid with one periodic boundary condition can be specified as

```
grid = pde.CartesianGrid([[0, 10], [0, 5]], [20, 10], periodic=[True, False])
```

This grid will have a rectangular shape of 10x5 with square unit cells of side length 0.5. Note that the grid will only be periodic in the x -direction.

3.2.2 Initializing a field

Fields specifying the values at the discrete points of the grid defined in the previous section. Most PDEs discussed in the package describe a scalar variable, which can be encoded th class *ScalarField*. However, tensors with rank 1 (vectors) and rank 2 are also supported using *VectorField* and *Tensor2Field*, respectively. In any case, a field is initialized using a pre-defined grid, e.g., `field = pde.ScalarField(grid)`. Optional values allow to set the value of the grid, as well as a label that is later used in plotting, e.g., `field1 = pde.ScalarField(grid, data=1, label="Ones")`. Moreover, fields can be initialized randomly (`field2 = pde.ScalarField.random_normal(grid, mean=0.5)`) or from a mathematical expression, which may depend on the coordinates of the grid (`field3 = pde.ScalarField.from_expression(grid, "x * y")`).

All field classes support basic arithmetic operations and can be used much like numpy arrays. Moreover, they have methods for applying differential operators, e.g., the result of applying the Laplacian to a scalar field is returned by calling the method `laplace()`, which returns another instance of `ScalarField`, whereas `gradient()` returns a `VectorField`. Combining these functions with ordinary arithmetics on fields allows to represent the right hand side of many partial differential equations that appear in physics. Importantly, the differential operators work with flexible boundary conditions.

3.2.3 Specifying the PDE

PDEs are also instances of special classes and a number of classical PDEs are already pre-defined in the module `pde.pdes`. Moreover, the special class `PDE` allows defining PDEs by simply specifying the expression on their right hand side. To see how this works in practice, let us consider the [Kuramoto–Sivashinsky equation](#), $\partial_t u = -\nabla^4 u - \nabla^2 u - \frac{1}{2}|\nabla u|^2$, which describes the time evolution of a scalar field u . A simple implementation of this equation reads

```
eq = pde.PDE({"u": "-gradient_squared(u) / 2 - laplace(u + laplace(u))"})
```

Here, the argument defines the evolution rate for all fields (in this case only u). The expression on the right hand side can contain typical mathematical functions and the operators defined by the package.

3.2.4 Running the simulation

To solve the PDE, we first need to generate an initial condition, i.e., the initial values of the fields that are evolved forward in time by the PDE. This field also defined the geometry on which the PDE is solved. In the simplest case, the solution is then obtain by running

```
result = eq.solve(field, t_range=10, dt=1e-2)
```

Here, `t_range` specifies the duration over which the PDE is considered and `dt` specifies the time step. The `result` field will be defined on the same grid as the initial condition `field`, but instead contain the data value at the final time. Note that all intermediate states are discarded in the simulation above and no information about the dynamical evolution is retained. To study the dynamics, one can either analyze the evolution on the fly or store its state for subsequent analysis. Both these tasks are achieved using `trackers`, which analyze the simulation periodically. For instance, to store the state for some time points in memory, one uses

```
storage = pde.MemoryStorage()
result = eq.solve(field, t_range=10, dt=1e-3, tracker=["progress", storage.
    ↪ tracker(1)])
```

Note that we also included the special identifier "progress" in the list of trackers, which shows a progress bar during the simulation. Another useful tracker is "plot" which displays the state on the fly.

3.2.5 Analyzing the results

Sometimes it suffices to plot the final result, which can be done using `result.plot()`. The final result can of course also be analyzed quantitatively, e.g., using `result.average` to obtain its mean value. If the intermediate states have been saved as indicated above, they can be analyzed subsequently:

```
for time, field in storage.items():
    print(f"t={time}, field={field.magnitude}")
```

Moreover, a movie of the simulation can be created using `pde.movie(storage, filename=FILE)`, where `FILE` determines where the movie is written.

3.3 Advanced usage

3.3.1 Boundary conditions

A crucial aspect of partial differential equations are boundary conditions, which need to be specified at the domain boundaries. For the simple domains contained in *py-pde*, all boundaries are orthogonal to one of the axes in the domain, so boundary conditions need to be applied to both sides of each axis. Here, the lower side of an axis can have a different condition than the upper side. For instance, one can enforce the value of a field to be 4 at the lower side and its derivative (in the outward direction) to be 2 on the upper side using the following code:

```
bc_lower = {"value": 4}
bc_upper = {"derivative": 2}
bc = [bc_lower, bc_upper]

grid = pde.UnitGrid([16])
field = pde.ScalarField(grid)
field.laplace(bc)
```

Here, the Laplace operator applied to the field in the last line will respect the boundary conditions. Note that it suffices to give one condition if both sides of the axis require the same condition. For instance, to enforce a value of 3 on both side, one could simply use `bc = {'value': 3}`. Vectorial boundary conditions, e.g., to calculate the vector gradient or tensor divergence, can have vectorial values for the boundary condition. Generally, only the normal components at a boundary need to be specified if an operator reduces the rank of a field, e.g., for divergences. Otherwise, e.g., for gradients and Laplacians, the full field needs to be specified at the boundary.

Boundary values that depend on space can be set by specifying a mathematical expression, which may depend on the coordinates of all axes:

```
# two different conditions for lower and upper end of x-axis
bc_x = [{"derivative": 0.1}, {"value": "sin(y / 2)"}]
# the same condition on the lower and upper end of the y-axis
bc_y = {"value": "sqrt(1 + cos(x))"}

grid = UnitGrid([32, 32])
field = pde.ScalarField(grid)
field.laplace(bc=[bc_x, bc_y])
```

Warning: To interpret arbitrary expressions, the package uses `exec()`. It should therefore not be used in a context where malicious input could occur.

Inhomogeneous values can also be specified by directly supplying an array, whose shape needs to be compatible with the boundary, i.e., it needs to have the same shape as the grid but with the dimension of the axis along which the boundary is specified removed.

There exist also special boundary conditions that impose a more complex value of the field (`bc='value_expression'`) or its derivative (`bc='derivative_expression'`). Beyond the spatial coordinates that are already supported for the constant conditions above, the expressions of these boundary conditions can depend on the time variable t . Moreover, these boundary conditions also accept python functions (with signature *adjacent_value*, *dx*, **coords*, *t*), thus greatly enlarging the flexibility with which boundary conditions can be expressed. Note that PDEs need to supply the current time t when setting the boundary conditions, e.g., when applying the differential operators. The pre-defined PDEs and the general class *PDE* already support time-dependent boundary conditions.

One important aspect about boundary conditions is that they need to respect the periodicity of the underlying grid. For instance, in a 2d grid with one periodic axis, the following boundary condition can be used:

```
grid = pde.UnitGrid([16, 16], periodic=[True, False])
field = pde.ScalarField(grid)
bc = ["periodic", {"derivative": 0}]
field.laplace(bc)
```

For convenience, this typical situation can be described with the special boundary condition *auto_periodic_neumann*, e.g., calling the Laplace operator using `field.laplace("auto_periodic_neumann")` is identical to the example above. Similarly, the special condition *auto_periodic_dirichlet* enforces periodic boundary conditions or Dirichlet boundary condition (vanishing value), depending on the periodicity of the underlying grid.

In summary, we have the following options for boundary conditions on a field c

Table 1: Supported boundary conditions

Name	Condition	Example
Dirichlet	$c = 0$	"dirichlet" or "value"
	$c = \text{const}$	{"value": 1.5}
	$c = f(x, t)$	{"value_expression": "sin(x)"}
	$c = f(x, t)$	{"value_expression": func} with function func(value, dx, *coords, t)
Neumann	$\partial_n c = 0$	"neumann" or "derivative"
	$\partial_n c = \text{const}$	{"derivative": -2}
	$\partial_n c = f(x, t)$	{"derivative_expression": "exp(t)"}
Robin	$\partial_n c + \text{value} \cdot c = \text{const}$	{"type": "mixed", "value": 2, "const": 7}
	$\partial_n c + \text{value} \cdot c = \text{const}$	{"type": "mixed_expression", "value": "exp(t)", "const": "3 * x"}
Curvature	$\partial_n^2 c = \text{const}$	{"curvature": 3}
Periodic	$c(0) = c(L)$	"periodic"
Anti-periodic	$c(0) = -c(L)$	"anti-periodic"
Periodic or Dirichlet	$c(0) = c(L)$ or $c = 0$	"auto_periodic_dirichlet"
Periodic or Neumann	$c(0) = c(L)$ or $\partial_n c = 0$	"auto_periodic_neumann"

Here, ∂_n denotes a derivative in outward normal direction, f denotes an arbitrary function given by an expression (see next section), x denotes coordinates along the boundary, t denotes time.

3.3.2 Expressions

Expressions are strings that describe mathematical expressions. They can be used in several places, most prominently in defining PDEs using *PDE*, in creating fields using *from_expression()*, and in defining boundary conditions; see section above. Expressions are parsed using *sympy*, so the expected syntax is defined by this python package. While we describe some common use cases below, it might be best to test the abilities using the *evaluate()* function.

Warning: To interpret arbitrary expressions, the package uses `exec()`. It should therefore not be used in a context where malicious input could occur.

Simple expressions can contain many standard mathematical functions, e.g., `sin(a) + b**2` is a valid expression. `PDE` and `evaluate()` furthermore accept differential operators defined in this package. Note that operators need to be specified with their full name, i.e., `laplace` for a scalar Laplacian and `vector_laplace` for a Laplacian operating on a vector field. Moreover, the dot product between two vector fields can be denoted by using `dot(field1, field2)` in the expression, and `outer(field1, field2)` calculates an outer product. In this case, boundary conditions for the operators can be specified using the `bc` argument, in which case the same boundary conditions are applied to all operators. The additional argument `bc_ops` provides a more fine-grained control, where conditions for each individual operator can be specified.

Field expressions can also directly depend on spatial coordinates. For instance, if a field is defined on a two-dimensional Cartesian grid, the variables `x` and `y` denote the local coordinates. To initialize a step profile in the x -direction, one can use either `(x > 5)` or `heaviside(x - 5, 0.5)`, where the second argument denotes the returned value in case the first argument is 0. Finally, expressions for equations in `PDE` can explicitly depend on time, which is denoted by the variable `t`.

Expressions also support user-defined functions via the `user_funcs` argument, which is a dictionary that maps the name of a function to an actual implementation. Finally, constants can be defined using the `consts` argument. Constants can either be individual numbers or spatially extended data, which provide values for each grid point. Note that in the latter case only the actual grid data should be supplied, i.e., the `data` attribute of a potential field class.

3.3.3 Custom PDE classes

To implement a new PDE in a way that all of the machinery of `py-pde` can be used, one needs to subclass `PDEBase` and overwrite at least the `evolution_rate()` method. A simple implementation for the Kuramoto–Sivashinsky equation could read

```
class KuramotoSivashinskyPDE(PDEBase):

    def evolution_rate(self, state, t=0):
        """ numpy implementation of the evolution equation """
        state_lapacian = state.laplace(bc="auto_periodic_neumann")
        state_gradient = state.gradient(bc="auto_periodic_neumann")
        return (- state_lapacian.laplace(bc="auto_periodic_neumann")
                - state_lapacian
                - 0.5 * state_gradient.to_scalar("squared_sum"))
```

A slightly more advanced example would allow for attributes that for instance define the boundary conditions and the diffusivity:

```
class KuramotoSivashinskyPDE(PDEBase):

    def __init__(self, diffusivity=1, bc="auto_periodic_neumann", bc_laplace="auto_
↳ periodic_neumann"):
        """ initialize the class with a diffusivity and boundary conditions
        for the actual field and its second derivative """
        self.diffusivity = diffusivity
        self.bc = bc
        self.bc_laplace = bc_laplace

    def evolution_rate(self, state, t=0):
        """ numpy implementation of the evolution equation """
        state_lapacian = state.laplace(bc=self.bc)
        state_gradient = state.gradient(bc=self.bc)
        return (- state_lapacian.laplace(bc=self.bc_laplace)
                - state_lapacian
                - 0.5 * self.diffusivity * (state_gradient @ state_gradient))
```

We here replaced the call to `to_scalar('squared_sum')` by a dot product with itself (using the `@` notation), which is equivalent. Note that the numpy implementation of the right hand side of the PDE is rather slow since it runs mostly in pure python and constructs a lot of intermediate field classes. While such an implementation is helpful for testing initial ideas, actual computations should be performed with compiled PDEs as described below.

3.3.4 Low-level operators

This section explains how to use the low-level version of the field operators. This is necessary for the numba-accelerated implementations described above and it might be necessary to use parts of the *py-pde* package in other packages.

Differential operators

Applying a differential operator to an instance of *ScalarField* is as simple as calling `field.laplace(bc)`, where *bc* denotes the boundary conditions. Calling this method returns another *ScalarField*, which in this case contains the discretized Laplacian of the original field. The equivalent call using the low-level interface is

```
apply_laplace = field.grid.make_operator("laplace", bc)

laplace_data = apply_laplace(field.data)
```

Here, the first line creates a function `apply_laplace` for the given grid `field.grid` and the boundary conditions *bc*. This function can be applied to `numpy.ndarray` instances, e.g. `field.data`. Note that the result of this call is again a `numpy.ndarray`.

Similarly, a gradient operator can be defined

```
grid = UnitGrid([6, 8])
apply_gradient = grid.make_operator("gradient", bc="auto_periodic_neumann")

data = np.random.random((6, 8))
gradient_data = apply_gradient(data)
assert gradient_data.shape == (2, 6, 8)
```

Note that this example does not even use the field classes. Instead, it directly defines a *grid* and the respective gradient operator. This operator is then applied to a random field and the resulting `numpy.ndarray` represents the 2-dimensional vector field.

The `make_operator` method of the grids generally supports the following differential operators: 'laplacian', 'gradient', 'gradient_squared', 'divergence', 'vector_gradient', 'vector_laplace', and 'tensor_divergence'. Moreover, generic operators that perform a derivative along a single axis are supported: Specifying 'd_dx' for instance performs a single derivative along the *x*-direction, 'd_dy_forward' uses a forward derivative along the *y*-direction, and 'd_d2r' performs a second derivative in *r*-direction. A complete list of operators supported by a certain grid class can be obtained from the class property `GridClass.operators`. New operators can be added using the class method `GridClass.register_operator()`.

Field integration

The integral of an instance of `ScalarField` is usually determined by accessing the property `field.integral`. Since the integral of a discretized field is basically a sum weighted by the cell volumes, calculating the integral using only `numpy` is easy:

```
cell_volumes = field.grid.cell_volumes
integral = (field.data * cell_volumes).sum()
```

Note that `cell_volumes` is a simple number for Cartesian grids, but is an array for more complicated grids, where the cell volume is not uniform.

Field interpolation

The fields defined in the `py-pde` package also support linear interpolation by calling `field.interpolate(point)`. Similarly to the differential operators discussed above, this call can also be translated to code that does not use the full package:

```
grid = UnitGrid([6, 8])
interpolate = grid.make_interpolator_compiled(bc="auto_periodic_neumann")

data = np.random.random((6, 8))
value = interpolate(data, np.array([3.5, 7.9]))
```

We first create a function `interpolate`, which is then used to interpolate the field data at a certain point. Note that the coordinates of the point need to be supplied as a `numpy.ndarray` and that only the interpolation at single points is supported. However, iteration over multiple points can be fast when the loop is compiled with `numba`.

Inner products

For vector and tensor fields, `py-pde` defines inner products that can be accessed conveniently using the `@`-syntax: `field1 @ field2` determines the scalar product between the two fields. The package also provides an implementation for an `dot`-operator:

```
grid = UnitGrid([6, 8])
field1 = VectorField.random_normal(grid)
field2 = VectorField.random_normal(grid)

dot_operator = field1.make_dot_operator()

result = dot_operator(field1.data, field2.data)
assert result.shape == (6, 8)
```

Here, `result` is the data of the scalar field resulting from the dot product.

3.3.5 Numba-accelerated PDEs

The compiled operators introduced in the previous section can be used to implement a compiled method for the evolution rate of PDEs. As an example, we now extend the class `KuramotoSivashinskyPDE` introduced above:

```
from pde.tools.numba import jit

class KuramotoSivashinskyPDE(PDEBase):

    def __init__(self, diffusivity=1, bc="auto_periodic_neumann", bc_laplace="auto_
    ↪periodic_neumann"):
        """ initialize the class with a diffusivity and boundary conditions
        for the actual field and its second derivative """
        self.diffusivity = diffusivity
        self.bc = bc
        self.bc_laplace = bc_laplace

    def evolution_rate(self, state, t=0):
        """ numpy implementation of the evolution equation """
        state_lapacian = state.laplace(bc=self.bc)
        state_gradient = state.gradient(bc="auto_periodic_neumann")
        return (- state_lapacian.laplace(bc=self.bc_laplace)
                - state_lapacian
                - 0.5 * self.diffusivity * (state_gradient @ state_gradient))

    def _make_pde_rhs_numba(self, state):
        """ the numba-accelerated evolution equation """
        # make attributes locally available
        diffusivity = self.diffusivity

        # create operators
        laplace_u = state.grid.make_operator("laplace", bc=self.bc)
        gradient_u = state.grid.make_operator("gradient", bc=self.bc)
        laplace2_u = state.grid.make_operator("laplace", bc=self.bc_laplace)
        dot = VectorField(state.grid).make_dot_operator()

        @jit
        def pde_rhs(state_data, t=0):
            """ compiled helper function evaluating right hand side """
            state_lapacian = laplace_u(state_data)
            state_grad = gradient_u(state_data)
            return (- laplace2_u(state_lapacian)
                    - state_lapacian
                    - diffusivity / 2 * dot(state_grad, state_grad))

        return pde_rhs
```

To activate the compiled implementation of the evolution rate, we simply have to overwrite the `_make_pde_rhs_numba()` method. This method expects an example of the state class (e.g., an instance of `ScalarField`) and returns a function that calculates the evolution rate. The `state` argument is necessary to define the grid and the dimensionality of the data that the returned function is supposed to be handling. The implementation of the compiled function is split in several parts, where we first copy the attributes that are required by the implementation. This is necessary, since `numba` freezes the values when compiling the function, so that in the example above the `diffusivity` cannot be altered without recompiling. In the next step, we create all operators that we need subsequently. Here, we use the boundary conditions defined by the attributes, which requires two different laplace operators, since their boundary

conditions might differ. In the last step, we define the actual implementation of the evolution rate as a local function that is compiled using the `jit` decorator. Here, we use the implementation shipped with *py-pde*, which sets some default values. However, we could have also used the usual numba implementation. It is important that the implementation of the evolution rate only uses python constructs that numba can compile.

One advantage of the numba compiled implementation is that we can now use loops, which will be much faster than their python equivalents. For instance, we could have written the dot product in the last line as an explicit loop:

```
[...]

def _make_pde_rhs_numba(self, state):
    """ the numba-accelerated evolution equation """
    # make attributes locally available
    diffusivity = self.diffusivity

    # create operators
    laplace_u = state.grid.make_operator("laplace", bc=self.bc)
    gradient_u = state.grid.make_operator("gradient", bc=self.bc)
    laplace2_u = state.grid.make_operator("laplace", bc=self.bc_laplace)
    dot = VectorField(state.grid).make_dot_operator()
    dim = state.grid.dim

    @jit
    def pde_rhs(state_data, t=0):
        """ compiled helper function evaluating right hand side """
        state_lapacian = laplace_u(state_data)
        state_grad = gradient_u(state_data)
        result = - laplace2_u(state_lapacian) - state_lapacian

        for i in range(state_data.size):
            for j in range(dim):
                result.flat[i] -= diffusivity / 2 * state_grad[j].flat[i]**2

        return result

    return pde_rhs
```

Here, we extract the total number of elements in the state using its `size` attribute and we obtain the dimensionality of the space from the grid attribute `dim`. Note that we access numpy arrays using their `flat` attribute to provide an implementation that works for all dimensions.

3.3.6 Configuration parameters

Configuration parameters affect how the package behaves. They can be set using a dictionary-like interface of the configuration `config`, which can be imported from the base package. Here is a list of all configuration options that can be adjusted in the package:

numba.debug

Determines whether numba uses the debug mode for compilation. If enabled, this emits extra information that might be useful for debugging. (**Default value: False**)

numba.fastmath

Determines whether the fastmath flag is set during compilation. If enabled, some mathematical operations might be faster, but less precise. This flag does not affect infinity detection and NaN handling. (**Default value: True**)

numba.multithreading

Determines whether multiple threads are used in numba-compiled code. Enabling this option accelerates a small subset of operators applied to fields defined on large grids. (**Default value: True**)

numba.multithreading_threshold

Minimal number of support points of grids before multithreading is enabled in numba compilations. Has no effect when `numba.multithreading` is `False`. **(Default value: 65536)**

Tip: To disable parallel computing in the package, the following code could be added to the start of the script:

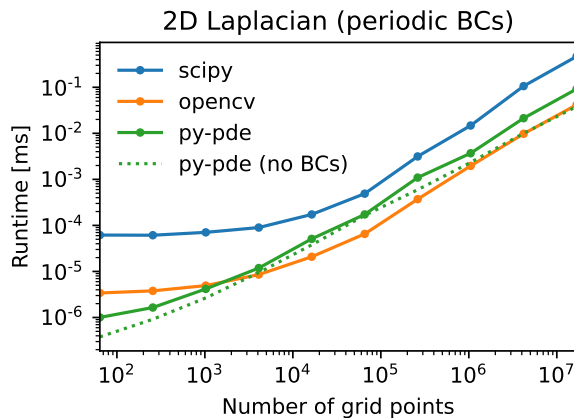
```
from pde import config
config["numba.multithreading"] = False

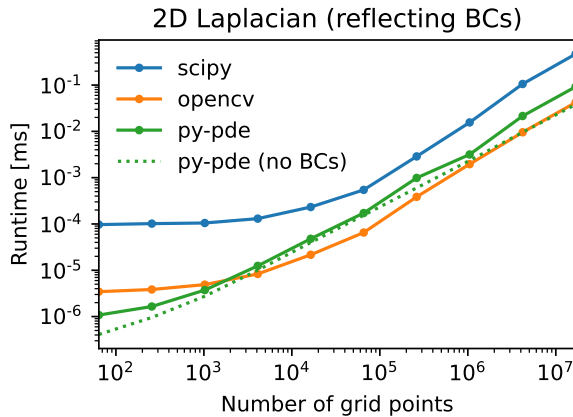
# actual code using py-pde
```

3.4 Performance

3.4.1 Measuring performance

The performance of the *py-pde* package depends on many details and general statements are thus difficult to make. However, since the core operators are just-in-time compiled using *numba*, many operations of the package proceed at performances close to most compiled languages. For instance, a simple Laplace operator applied to fields defined on a Cartesian grid has performance that is similar to the operators supplied by the popular *OpenCV* package. The following figures illustrate this by showing the duration of evaluating the Laplacian on grids of increasing number of support points for two different boundary conditions (lower duration is better):





Note that the call overhead is lower in the *py-pde* package, so that the performance on small grids is particularly good. However, realistic use-cases probably need more complicated operations and it is thus always necessary to profile the respective code. This can be done using the function `estimate_computation_speed()` or the traditional `timeit`, `profile`, or even more sophisticated profilers like `pyinstrument`.

3.4.2 Improving performance

Beside the underlying implementation of the operators, a major factor for performance is numerical problem at hand and the methods that are used to solve it. As a rule of thumb, simulations run faster when there are fewer degrees of freedom. In the case of partial differential equations, this often means using a coarser grid with fewer support points. However, there often also is an lower bound to the number of support points if structures of a certain length scales need to be resolved. Reducing the number of support points not only reduces the number of variables to be treated, but it can also allow for larger time steps. This is particularly transparent for the simple diffusion equation, where a [von Neumann stability analysis](#) reveals that the maximal time step scales as one over the discretization length squared! Choosing the right time step obviously also affects performance of a simulation. The package supports automatic choice of suitable time steps, using adaptive stepping schemes. To enable those, it's best to specify an initial time step, like so

```
eq.solve(t_range=10, dt=1e-3, adaptive=True)
```

An additional advantage of this choice is that it selects *ExplicitSolver*, which is also compiled with `numba` for speed. Alternatively, if only `t_range` is specified, the generic `scipy`-solver *ScipySolver*, which can be significantly slower.

Additional factors influencing the performance of the package include the compiler used for `numpy`, `scipy`, and of course `numba`. Moreover, the BLAS and LAPACK libraries might make a difference. The package has some basic support for multithreading, which can be accelerated using the *Threading Building Blocks* library. Finally, it can help to install the intel short vector math library (SVML). However, this is not distributed with `macports` and might thus be more difficult to enable.

Using `macports`, one could for instance install the following variants of typical packages

```
port install py37-numpy +gcc8+openblas
port install py37-scipy +gcc8+openblas
port install py37-numba +tbb
```

Note that you can disable the automatic multithreading via *Configuration parameters*.

3.4.3 Multiprocessing using MPI

The package also supports parallel simulations of PDEs using the [Message Passing Interface \(MPI\)](#), which allows combining the power of CPU cores that do not share memory. To use this advanced simulation technique, a working implementation of MPI needs to be installed on the computer. Usually, this is done automatically, when the optional package `numba-mpi` is installed via `pip` or `conda`.

To run simulations in parallel, the special solver `ExplicitMPSolver` needs to be used and the entire script needs to be started using `mpiexec`. Taken together, a minimal example reads

```
from pde import DiffusionPDE, ScalarField, UnitGrid

grid = UnitGrid([64, 64])
state = ScalarField.random_uniform(grid, 0.2, 0.3)

eq = DiffusionPDE(diffusivity=0.1)
result = eq.solve(state, t_range=10, dt=0.1, method="explicit_mpi")

if result is not None: # restrict the output to the main node
    result.plot()
```

Saving this script as `multiprocessing.py`, we can evoke a parallel simulation using

```
mpiexec -n 2 python3 multiprocessing.py
```

Here, the number 2 determines the number of cores that will be used. Note that macOS might require an additional hint on how to connect the processes even when they are run on the same machine (e.g., your workstation). It might help to run `mpiexec -n 2 -host localhost:2 python3 multiprocessing.py` in this case.

In the example above, two python processes will start in parallel and run independently at first. In particular, both processes will load all packages and create the initial `state` field as well as the PDE class `eq`. Once the `explicit_mpi` solver is evoked, the processes will start communicating. `py-pde` will split up the full grid into two sub-grids, in this case of shape 32x64, distribute the associated sub-fields to both processes and ask each process to evolve the PDE for their sub-field. Note that boundary conditions are treated and boundary values are exchanged between neighboring sub-grids automatically. To avoid confusion, trackers will only be used on one process and also the result is only returned in one process to avoid problems where multiple process write data simultaneously. Consequently, the example above checked whether `result` is `None` (in which case the corresponding process is a child process) and only resumes analysis when the result is actually present.

The automatic treatment tries to use sensible default values, so typical simulations work out of the box. However, in some situations it might be advantageous to adjust these values. For instance, the decomposition of the grid can be affected by an argument `decomposition`, which can be passed to the `solve()` method or the `ExplicitMPSolver`. The argument should be a list with one integer for each axis in the grid, which specifies how often the particular axis is divided.

Warning: The automatic division of the grid into sub-grids can lead to unexpected behavior, particularly in custom PDEs that were not designed for this use case. As a rule of thumb, all local operations are fine (since they can be performed on each subgrid), while global operations might need synchronization between all subgrids. One example is integration, which has been implemented properly in `py-pde`. Consequently, it is safe to use `integral`.

3.5 Contributing code

3.5.1 Structure of the package

The functionality of the `pde` package is split into multiple sub-package. The domain, together with its symmetries, periodicities, and discretizations, is described by classes defined in `grids`. Discretized fields are represented by classes in `fields`, which have methods for differential operators with various boundary conditions collected in `boundaries`. The actual pdes are collected in `pdes` and the respective solvers are defined in `solvers`.

3.5.2 Extending functionality

All code is build on a modular basis, making it easy to introduce new classes that integrate with the rest of the package. For instance, it is simple to define a new partial differential equation by subclassing `PDEBase`. Alternatively, PDEs can be defined by specifying their evolution rates using mathematical expressions by creating instances of the class `PDE`. Moreover, new grids can be introduced by subclassing `GridBase`. It is also possible to only use parts of the package, e.g., the discretized differential operators from `operators`.

New operators can be associated with grids by registering them using `register_operator()`. For instance, to create a new operator for the cylindrical grid one needs to define a factory function that creates the operator. This factory function takes an instance of `Boundaries` as an argument and returns a function that takes as an argument the actual data array for the grid. Note that the grid itself is an attribute of `Boundaries`. This operator would be registered with the grid by calling `CylindricalSymGrid.register_operator("operator", make_operator)`, where the first argument is the name of the operator and the second argument is the factory function.

3.5.3 Design choices

The data layout of field classes (subclasses of `FieldBase`) was chosen to allow for a simple decomposition of different fields and tensor components. Consequently, the data is laid out in memory such that spatial indices are last. For instance, the data of a vector field `field` defined on a 2d Cartesian grid will have three dimensions and can be accessed as `field.data[vector_component, x, y]`, where `vector_component` is either 0 or 1.

3.5.4 Coding style

The coding style is enforced using `isort` and `black`. Moreover, we use `Google Style docstrings`, which might be best [learned by example](#). The documentation, including the docstrings, are written using `reStructuredText`, with examples in the following [cheatsheet](#). To ensure the integrity of the code, we also try to provide many test functions, contained in the separate sub-folder `tests`. These tests can be ran using scripts in the `scripts` subfolder in the root folder. This folder also contain a script `tests_types.sh`, which uses `mypy` to check the consistency of the python type annotations. We use these type annotations for additional documentation and they have also already been useful for finding some bugs.

We also have some conventions that should make the package more consistent and thus easier to use. For instance, we try to use `properties` instead of getter and setter methods as often as possible. Because we use a lot of `numba` just-in-time compilation to speed up computations, we need to pass around (compiled) functions regularly. The names of the methods and functions that make such functions, i.e. that return callables, should start with `'make_*` where the wildcard should describe the purpose of the function being created.

3.5.5 Running unit tests

The `pde` package contains several unit tests, collection in the `tests` folder in the project root. These tests ensure that basic functions work as expected, in particular when code is changed in future versions. To run all tests, there are a few convenience scripts in the root directory `scripts`. The most basic script is `tests_run.sh`, which uses `pytest` to run the tests. Clearly, the python package `pytest` needs to be installed. There are also additional scripts that for instance run tests in parallel (needs the python package `pytest-xdist` installed), measure test coverage (needs package `pytest-cov` installed), and make simple performance measurements. Moreover, there is a script `test_types.sh`, which uses `mypy` to check the consistency of the python type annotations and there is a script `format_code.sh`, which formats the code automatically to adhere to our style.

Before committing a change to the code repository, it is good practice to run the tests, check the type annotations, and the coding style with the scripts described above.

3.6 Citing the package

To cite or reference *py-pde* in other work, please refer to the [publication in the Journal of Open Source Software](#). Here are the respective bibliographic records in Bibtex format:

```
@article{py-pde,
  Author = {David Zwicker},
  Doi = {10.21105/joss.02158},
  Journal = {Journal of Open Source Software},
  Number = {48},
  Pages = {2158},
  Publisher = {The Open Journal},
  Title = {py-pde: A Python package for solving partial differential equations},
  Url = {https://doi.org/10.21105/joss.02158},
  Volume = {5},
  Year = {2020}
}
```

and in RIS format:

```
TY  - JOUR
AU  - Zwicker, David
JO  - Journal of Open Source Software
IS  - 48
SP  - 2158
PB  - The Open Journal
T1  - py-pde: A Python package for solving partial differential equations
UR  - https://doi.org/10.21105/joss.02158
VL  - 5
PY  - 2020
```

3.7 Code of Conduct

3.7.1 Our Pledge

In the interest of fostering an open and welcoming environment, we as contributors and maintainers pledge to making participation in our project and our community a harassment-free experience for everyone, regardless of age, body size, disability, ethnicity, sex characteristics, gender identity and expression, level of experience, education, socio-economic status, nationality, personal appearance, race, religion, or sexual identity and orientation.

3.7.2 Our Standards

Examples of behavior that contributes to creating a positive environment include:

- Using welcoming and inclusive language
- Being respectful of differing viewpoints and experiences
- Gracefully accepting constructive criticism
- Focusing on what is best for the community
- Showing empathy towards other community members

Examples of unacceptable behavior by participants include:

- The use of sexualized language or imagery and unwelcome sexual attention or advances
- Trolling, insulting/derogatory comments, and personal or political attacks
- Public or private harassment
- Publishing others' private information, such as a physical or electronic address, without explicit permission
- Other conduct which could reasonably be considered inappropriate in a professional setting

3.7.3 Our Responsibilities

Project maintainers are responsible for clarifying the standards of acceptable behavior and are expected to take appropriate and fair corrective action in response to any instances of unacceptable behavior.

Project maintainers have the right and responsibility to remove, edit, or reject comments, commits, code, wiki edits, issues, and other contributions that are not aligned to this Code of Conduct, or to ban temporarily or permanently any contributor for other behaviors that they deem inappropriate, threatening, offensive, or harmful.

3.7.4 Scope

This Code of Conduct applies both within project spaces and in public spaces when an individual is representing the project or its community. Examples of representing a project or community include using an official project e-mail address, posting via an official social media account, or acting as an appointed representative at an online or offline event. Representation of a project may be further defined and clarified by project maintainers.

3.7.5 Enforcement

Instances of abusive, harassing, or otherwise unacceptable behavior may be reported by contacting the project team at david.zwicker@ds.mpg.de. All complaints will be reviewed and investigated and will result in a response that is deemed necessary and appropriate to the circumstances. The project team is obligated to maintain confidentiality with regard to the reporter of an incident. Further details of specific enforcement policies may be posted separately.

Project maintainers who do not follow or enforce the Code of Conduct in good faith may face temporary or permanent repercussions as determined by other members of the project's leadership.

3.7.6 Attribution

This Code of Conduct is adapted from the [Contributor Covenant](https://www.contributor-covenant.org/version/1/4/code-of-conduct.html), version 1.4, available at <https://www.contributor-covenant.org/version/1/4/code-of-conduct.html>

For answers to common questions about this code of conduct, see <https://www.contributor-covenant.org/faq>

REFERENCE MANUAL

The py-pde package provides classes and methods for solving partial differential equations.

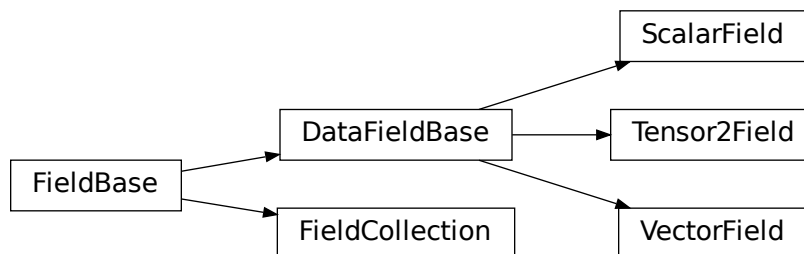
Subpackages:

4.1 `pde.fields` package

Defines fields, which contain the actual data stored on a discrete grid.

<i>ScalarField</i>	Scalar field discretized on a grid
<i>VectorField</i>	Vector field discretized on a grid
<i>Tensor2Field</i>	Tensor field of rank 2 discretized on a grid
<i>FieldCollection</i>	Collection of fields defined on the same grid

Inheritance structure of the classes:



The details of the classes are explained below:

4.1.1 `pde.fields.base` module

Defines base classes of fields, which are discretized on grids

class `DataFieldBase` (*grid*, *data*='zeros', *, *label*=None, *dtype*=None, *with_ghost_cells*=False)

Bases: `FieldBase`

abstract base class for describing fields of single entities

Parameters

- **grid** (`GridBase`) – Grid defining the space on which this field is defined.
- **data** (Number or `ndarray`, optional) – Field values at the support points of the grid. The flag *with_ghost_cells* determines whether this data array contains values for the ghost cells, too. The resulting field will contain real data unless the *data* argument contains complex values. Special values are “zeros” or None, initializing the field with zeros, and “empty”, just allocating memory with unspecified values.
- **label** (`str`, optional) – Name of the field
- **dtype** (`numpy dtype`) – The data type of the field. If omitted, it will be determined from *data* automatically.
- **with_ghost_cells** (`bool`) – Indicates whether the ghost cells are included in data

apply_operator (*operator*, *bc*, *out*=None, *, *label*=None, *args*=None, ***kwargs*)

apply a (differential) operator and return result as a field

Parameters

- **operator** (`str`) – An identifier determining the operator. Note that not all grids support the same operators.
- **bc** (`BoundariesData` | `None`) – Boundary conditions applied to the field before applying the operator. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value `None` is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (`DataFieldBase`, optional) – Optional field to which the result is written.
- **label** (`str`, optional) – Name of the returned field
- **args** (`dict`) – Additional arguments for the boundary conditions
- ****kwargs** – Additional arguments affecting how the operator behaves.

Returns

Field data after applying the operator. This field is identical to *out* if this argument was specified.

Return type

`DataFieldBase`

property average: `int | float | complex | ndarray`

the average of data

This is calculated by integrating each component of the field over space and dividing by the grid volume

Type

float or `ndarray`

copy (*, *label=None*, *dtype=None*)

return a new field with the data (but not the grid) copied

Parameters

- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically or the dtype of the current field is used.
- **self** (*TDataField*) –

Returns

A copy of the current field

Return type

`DataFieldBase`

property data_shape: `tuple[int, ...]`

the shape of the data at each grid point

Type

`tuple`

property fluctuations: `int | float | complex | ndarray`

quantification of the average fluctuations

The fluctuations are defined as the standard deviation of the data scaled by the cell volume. This definition makes the fluctuations independent of the discretization. It corresponds to the physical scaling available in the `random_normal()`.

Returns

A tensor with the same rank of the field, specifying the fluctuations of each component of the tensor field individually. Consequently, a simple scalar is returned for a `ScalarField`.

Return type

`ndarray`

Type

float or `ndarray`

classmethod from_state (*attributes*, *data=None*)

create a field from given state.

Parameters

- **attributes** (*dict*) – The attributes that describe the current instance
- **data** (*ndarray*, *optional*) – Data values at the support points of the grid defining the field

Returns

The instance created from the stored state

Return type

`DataFieldBase`

get_boundary_values (*axis*, *upper*, *bc=None*)

get the field values directly on the specified boundary

Parameters

- **axis** (*int*) – The axis perpendicular to the boundary
- **upper** (*bool*) – Whether the boundary is at the upper side of the axis
- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.

Returns

The discretized values on the boundary

Return type

`ndarray`

classmethod get_class_by_rank (*rank*)

return a `DataFieldBase` subclass describing a field with a given rank

Parameters

rank (*int*) – The rank of the tensor field

Returns

The DataField class that corresponds to the rank

Return type

`type[DataFieldBase]`

get_image_data (*scalar='auto'*, *transpose=False*, ***kwargs*)

return data for plotting an image of the field

Parameters

- **scalar** (*str* or *int*) – The method for extracting scalars as described in `DataFieldBase.to_scalar()`.
- **transpose** (*bool*) – Determines whether the transpose of the data should be plotted
- ****kwargs** – Additional parameters are forwarded to `grid.get_image_data`

Returns

Information useful for plotting an image of the field

Return type

`dict`

get_line_data (*scalar='auto'*, *extract='auto'*)

return data for a line plot of the field

Parameters

- **scalar** (*str* or *int*) – The method for extracting scalars as described in `DataFieldBase.to_scalar()`.
- **extract** (*str*) – The method used for extracting the line data. See the docstring of the grid method `get_line_data` to find supported values.

Returns

Information useful for performing a line plot of the field

Return type

`dict`

get_vector_data (*transpose=False, **kwargs*)

return data for a vector plot of the field

Parameters

- ****kwargs** – Additional parameters are forwarded to `grid.get_image_data`
- **transpose** (*bool*) –

Returns

Information useful for plotting an vector field

Return type

`dict`

insert (*point, amount*)

adds an (integrated) value to the field at an interpolated position

Parameters

- **point** (*ndarray*) – The point inside the grid where the value is added. This is given in grid coordinates.
- **amount** (Number or *ndarray*) – The amount that will be added to the field. The value describes an integrated quantity (given by the field value times the discretization volume). This is important for consistency with different discretizations and in particular grids with non-uniform discretizations.

Return type

`None`

abstract property integral: `int` | `float` | `complex` | `ndarray`

integral of the scalar field over space

interpolate (*point, *, bc=None, fill=None*)

interpolate the field to points between support points

Parameters

- **point** (*ndarray*) – The points at which the values should be obtained. This is given in grid coordinates.
- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field, which affects values close to the boundary. If omitted, the argument *fill* is used to determine values outside the domain. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by

`{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.

- **fill** (*Number*, *optional*) – Determines how values out of bounds are handled. If *None*, a *ValueError* is raised when out-of-bounds points are requested. Otherwise, the given value is returned.

Returns

the values of the field

Return type

`ndarray`

interpolate_to_grid (*grid*, *, *bc=None*, *fill=None*, *label=None*)

interpolate the data of this field to another grid.

Parameters

- **grid** (*GridBase*) – The grid of the new field onto which the current field is interpolated.
- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field, which affects values close to the boundary. If omitted, the argument *fill* is used to determine values outside the domain. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by 'periodic' and 'anti-periodic'). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{'value': NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **fill** (*Number*, *optional*) – Determines how values out of bounds are handled. If *None*, a *ValueError* is raised when out-of-bounds points are requested. Otherwise, the given value is returned.
- **label** (*str*, *optional*) – Name of the returned field
- **self** (*TDataField*) –

Returns

Field of the same rank as the current one.

Return type

TDataField

property magnitude: `float`

determine the (scalar) magnitude of the field

This is calculated by getting a scalar field using the default arguments of the `to_scalar()` method, averaging the result over the whole grid, and taking the absolute value.

Type

`float`

make_dot_operator (*backend='numba'*, *, *conjugate=True*)

return operator calculating the dot product between two fields

This supports both products between two vectors as well as products between a vector and a tensor.

Parameters

- **backend** (*str*) – Can be *numba* or *numpy*, deciding how the function is constructed
- **conjugate** (*bool*) – Whether to use the complex conjugate for the second operand

Returns

function that takes two instance of `ndarray`, which contain the discretized data of the two operands. An optional third argument can specify the output array to which the result is written.

Return type

`Callable[[ndarray, ndarray, ndarray | None], ndarray]`

make_interpolator (*, *fill=None*, *with_ghost_cells=False*)

returns a function that can be used to interpolate values.

Parameters

- **fill** (*Number*, *optional*) – Determines how values out of bounds are handled. If *None*, a *ValueError* is raised when out-of-bounds points are requested. Otherwise, the given value is returned.
- **with_ghost_cells** (*bool*) – Flag indicating that the interpolator should work on the full data array that includes values for the ghost points. If this is the case, the boundaries are not checked and the coordinates are used as is.

Returns

A function which returns interpolated values when called with arbitrary positions within the space of the grid.

Return type

`Callable[[ndarray, ndarray], int | float | complex | ndarray]`

plot (*kind='auto'*, **args*, *title=None*, *filename=None*, *action='auto'*, *ax_style=None*, *fig_style=None*, *ax=None*, ***kwargs*)

visualize the field

Parameters

- **kind** (*str*) – Determines the visualizations. Supported values are *image*, *line*, *vector*, or *interactive*. Alternatively, *auto* determines the best visualization based on the field itself.
- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically.
- **filename** (*str*, *optional*) – If given, the plot is written to the specified file.
- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **ax_style** (*dict*) – Dictionary with properties that will be changed on the axis after the plot has been drawn by calling `matplotlib.pyplot.setp()`. A special item in this dictionary is *use_offset*, which is flag that can be used to control whether offset are shown along the axes of the plot.
- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.

- **ax** (`matplotlib.axes.Axes`) – Figure axes to be used for plotting. The special value “create” creates a new figure, while “reuse” attempts to reuse an existing figure, which is the default.
- ****kwargs** – All additional keyword arguments are forwarded to the actual plotting function determined by *kind*.

Returns

Instance that contains information to update the plot with new data later.

Return type

PlotReference

Tip: Typical additional arguments for the various plot kinds include

- `kind == "line"`:
 - *scalar*: Sets method for extracting scalars as described in `DataFieldBase.to_scalar()`.
 - *extract*: Method used for extracting the line data.
 - *ylabel*: Label of the y-axis.
 - *ylim*: Data limits of the y-axis.
 - Additional arguments are passed to `matplotlib.pyplot.plot()`
 - `kind == "image"`:
 - *colorbar*: Determines whether a colorbar is shown
 - **scalar**: Sets method for extracting scalars as described in `DataFieldBase.to_scalar()`.
 - *transpose* Determines whether the transpose of the data is plotted
 - Most remaining arguments are passed to `matplotlib.pyplot.imshow()`
 - `kind == "vector"`:
 - *method* Can be either *quiver* or *streamplot*
 - *transpose* Determines whether the transpose of the data is plotted
 - *max_points* Sets max. number of points along each axis in quiver plots
 - Additional arguments are passed to `matplotlib.pyplot.quiver()` or `matplotlib.pyplot.streamplot()`.
-

classmethod random_colored (*grid*, *exponent=0*, *scale=1*, *, *label=None*, *dtype=None*, *rng=None*)

create a field of random values with colored noise

The spatially correlated values obey

$$\langle c_i(\mathbf{k}) c_j(\mathbf{k}') \rangle = \Gamma^2 |\mathbf{k}|^\nu \delta_{ij} \delta(\mathbf{k} - \mathbf{k}')$$

in spectral space, where \mathbf{k} is the wave vector. The special case $\nu = 0$ corresponds to white noise. Note that the spatial correlations always assume periodic boundary conditions (even if the underlying grid does not) and that the components of tensor fields are uncorrelated.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined

- **exponent** (*float*) – Exponent ν of the power spectrum
- **scale** (*float*) – Scaling factor Γ determining noise strength
- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it defaults to *double*.
- **rng** (*Generator*) – Random number generator (default: `default_rng()`)

Return type*TDataField*

classmethod random_harmonic (*grid*, *modes=3*, *harmonic=<ufunc 'cos'>*, *axis_combination=<ufunc 'multiply'>*, *, *label=None*, *dtype=None*, *rng=None*)

create a random field build from harmonics

The resulting fields will be highly correlated in space and can thus serve for testing differential operators.

With the default settings, the resulting field $c_i(\mathbf{x})$ is given by

$$c_i(\mathbf{x}) = \prod_{\alpha=1}^N \sum_{j=1}^M a_{ij\alpha} \cos\left(\frac{2\pi x_\alpha}{jL_\alpha}\right),$$

where N is the number of spatial dimensions, each with length L_α , M is the number of modes given by *modes*, and $a_{ij\alpha}$ are random amplitudes, chosen from a uniform distribution over the interval $[0, 1]$.

Note that the product could be replaced by a sum when *axis_combination* = *numpy.add* and the `cos()` could be any other function given by the parameter *harmonic*.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **modes** (*int*) – Number M of harmonic modes
- **harmonic** (*callable*) – Determines which harmonic function is used. Typical values are `numpy.sin()` and `numpy.cos()`, which basically relate to different boundary conditions applied at the grid boundaries.
- **axis_combination** (*callable*) – Determines how values from different axis are combined. Typical choices are `numpy.multiply()` and `numpy.add()` resulting in products and sums of the values along axes, respectively.
- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it defaults to *double*.
- **rng** (*Generator*) – Random number generator (default: `default_rng()`)

Return type*TDataField*

classmethod random_normal (*grid*, *mean=0*, *std=1*, *, *scaling='none'*, *label=None*, *dtype=None*, *rng=None*)

create field with normal distributed random values

These values are uncorrelated in space. A complex field is returned when either *mean* or *std* is a complex number. In this case, the real and imaginary parts of these arguments are used to determine the distribution of the real and imaginary parts of the resulting field. Consequently, `ScalarField.random_normal(grid, 0, 1 + 1j)` creates a complex field where the real and imaginary parts are chosen from a standard normal distribution.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **mean** (*float*) – Mean of the Gaussian distribution
- **std** (*float*) – Standard deviation of the Gaussian distribution.
- **scaling** (*str*) – Determines how the values are scaled. Possible choices are ‘none’ (values are drawn from a normal distribution with given mean and standard deviation) or ‘physical’ (the variance of the random number is scaled by the inverse volume of the grid cell; this is for instance useful for concentration fields, which vary less in larger volumes).
- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it defaults to *double* if both *mean* and *std* are real, otherwise it is *complex*.
- **rng** (*Generator*) – Random number generator (default: `default_rng()`)

Return type*TDataField***classmethod random_uniform** (*grid*, *vmin=0*, *vmax=1*, ***, *label=None*, *dtype=None*, *rng=None*)

create field with uniform distributed random values

These values are uncorrelated in space.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **vmin** (*float*) – Smallest possible random value
- **vmax** (*float*) – Largest random value
- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it defaults to *double* if both *vmin* and *vmax* are real, otherwise it is *complex*.
- **rng** (*Generator*) – Random number generator (default: `default_rng()`)

Return type*TDataField***rank:** *int***set_ghost_cells** (*bc*, ***, *set_corners=False*, *args=None*)

set the boundary values on virtual points for all boundaries

Parameters

- **bc** (*str or list or tuple or dict*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **set_corners** (*bool*) – Determines whether the corner cells are set using interpolation
- **args** – Additional arguments that might be supported by special boundary conditions.

Return type

None

smooth (*sigma*=1, *, *out*=None, *label*=None)

applies Gaussian smoothing with the given standard deviation

This function respects periodic boundary conditions of the underlying grid, using reflection when no periodicity is specified.

Parameters

- **sigma** (*float*) – Gives the standard deviation of the smoothing in real length units (default: 1)
- **out** (*FieldBase*, *optional*) – Optional field into which the smoothed data is stored. Setting this to the input field enables in-place smoothing.
- **label** (*str*, *optional*) – Name of the returned field
- **self** (*TDataField*) –

ReturnsField with smoothed data. This is stored at *out* if given.**Return type***TDataField***abstract to_scalar** (*scalar*='auto', *, *label*=None)

return scalar variant of the field

Parameters

- **scalar** (*str*) –
- **label** (*str* | *None*) –

Return type*ScalarField***classmethod unserialize_attributes** (*attributes*)

unserializes the given attributes

Parameters**attributes** (*dict*) – The serialized attributes**Returns**

The unserialized attributes

Return type*dict***class FieldBase** (*grid*, *data*, *, *label*=None)Bases: *object*

abstract base class for describing (discretized) fields

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **data** (*ndarray*, *optional*) – Field values at the support points of the grid and the ghost cells
- **label** (*str*, *optional*) – Name of the field

apply (*func*, *out=None*, *, *label=None*, *evaluate_args=None*)

applies a function/expression to the data and returns it as a field

Parameters

- **func** (*callable* or *str*) – The (vectorized) function being applied to the data or an expression that can be parsed using sympy (`evaluate()` is used in this case). The local field values can be accessed using the field labels for a field collection and via the variable *c* otherwise.
- **out** (*FieldBase*, *optional*) – Optional field into which the data is written
- **label** (*str*, *optional*) – Name of the returned field
- **evaluate_args** (*dict*) – Additional arguments passed to `evaluate()`. Only used when *func* is a string.
- **self** (*TField*) –

Returns

Field with new data. Identical to *out* if given.

Return type

FieldBase

assert_field_compatible (*other*, *accept_scalar=False*)

checks whether *other* is compatible with the current field

Parameters

- **other** (*FieldBase*) – The other field this one is compared to
- **accept_scalar** (*bool*, *optional*) – Determines whether it is acceptable that *other* is an instance of `ScalarField`.

Return type

None

property attributes: `dict[str, Any]`

describes the state of the instance (without the data)

Type

`dict`

property attributes_serialized: `dict[str, str]`

serialized version of the attributes

Type

`dict`

conjugate ()

returns complex conjugate of the field

Returns

the complex conjugated field

Return type

FieldBase

Parameters

self (*TField*) –

abstract copy (*, *label=None*, *dtype=None*)

return a new field with the data (but not the grid) copied

Parameters

- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically or the dtype of the current field is used.
- **self** (*TField*) –

Returns

A copy of the current field

Return type

DataFieldBase

property data: *ndarray*

discretized data at the support points

Type

ndarray

property dtype: *dtype[Any] | None | type[Any] | _SupportsDType[dtype[Any]] | str | tuple[Any, int] | tuple[Any, SupportsIndex] | Sequence[SupportsIndex] | list[Any] | _DTypeDict | tuple[Any, Any]*

the numpy dtype of the underlying data

Type

DTypeLike

classmethod from_file (*filename*)

create field from data stored in a file

Field can be written to a file using *FieldBase.to_file()*.

Example

Write a field to a file and then read it back:

```
field = pde.ScalarField(...)
field.write_to("test.hdf5")

field_copy = pde.FieldBase.from_file("test.hdf5")
```

Parameters

filename (*str*) – Path to the file being read

Returns

The field with the appropriate sub-class

Return type

FieldBase

classmethod from_state (*attributes*, *data=None*)

create a field from given state.

Parameters

- **attributes** (*dict*) – The attributes that describe the current instance
- **data** (*ndarray*, optional) – Data values at the support points of the grid defining the field

Returns

The field created from the state

Return type

FieldBase

abstract `get_image_data()`

return data for plotting an image of the field

Parameters

- **scalar** (*str* or *int*) – The method for extracting scalars as described in *DataFieldBase.to_scalar()*.
- **transpose** (*bool*) – Determines whether the transpose of the data should be plotted
- ****kwargs** – Additional parameters are forwarded to *grid.get_image_data*

Returns

Information useful for plotting an image of the field

Return type

dict

abstract `get_line_data(scalar='auto', extract='auto')`

return data for a line plot of the field

Parameters

- **scalar** (*str* or *int*) – The method for extracting scalars as described in *DataFieldBase.to_scalar()*.
- **extract** (*str*) – The method used for extracting the line data. See the docstring of the grid method *get_line_data* to find supported values.

Returns

Information useful for performing a line plot of the field

Return type

dict

property `grid`: *GridBase*

The grid on which the field is defined

Type

base, GridBase

property `imag`: *TField*

Imaginary part of the field

Type

FieldBase

property `is_complex`: *bool*

whether the field contains real or complex data

Type

bool

property label: `str` | `None`

the name of the field

Type

`str`

abstract plot (**args, **kwargs*)

visualize the field

plot_interactive (*viewer_args=None, **kwargs*)

create an interactive plot of the field using `napari`

For a detailed description of the launched program, see the [napari webpage](#).

Parameters

- **viewer_args** (*dict*) – Arguments passed to `napari.viewer.Viewer` to affect the viewer.
- ****kwargs** – Extra arguments passed to the plotting function

Return type

`None`

property real: `TField`

Real part of the field

Type

`FieldBase`

split_mpi (*decomposition=-1*)

splits the field onto subgrids in an MPI run

In a normal serial simulation, the method simply returns the field itself. In contrast, in an MPI simulation, the field provided on the main node is split onto all nodes using the given decomposition. The field data provided on all other nodes is not used.

Parameters

- **decomposition** (*list of ints*) – Number of subdivision in each direction. Should be a list of length `field.grid.num_axes` specifying the number of nodes for this axis. If one value is `-1`, its value will be determined from the number of available nodes. The default value decomposed the first axis using all available nodes
- **self** (*TField*) –

Returns

The part of the field that corresponds to the subgrid associated with the current MPI node.

Return type

`FieldBase`

to_file (*filename, **kwargs*)

store field in a file

The extension of the filename determines what format is being used. If it ends in `.h5` or `.hdf`, the Hierarchical Data Format is used. The other supported format are images, where only the most typical formats are supported.

To load the field back from the file, you may use `FieldBase.from_file()`.

Example

Write a field to a file and then read it back:

```
field = pde.ScalarField(...)
field.write_to("test.hdf5")

field_copy = pde.FieldBase.from_file("test.hdf5")
```

Parameters

- **filename** (*str*) – Path where the data is stored
- ****kwargs** – Additional parameters may be supported for some formats

Return type

None

classmethod unserialize_attributes (*attributes*)

unserializes the given attributes

Parameters

attributes (*dict*) – The serialized attributes

Returns

The unserialized attributes

Return type

dict

property writeable: *bool*

whether the field data can be changed or not

Type

bool

exception RankError

Bases: *TypeError*

error indicating that the field has the wrong rank

4.1.2 pde.fields.collection module

Defines a collection of fields to represent multiple fields defined on a common grid.

class FieldCollection (*fields*, *, *copy_fields=False*, *label=None*, *labels=None*, *dtype=None*)

Bases: *FieldBase*

Collection of fields defined on the same grid

Note: All fields in a collection must have the same data type. This might lead to up-casting, where for instance a combination of a real-valued and a complex-valued field will be both stored as complex fields.

Parameters

- **fields** (sequence or mapping of *DataFieldBase*) – Sequence or mapping of the individual fields. If a mapping is used, the keys set the names of the individual fields.

- **copy_fields** (*bool*) – Flag determining whether the individual fields given in *fields* are copied. Note that fields are always copied if some of the supplied fields are identical. If fields are copied the original fields will be left untouched. Conversely, if *copy_fields* == *False*, the original fields are modified so their data points to the collection. It is thus basically impossible to have fields that are linked to multiple collections at the same time.
- **label** (*str*) – Label of the field collection
- **labels** (*list of str*) – Labels of the individual fields. If omitted, the labels from the *fields* argument are used.
- **dtype** (*numpy dtype*) – The data type of the field. All the numpy dtypes are supported. If omitted, it will be determined from *data* automatically.

append (**fields*, *label=None*)

create new collection with appended field(s)

Parameters

- **fields** (*FieldCollection* or *DataFieldBase*) – A sequence of single fields or collection of fields that will be appended to the fields in the current collection. The data of all fields will be copied.
- **label** (*str*) – Label of the new field collection. If omitted, the current label is used

Returns

A new field collection, which combines the current one with fields given by *fields*.

Return type

FieldCollection

assert_field_compatible (*other*, *accept_scalar=False*)

checks whether *other* is compatible with the current field

Parameters

- **other** (*FieldBase*) – Other field this is compared to
- **accept_scalar** (*bool*, *optional*) – Determines whether it is acceptable that *other* is an instance of *ScalarField*.

property attributes: *dict[str, Any]*

describes the state of the instance (without the data)

Type

dict

property attributes_serialized: *dict[str, str]*

serialized version of the attributes

Type

dict

property averages: *list*

averages of all fields

copy (*, *label=None*, *dtype=None*)

return a copy of the data, but not of the grid

Parameters

- **label** (*str*, *optional*) – Name of the returned field

- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.
- **self** (*FieldCollection*) –

Return type*FieldCollection***property fields:** *list* [*DataFieldBase*]

the fields of this collection

Type*list***classmethod from_data** (*field_classes*, *grid*, *data*, *, *with_ghost_cells=True*, *label=None*, *labels=None*, *dtype=None*)

create a field collection from classes and data

Parameters

- **field_classes** (*list*) – List of the classes that define the individual fields
- **data** (*ndarray*, optional) – Data values of all fields at support points of the grid
- **grid** (*GridBase*) – Grid defining the space on which this field is defined.
- **with_ghost_cells** (*bool*) – Indicates whether the ghost cells are included in data
- **label** (*str*) – Label of the field collection
- **labels** (*list of str*) – Labels of the individual fields. If omitted, the labels from the *fields* argument are used.
- **dtype** (*numpy dtype*) – The data type of the field. All the numpy dtypes are supported. If omitted, it will be determined from *data* automatically.

classmethod from_scalar_expressions (*grid*, *expressions*, *, *user_funcs=None*, *consts=None*, *label=None*, *labels=None*, *dtype=None*)

create a field collection on a grid from given expressions

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **expressions** (*list of str*) – A list of mathematical expression, one for each field in the collection. The expressions determine the values as a function of the position on the grid. The expressions may contain standard mathematical functions and they may depend on the axes labels of the grid. More information can be found in the [expression documentation](#).
- **user_funcs** (*dict*, optional) – A dictionary with user defined functions that can be used in the expression
- **consts** (*dict*, optional) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or *ndarray*.
- **label** (*str*, optional) – Name of the whole collection
- **labels** (*list of str*, optional) – Names of the individual fields

- **dtype** (*numpy dtype*) – The data type of the field. All the numpy dtypes are supported. If omitted, it will be determined from *data* automatically.

Return type*FieldCollection***classmethod** `from_state` (*attributes*, *data=None*)

create a field collection from given state.

Parameters

- **attributes** (*dict*) – The attributes that describe the current instance
- **data** (*ndarray*, optional) – Data values at support points of the grid defining all fields

Return type*FieldCollection***get_image_data** (*index=0*, ***kwargs*)

return data for plotting an image of the field

Parameters

- **index** (*int*) – Index of the field whose data is returned
- ****kwargs** – Arguments forwarded to the *get_image_data* method

Returns

Information useful for plotting an image of the field

Return type*dict***get_line_data** (*index=0*, *scalar='auto'*, *extract='auto'*)

return data for a line plot of the field

Parameters

- **index** (*int*) – Index of the field whose data is returned
- **scalar** (*str* or *int*) – The method for extracting scalars as described in *DataFieldBase.to_scalar()*.
- **extract** (*str*) – The method used for extracting the line data. See the docstring of the grid method *get_line_data* to find supported values.

Returns

Information useful for performing a line plot of the field

Return type*dict***property** `integrals`: *list*

integrals of all fields

interpolate_to_grid (*grid*, ***, *fill=None*, *label=None*)

interpolate the data of this field collection to another grid.

Parameters

- **grid** (*GridBase*) – The grid of the new field onto which the current field is interpolated.

- **fill** (*Number, optional*) – Determines how values out of bounds are handled. If *None*, a *ValueError* is raised when out-of-bounds points are requested. Otherwise, the given value is returned.
- **label** (*str, optional*) – Name of the returned field collection

Returns

Interpolated data

Return type

`FieldCollection`

property labels: `_FieldLabels`

the labels of all fields

Note: The attribute returns a special class `_FieldLabels` to allow specific manipulations of the field labels. The returned object behaves much like a list, but assigning values will modify the labels of the fields in the collection.

Type

`_FieldLabels`

property magnitudes: `ndarray`

scalar magnitudes of all fields

Type

`ndarray`

plot (*kind='auto', figsize='auto', arrangement='horizontal', subplot_args=None, *args, title=None, constrained_layout=True, filename=None, action='auto', fig_style=None, fig=None, **kwargs*)

visualize all the fields in the collection

Parameters

- **kind** (*str or list of str*) – Determines the kind of the visualizations. Supported values are *image*, *line*, *vector*, *interactive*, or *merged*. Alternatively, *auto* determines the best visualization based on each field itself. Instead of a single value for all fields, a list with individual values can be given, unless *merged* is chosen.
- **figsize** (*str or tuple of numbers*) – Determines the figure size. The figure size is unchanged if the string *default* is passed. Conversely, the size is adjusted automatically when *auto* is passed. Finally, a specific figure size can be specified using two values, using `matplotlib.figure.Figure.set_size_inches()`.
- **arrangement** (*str*) – Determines how the subpanels will be arranged. The default value *horizontal* places all subplots next to each other. The alternative value *vertical* puts them below each other.
- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically. This is shown above all panels.
- **constrained_layout** (*bool*) – Whether to use *constrained_layout* in `matplotlib.pyplot.figure()` call to create a figure. This affects the layout of all plot elements. Generally, spacing might be better with this flag enabled, but it can also lead to problems when plotting multiple plots successively, e.g., when creating a movie.
- **filename** (*str, optional*) – If given, the figure is written to the specified file.

- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.
- **fig** (`matplotlib.figure.Figure`) – Figure that is used for plotting. If omitted, a new figure is created.
- **subplot_args** (*list*) – Additional arguments for the specific subplots. Should be a list with a dictionary of arguments for each subplot. Supplying an empty dict allows to keep the default setting of specific subplots.
- ****kwargs** – All additional keyword arguments are forwarded to the actual plotting function of all subplots.

Returns

Instances that contain information to update all the plots with new data later.

Return type

List of `PlotReference`

classmethod scalar_random_uniform (*num_fields*, *grid*, *vmin*=0, *vmax*=1, *, *label*=None, *labels*=None, *rng*=None)

create scalar fields with random values between *vmin* and *vmax*

Parameters

- **num_fields** (*int*) – The number of fields to create
- **grid** (`GridBase`) – Grid defining the space on which the fields are defined
- **vmin** (*float*) – Lower bound. Can be complex to create complex fields
- **vmax** (*float*) – Upper bound. Can be complex to create complex fields
- **label** (*str*, *optional*) – Name of the field collection
- **labels** (*list of str*, *optional*) – Names of the individual fields
- **rng** (`Generator`) – Random number generator (default: `default_rng()`)

Return type

`FieldCollection`

smooth (*sigma*=1, *, *out*=None, *label*=None)

applies Gaussian smoothing with the given standard deviation

This function respects periodic boundary conditions of the underlying grid, using reflection when no periodicity is specified.

sigma (float):

Gives the standard deviation of the smoothing in real length units (default: 1)

out (FieldCollection, optional):

Optional field into which the smoothed data is stored

label (str, optional):

Name of the returned field

Returns

Field collection with smoothed data, stored at *out* if given.

Parameters

- **sigma** (*float*) –
- **out** (*FieldCollection* / *None*) –
- **label** (*str* / *None*) –

Return type

FieldCollection

classmethod **unserialize_attributes** (*attributes*)

unserializes the given attributes

Parameters

attributes (*dict*) – The serialized attributes

Returns

The unserialized attributes

Return type

dict

4.1.3 `pde.fields.scalar` module

Defines a scalar field over a grid

class **ScalarField** (*grid*, *data*='zeros', *, *label*=None, *dtype*=None, *with_ghost_cells*=False)

Bases: *DataFieldBase*

Scalar field discretized on a grid

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined.
- **data** (Number or *ndarray*, optional) – Field values at the support points of the grid. The flag *with_ghost_cells* determines whether this data array contains values for the ghost cells, too. The resulting field will contain real data unless the *data* argument contains complex values. Special values are “zeros” or None, initializing the field with zeros, and “empty”, just allocating memory with unspecified values.
- **label** (*str*, optional) – Name of the field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.
- **with_ghost_cells** (*bool*) – Indicates whether the ghost cells are included in data

classmethod **from_expression** (*grid*, *expression*, *, *user_funcs*=None, *consts*=None, *label*=None, *dtype*=None)

create a scalar field on a grid from a given expression

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **expression** (*str*) – Mathematical expression for the scalar value as a function of the position on the grid. The expression may contain standard mathematical functions and it may depend on the axes labels of the grid. More information can be found in the [expression documentation](#).
- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that can be used in the expression
- **consts** (*dict*, *optional*) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or `ndarray`.
- **label** (*str*, *optional*) – Name of the field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.

Return type[ScalarField](#)**classmethod** `from_image` (*path*, *bounds=None*, *periodic=False*, *, *label=None*)

create a scalar field from an image

Parameters

- **path** (*Path* or *str*) – The path to the image file
- **bounds** (*tuple*, *optional*) – Gives the coordinate range for each axis. This should be two tuples of two numbers each, which mark the lower and upper bound for each axis.
- **periodic** (*bool* or *list*) – Specifies which axes possess periodic boundary conditions. This is either a list of booleans defining periodicity for each individual axis or a single boolean value specifying the same periodicity for all axes.
- **label** (*str*, *optional*) – Name of the field

Return type[ScalarField](#)**get_boundary_field** (*index*, *bc=None*, *, *label=None*)

get the field on the specified boundary

Parameters

- **index** (*str* or *tuple*) – Index specifying the boundary. Can be either a string given in [boundary_names](#), like "left", or a tuple of the axis index perpendicular to the boundary and a boolean specifying whether the boundary is at the upper side of the axis or not, e.g., (1, True).
- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by 'periodic' and 'anti-periodic'). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by {'value': NUM}) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by {'derivative': DERIV}) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis

and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.

- **label** (*str*) – Label of the returned field

Returns

The field on the boundary

Return type

ScalarField

gradient (*bc*, *out=None*, ***kwargs*)

apply gradient operator and return result as a field

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (*VectorField*, *optional*) – Optional vector field to which the result is written.
- **label** (*str*, *optional*) – Name of the returned field

Returns

result of applying the operator

Return type

VectorField

gradient_squared (*bc*, *out=None*, ***kwargs*)

apply squared gradient operator and return result as a field

This evaluates $|\nabla\phi|^2$ for the scalar field ϕ

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (*ScalarField*, *optional*) – Optional vector field to which the result is written.
- **label** (*str*, *optional*) – Name of the returned field

- **central** (*bool*) – Determines whether a central difference approximation is used for the gradient operator or not. If not, the squared gradient is calculated as the mean of the squared values of the forward and backward derivatives, which thus includes the value at a support point in the result at the same point.

Returns

the squared gradient of the field

Return type

ScalarField

property integral: *int* | *float* | *complex*

integral of the scalar field over space

Type

Number

interpolate_to_grid (*grid*, *, *bc=None*, *fill=None*, *label=None*)

interpolate the data of this scalar field to another grid.

Parameters

- **grid** (*GridBase*) – The grid of the new field onto which the current field is interpolated.
- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field, which affects values close to the boundary. If omitted, the argument *fill* is used to determine values outside the domain. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **fill** (*Number*, *optional*) – Determines how values out of bounds are handled. If *None*, a *ValueError* is raised when out-of-bounds points are requested. Otherwise, the given value is returned.
- **label** (*str*, *optional*) – Name of the returned field
- **self** (*ScalarField*) –

Returns

Field of the same rank as the current one.

Return type

ScalarField

laplace (*bc*, *out=None*, ***kwargs*)

apply Laplace operator and return result as a field

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value

NUM (specified by `{'value': NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value `None` is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.

- **out** (`ScalarField`, *optional*) – Optional scalar field to which the result is written.
- **label** (`str`, *optional*) – Name of the returned field
- **backend** (`str`) – The backend (e.g., 'numba' or 'scipy') used for this operator.

Returns

the Laplacian of the field

Return type

`ScalarField`

project (`axes`, `method='integral'`, `label=None`)

project scalar field along given axes

Parameters

- **axes** (*list of str*) – The names of the axes that are removed by the projection operation. The valid names for a given grid are the ones in the `GridBase.axes` attribute.
- **method** (`str`) – The projection method. This can be either 'integral' to integrate over the removed axes or 'average' to perform an average instead.
- **label** (`str`, *optional*) – The label of the returned field

Returns

The projected data in a scalar field with a subgrid of the original grid.

Return type

`ScalarField`

rank: `int` = 0

slice (`position`, `*`, `method='nearest'`, `label=None`)

slice data at a given position

Note: This method should not be used to evaluate fields right at the boundary since it does not respect boundary conditions. Use `get_boundary_field()` to obtain the values directly on the boundary.

Parameters

- **position** (*dict*) – Determines the location of the slice using a dictionary supplying coordinate values for a subset of axes. Axes not mentioned in the dictionary are retained and form the slice. For instance, in a 2d Cartesian grid, `position = {'x': 1}` slices along the y-direction at x=1. Additionally, the special positions 'low', 'mid', and 'high' are supported to reference relative positions along the axis.
- **method** (`str`) – The method used for slicing. Currently, we only support *nearest*, which takes data from cells defined on the grid.
- **label** (`str`, *optional*) – The label of the returned field

Returns

The sliced data in a scalar field with a subgrid of the original grid.

Return type*ScalarField***to_scalar** (*scalar*='auto', *, *label*=None)return a modified scalar field by applying method *scalar***Parameters**

- **scalar** (*str* or *callable*) – Determines the method used for obtaining the scalar. If this is a callable, it is simply applied to self.data and a new scalar field with this data is returned. Alternatively, pre-defined methods can be selected using strings. Here, *abs* and *norm* denote the norm of each entry of the field, while *norm_squared* returns the squared norm. The default *auto* is to return a (unchanged) copy of a real field and the norm of a complex field.
- **label** (*str*, *optional*) – Name of the returned field

Returns

Scalar field after applying the operation

Return type*ScalarField*

4.1.4 pde.fields.tensorial module

Defines a tensorial field of rank 2 over a grid

class Tensor2Field (*grid*, *data*='zeros', *, *label*=None, *dtype*=None, *with_ghost_cells*=False)Bases: *DataFieldBase*

Tensor field of rank 2 discretized on a grid

Warning: Components of the tensor field are given in the local basis. While the local basis is identical to the global basis in Cartesian coordinates, the local basis depends on position in curvilinear coordinate systems. Moreover, the field always contains all components, even if the underlying grid assumes symmetries.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined.
- **data** (Number or *ndarray*, *optional*) – Field values at the support points of the grid. The flag *with_ghost_cells* determines whether this data array contains values for the ghost cells, too. The resulting field will contain real data unless the *data* argument contains complex values. Special values are “zeros” or None, initializing the field with zeros, and “empty”, just allocating memory with unspecified values.
- **label** (*str*, *optional*) – Name of the field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.
- **with_ghost_cells** (*bool*) – Indicates whether the ghost cells are included in data

divergence (*bc*, *out=None*, ***kwargs*)

apply tensor divergence and return result as a field

The tensor divergence is a vector field v_α resulting from a contracting of the derivative of the tensor field $t_{\alpha\beta}$:

$$v_\alpha = \sum_\beta \frac{\partial t_{\alpha\beta}}{\partial x_\beta}$$

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (*VectorField*, *optional*) – Optional scalar field to which the result is written.
- **label** (*str*, *optional*) – Name of the returned field
- ****kwargs** – Additional arguments affecting how the operator behaves.

Returns

result of applying the operator

Return type

VectorField

dot (*other*, *out=None*, ***, *conjugate=True*, *label='dot product'*)

calculate the dot product involving a tensor field

This supports the dot product between two tensor fields as well as the product between a tensor and a vector. The resulting fields will be a tensor or vector, respectively.

Parameters

- **other** (*VectorField* or *Tensor2Field*) – the second field
- **out** (*VectorField* or *Tensor2Field*, *optional*) – Optional field to which the result is written.
- **conjugate** (*bool*) – Whether to use the complex conjugate for the second operand
- **label** (*str*, *optional*) – Name of the returned field

Returns

VectorField or *Tensor2Field*: result of applying the dot operator

Return type

VectorField | *Tensor2Field*

classmethod from_expression (*grid*, *expressions*, ***, *user_funcs=None*, *consts=None*, *label=None*, *dtype=None*)

create a tensor field on a grid from given expressions

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **expressions** (*list of str*) – A 2d list of mathematical expression, one for each component of the tensor field. The expressions determine the values as a function of the position on the grid. The expressions may contain standard mathematical functions and they may depend on the axes labels of the grid. More information can be found in the [expression documentation](#).
- **user_funcs** (*dict, optional*) – A dictionary with user defined functions that can be used in the expression
- **consts** (*dict, optional*) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or `ndarray`.
- **label** (*str, optional*) – Name of the field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.

Return type

`Tensor2Field`

property integral: `ndarray`

integral of each component over space

Type

`ndarray`

plot_components (*kind='auto', *args, title=None, constrained_layout=True, filename=None, action='auto', fig_style=None, fig=None, **kwargs*)

visualize all the components of this tensor field

Parameters

- **kind** (*str or list of str*) – Determines the kind of the visualizations. Supported values are *image* or *line*. Alternatively, *auto* determines the best visualization based on the grid.
- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically. This is shown above all panels.
- **constrained_layout** (*bool*) – Whether to use *constrained_layout* in `matplotlib.pyplot.figure()` call to create a figure. This affects the layout of all plot elements. Generally, spacing might be better with this flag enabled, but it can also lead to problems when plotting multiple plots successively, e.g., when creating a movie.
- **filename** (*str, optional*) – If given, the figure is written to the specified file.
- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.

- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.
- **fig** (`matplotlib.figure.Figure`) – Figure that is used for plotting. If omitted, a new figure is created.
- ****kwargs** – All additional keyword arguments are forwarded to the actual plotting function of all subplots.

Returns

Instances that contain information to update all the plots with new data later.

Return type

2d list of `PlotReference`

rank: `int` = 2

symmetrize (*make_traceless=False, inplace=False*)

symmetrize the tensor field in place

Parameters

- **make_traceless** (*bool*) – Determines whether the result is also traceless
- **inplace** (*bool*) – Flag determining whether to symmetrize the current field or return a new one

Returns

result of the operation

Return type

Tensor2Field

to_scalar (*scalar='auto', *, label='scalar {scalar}'*)

return scalar variant of the field

The invariants of the tensor field \mathbf{A} are

$$\begin{aligned}I_1 &= \text{tr}(\mathbf{A}) \\I_2 &= \frac{1}{2} \left[(\text{tr}(\mathbf{A}))^2 - \text{tr}(\mathbf{A}^2) \right] \\I_3 &= \det(\mathbf{A})\end{aligned}$$

where *tr* denotes the trace and *det* denotes the determinant. Note that the three invariants can only be distinct and non-zero in three dimensions. In two dimensional spaces, we have the identity $2I_2 = I_3$ and in one-dimensional spaces, we have $I_1 = I_3$ as well as $I_2 = 0$.

Parameters

- **scalar** (*str*) – The method to calculate the scalar. Possible choices include *norm* (the default chosen when the value is *auto*), *min*, *max*, *squared_sum*, *norm_squared*, *trace* (or *invariant1*), *invariant2*, and *determinant* (or *invariant3*)
- **label** (*str, optional*) – Name of the returned field

Returns

the scalar field after applying the operation

Return type

ScalarField

trace (*label='trace'*)

return the trace of the tensor field as a scalar field

Parameters

label (*str*, *optional*) – Name of the returned field

Returns

scalar field of traces

Return type

ScalarField

transpose (*label='transpose'*)

return the transpose of the tensor field

Parameters

label (*str*, *optional*) – Name of the returned field

Returns

transpose of the tensor field

Return type

Tensor2Field

4.1.5 pde.fields.vectorial module

Defines a vectorial field over a grid

class VectorField (*grid*, *data='zeros'*, *, *label=None*, *dtype=None*, *with_ghost_cells=False*)

Bases: *DataFieldBase*

Vector field discretized on a grid

Warning: Components of the vector field are given in the local basis. While the local basis is identical to the global basis in Cartesian coordinates, the local basis depends on position in curvilinear coordinate systems. Moreover, the field always contains all components, even if the underlying grid assumes symmetries.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined.
- **data** (Number or *ndarray*, *optional*) – Field values at the support points of the grid. The flag *with_ghost_cells* determines whether this data array contains values for the ghost cells, too. The resulting field will contain real data unless the *data* argument contains complex values. Special values are “zeros” or *None*, initializing the field with zeros, and “empty”, just allocating memory with unspecified values.
- **label** (*str*, *optional*) – Name of the field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.
- **with_ghost_cells** (*bool*) – Indicates whether the ghost cells are included in data

divergence (*bc*, *out=None*, ***kwargs*)

apply divergence operator and return result as a field

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (*ScalarField*, *optional*) – Optional scalar field to which the result is written.
- **label** (*str*, *optional*) – Name of the returned field
- ****kwargs** – Additional arguments affecting how the operator behaves.

Returns

Divergence of the field

Return type

ScalarField

dot (*other*, *out=None*, ***, *conjugate=True*, *label='dot product'*)

calculate the dot product involving a vector field

This supports the dot product between two vectors fields as well as the product between a vector and a tensor. The resulting fields will be a scalar or vector, respectively.

Parameters

- **other** (*VectorField* or *Tensor2Field*) – the second field
- **out** (*ScalarField* or *VectorField*, *optional*) – Optional field to which the result is written.
- **conjugate** (*bool*) – Whether to use the complex conjugate for the second operand
- **label** (*str*, *optional*) – Name of the returned field

Returns

ScalarField or *VectorField*: result of applying the operator

Return type

ScalarField | *VectorField*

classmethod from_expression (*grid*, *expressions*, ***, *user_funcs=None*, *consts=None*, *label=None*, *dtype=None*)

create a vector field on a grid from given expressions

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – Grid defining the space on which this field is defined
- **expressions** (*list of str*) – A list of mathematical expression, one for each component of the vector field. The expressions determine the values as a function of the position

on the grid. The expressions may contain standard mathematical functions and they may depend on the axes labels of the grid. More information can be found in the [expression documentation](#).

- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that can be used in the expression
- **consts** (*dict*, *optional*) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or `ndarray`.
- **label** (*str*, *optional*) – Name of the field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.

Return type

`VectorField`

classmethod from_scalars (*fields*, *, *label=None*, *dtype=None*)

create a vector field from a list of `ScalarFields`

Note that the data of the scalar fields is copied in the process

Parameters

- **fields** (*list*) – The list of (compatible) scalar fields
- **label** (*str*, *optional*) – Name of the returned field
- **dtype** (*numpy dtype*) – The data type of the field. If omitted, it will be determined from *data* automatically.

Returns

the resulting vector field

Return type

`VectorField`

get_vector_data (*transpose=False*, *max_points=None*, ***kwargs*)

return data for a vector plot of the field

Parameters

- **transpose** (*bool*) – Determines whether the transpose of the data should be plotted.
- **max_points** (*int*) – The maximal number of points that is used along each axis. This option can be used to sub-sample the data.
- ****kwargs** – Additional parameters forwarded to `grid.get_image_data`

Returns

Information useful for plotting an vector field

Return type

`dict`

gradient (*bc*, *out=None*, ***kwargs*)

apply vector gradient operator and return result as a field

The vector gradient field is a tensor field $t_{\alpha\beta}$ that specifies the derivatives of the vector field v_α with respect to all coordinates x_β .

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions need to determine all components of the vector field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (*VectorField*, *optional*) – Optional vector field to which the result is written.
- **label** (*str*, *optional*) – Name of the returned field
- ****kwargs** – Additional arguments affecting how the operator behaves.

Returns

Gradient of the field

Return type

Tensor2Field

property integral: *ndarray*

integral of each component over space

Type

ndarray

interpolate_to_grid (*grid*, *, *bc=None*, *fill=None*, *label=None*)

interpolate the data of this vector field to another grid.

Parameters

- **grid** (*GridBase*) – The grid of the new field onto which the current field is interpolated.
- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field, which affects values close to the boundary. If omitted, the argument *fill* is used to determine values outside the domain. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **fill** (*Number*, *optional*) – Determines how values out of bounds are handled. If *None*, a *ValueError* is raised when out-of-bounds points are requested. Otherwise, the given value is returned.
- **label** (*str*, *optional*) – Name of the returned field
- **self** (*VectorField*) –

Returns

Field of the same rank as the current one.

Return type*VectorField***laplace** (*bc*, *out=None*, ***kwargs*)

apply vector Laplace operator and return result as a field

The vector Laplacian is a vector field L_α containing the second derivatives of the vector field v_α with respect to the coordinates x_β :

$$L_\alpha = \sum_\beta \frac{\partial^2 v_\alpha}{\partial x_\beta \partial x_\beta}$$

Parameters

- **bc** (*BoundariesData* | *None*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#). If the special value *None* is given, no boundary conditions are enforced. The user then needs to ensure that the ghost cells are set accordingly.
- **out** (*VectorField*, *optional*) – Optional vector field to which the result is written.
- **label** (*str*, *optional*) – Name of the returned field
- ****kwargs** – Additional arguments affecting how the operator behaves.

Returns

Laplacian of the field

Return type*VectorField***make_outer_prod_operator** (*backend='numba'*)

return operator calculating the outer product of two vector fields

Warning: This function does not check types or dimensions.

Parameters

backend (*str*) – The backend (e.g., ‘numba’ or ‘scipy’) used for this operator.

Returns

function that takes two instance of *ndarray*, which contain the discretized data of the two operands. An optional third argument can specify the output array to which the result is written. Note that the returned function is jitted with numba for speed.

Return type*Callable*[*[ndarray, ndarray, ndarray* | *None]*, *ndarray*]**outer_product** (*other*, *out=None*, ***, *label=None*)

calculate the outer product of this vector field with another

Parameters

- **other** (*VectorField*) – The second vector field
- **out** (*Tensor2Field*, optional) – Optional tensorial field to which the result is written.
- **label** (*str*, optional) – Name of the returned field

Returns

result of the operation

Return type

Tensor2Field

rank: `int` = 1

to_scalar (*scalar*='auto', *, *label*='scalar {scalar}')

return scalar variant of the field

Parameters

- **scalar** (*str*) – Choose the method to use. Possible choices are *norm*, *max*, *min*, *squared_sum*, *norm_squared*, or an integer specifying which component is returned (indexing starts at 0). The default value *auto* picks the method automatically: The first (and only) component is returned for real fields on one-dimensional spaces, while the norm of the vector is returned otherwise.
- **label** (*str*, optional) – Name of the returned field

Returns

The scalar field after applying the operation

Return type

pde.fields.scalar.ScalarField

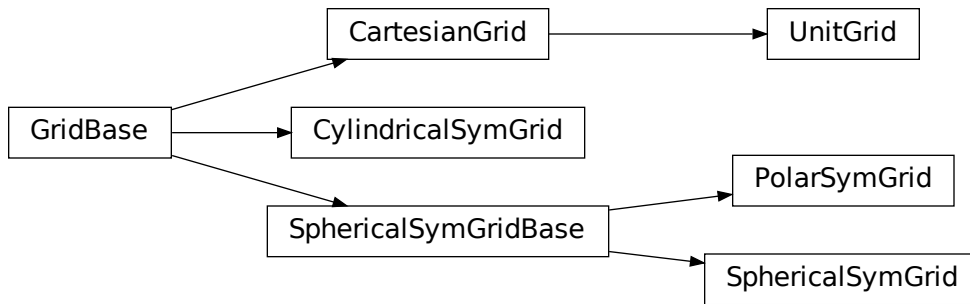
4.2 pde.grids package

Grids define the domains on which PDEs will be solved. In particular, symmetries, periodicities, and the discretizations are defined by the underlying grid.

We only consider regular, orthogonal grids, which are constructed from orthogonal coordinate systems with equidistant discretizations along each axis. The dimension of the space that the grid describes is given by the attribute `dim`. Cartesian coordinates can be mapped to grid coordinates and the corresponding discretization cells using the method `transform()`.

<i>UnitGrid</i>	d-dimensional Cartesian grid with unit discretization in all directions
<i>CartesianGrid</i>	d-dimensional Cartesian grid with uniform discretization for each axis
<i>PolarSymGrid</i>	2-dimensional polar grid assuming angular symmetry
<i>SphericalSymGrid</i>	3-dimensional spherical grid assuming spherical symmetry
<i>CylindricalSymGrid</i>	3-dimensional cylindrical grid assuming polar symmetry

Inheritance structure of the classes:



Subpackages:

4.2.1 `pde.grids.boundaries` package

This package contains classes for handling the boundary conditions of fields.

Boundary conditions

The mathematical details of boundary conditions for partial differential equations are treated in more detail in the `documentation` document. Since the `pde` package only supports orthogonal grids, boundary conditions need to be applied at the end of each axis. Consequently, methods expecting boundary conditions typically receive a list of conditions for each axes:

```
field = ScalarField(UnitGrid([16, 16], periodic=[True, False]))
field.laplace(bc=[bc_x, bc_y])
```

If an axis is periodic (like the first one in the example above), the only valid boundary conditions are ‘periodic’ and its cousin ‘anti-periodic’, which imposes opposite signs on both sides. For non-periodic axes (e.g., the second axis), different boundary conditions can be specified for the lower and upper end of the axis, which is done using a tuple of two conditions. Typical choices for individual conditions are Dirichlet conditions that enforce a value `NUM` (specified by `{‘value’: NUM}`) and Neumann conditions that enforce the value `DERIV` for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`). The specific choices for the example above could be

```
bc_x = "periodic"
bc_y = ({"value": 2}, {"derivative": -1})
```

which enforces a value of 2 at the lower side of the y-axis and a derivative (in outward normal direction) of -1 on the upper side. Instead of plain numbers, which enforce the same condition along the whole boundary, expressions can be used to support inhomogeneous boundary conditions. These mathematical expressions are given as a string that can be parsed by `sympy`. They can depend on all coordinates of the grid. An alternative boundary condition to the example above could thus read

```
bc_y = ({"value": "y**2"}, {"derivative": "-sin(x)"})
```

Warning: To interpret arbitrary expressions, the package uses `exec()`. It should therefore not be used in a context where malicious input could occur.

Inhomogeneous values can also be specified by directly supplying an array, whose shape needs to be compatible with the boundary, i.e., it needs to have the same shape as the grid but with the dimension of the axis along which the boundary is specified removed.

The package also supports mixed boundary conditions (depending on both the value and the derivative of the field) and imposing a second derivative. An example is

```
bc_y = ({ "type": "mixed", "value": 2, "const": 7 },
        { "curvature": 2 })
```

which enforces the condition $\partial_n c + 2c = 7$ and $\partial_n^2 c = 2$ onto the field c on the lower and upper side of the axis, respectively.

Beside the full specification of the boundary conditions, various short-hand notations are supported. If both sides of an axis have the same boundary condition, only one needs to be specified (instead of the tuple). For instance, `bc_y = { 'value': 2 }` imposes a value of 2 on both sides of the y-axis. Similarly, if all axes have the same boundary conditions, only one axis needs to be specified (instead of the list). For instance, the following example

```
field = ScalarField(UnitGrid([16, 16], periodic=False))
field.laplace(bc={ "value": 2 })
```

imposes a value of 2 on all sides of the grid. Finally, the special values ‘auto_periodic_neumann’ and ‘auto_periodic_dirichlet’ impose periodic boundary conditions for periodic axis and a vanishing derivative or value otherwise. For example,

```
field = ScalarField(UnitGrid([16, 16], periodic=[True, False]))
field.laplace(bc="auto_periodic_neumann")
```

enforces periodic boundary conditions on the first axis, while the second one has standard Neumann conditions.

Note: Derivatives are given relative to the outward normal vector, such that positive derivatives correspond to a function that increases across the boundary.

Boundaries overview

The `boundaries` package defines the following classes:

Local boundary conditions:

- `DirichletBC`: Imposing a constant value of the field at the boundary
- `ExpressionValueBC`: Imposing the value of the field at the boundary given by an expression or a python function
- `NeumannBC`: Imposing a constant derivative of the field in the outward normal direction at the boundary
- `ExpressionDerivativeBC`: Imposing the derivative of the field in the outward normal direction at the boundary given by an expression or a python function
- `MixedBC`: Imposing the derivative of the field in the outward normal direction proportional to its value at the boundary

- *ExpressionMixedBC*: Imposing the derivative of the field in the outward normal direction proportional to its value at the boundary with coefficients given by expressions or python functions
- *CurvatureBC*: Imposing a constant second derivative (curvature) of the field at the boundary

There are corresponding classes that only affect the normal component of a field, which can be useful when dealing with vector and tensor fields: *NormalDirichletBC*, *NormalNeumannBC*, *NormalMixedBC*, and *NormalCurvatureBC*.

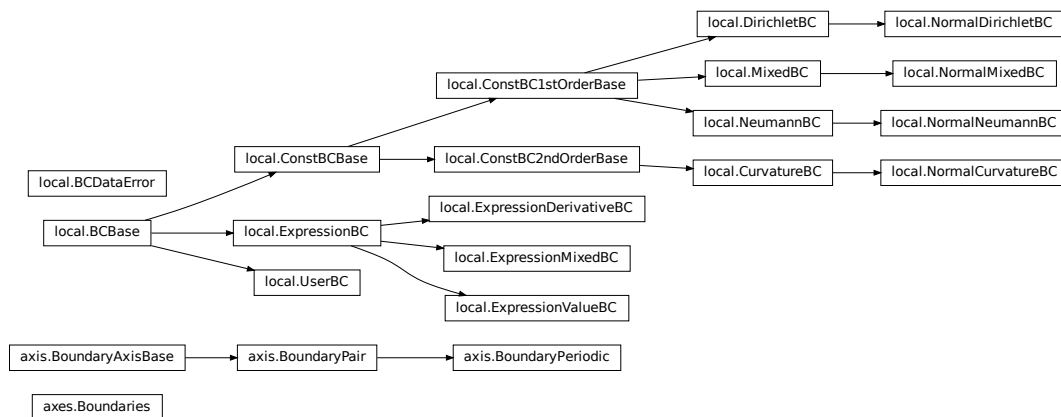
Boundaries for an axis:

- *BoundaryPair*: Uses the local boundary conditions to specify the two boundaries along an axis
- *BoundaryPeriodic*: Indicates that an axis has periodic boundary conditions

Boundaries for all axes of a grid:

- *Boundaries*: Collection of boundaries to describe conditions for all axes

Inheritance structure of the classes:



The details of the classes are explained below:

pde.grids.boundaries.axes module

This module handles the boundaries of all axes of a grid. It only defines *Boundaries*, which acts as a list of *BoundaryAxisBase*.

class Boundaries (*boundaries*)

Bases: `list`

class that bundles all boundary conditions for all axes

initialize with a list of boundaries

property boundaries: `Iterator[BCBase]`

iterator over all non-periodic boundaries

check_value_rank (*rank*)

check whether the values at the boundaries have the correct rank

Parameters

rank (*int*) – The tensorial rank of the field for this boundary condition

Return type

None

Throws:

RuntimeError: if any value does not have rank *rank*

copy ()

create a copy of the current boundaries

Return type

[Boundaries](#)

classmethod from_data (*grid, boundaries, rank=0*)

Creates all boundaries from given data

Parameters

- **grid** ([GridBase](#)) – The grid with which the boundary condition is associated
- **boundaries** (*str or list or tuple or dict*) – Data that describes the boundaries. This can either be a list of specifications for each dimension or a single one, which is then applied to all dimensions. The boundary for a dimensions can be specified by one of the following formats:
 - string specifying a single type for all boundaries
 - dictionary specifying the type and values for all boundaries
 - tuple pair specifying the low and high boundary individually
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

Return type

[Boundaries](#)

classmethod get_help ()

Return information on how boundary conditions can be set

Return type

[str](#)

get_mathematical_representation (*field_name='C'*)

return mathematical representation of the boundary condition

Parameters

field_name (*str*) –

Return type

[str](#)

grid: [GridBase](#)

grid for which boundaries are defined

Type

[GridBase](#)

make_ghost_cell_setter()

return function that sets the ghost cells on a full array

Return type

[GhostCellSetter](#)

property periodic: [list\[bool\]](#)

a boolean array indicating which dimensions are periodic according to the boundary conditions

Type

[ndarray](#)

set_ghost_cells(*data_full*, *, *set_corners=False*, *args=None*)

set the ghost cells for all boundaries

Parameters

- **data_full** ([ndarray](#)) – The full field data including ghost points
- **set_corners** ([bool](#)) – Determines whether the corner cells are set using interpolation
- **args** – Additional arguments that might be supported by special boundary conditions.

Return type

None

pde.grids.boundaries.axis module

This module handles the boundaries of a single axis of a grid. There are generally only two options, depending on whether the axis of the underlying grid is defined as periodic or not. If it is periodic, the class [BoundaryPeriodic](#) should be used, while non-periodic axes have more option, which are represented by [BoundaryPair](#).

class BoundaryAxisBase(*low*, *high*)

Bases: [object](#)

base class for defining boundaries of a single axis in a grid

Parameters

- **low** ([BCBase](#)) – Instance describing the lower boundary
- **high** ([BCBase](#)) – Instance describing the upper boundary

property axis: [int](#)

The axis along which the boundaries are defined

Type

[int](#)

copy()

return a copy of itself, but with a reference to the same grid

Return type

[BoundaryAxisBase](#)

classmethod get_help()

Return information on how boundary conditions can be set

Return type

[str](#)

get_mathematical_representation (*field_name*='C')

return mathematical representation of the boundary condition

Parameters

field_name (*str*) –

Return type

`tuple[str, str]`

get_sparse_matrix_data (*idx*)

sets the elements of the sparse representation of this condition

Parameters

idx (*tuple*) – The index of the point that must lie on the boundary condition

Returns

A constant value and a dictionary with indices and factors that can be used to calculate this virtual point

Return type

`float, dict`

property grid: `GridBase`

Underlying grid

Type

`GridBase`

high: `BCBase`

Boundary condition at upper end

Type

`BCBase`

low: `BCBase`

Boundary condition at lower end

Type

`BCBase`

make_ghost_cell_setter ()

return function that sets the ghost cells for this axis on a full array

Return type

`GhostCellSetter`

property periodic: `bool`

whether the axis is periodic

Type

`bool`

property rank: `int`

rank of the associated boundary condition

Type

`int`

set_ghost_cells (*data_full*, *, *args=None*)

set the ghost cell values for all boundaries

Parameters

- **data_full** (*ndarray*) – The full field data including ghost points
- **args** – Additional arguments that might be supported by special boundary conditions.

Return type

None

class **BoundaryPair** (*low, high*)Bases: *BoundaryAxisBase*

represents the two boundaries of an axis along a single dimension

Parameters

- **low** (*BCBase*) – Instance describing the lower boundary
- **high** (*BCBase*) – Instance describing the upper boundary

check_value_rank (*rank*)

check whether the values at the boundaries have the correct rank

Parameters

- **rank** (*int*) – The tensorial rank of the field for this boundary condition

Return type

None

Throws:RuntimeError: if the value does not have rank *rank***classmethod** **from_data** (*grid, axis, data, rank=0*)

create boundary pair from some data

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **data** (*str or dict*) – Data that describes the boundary pair
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

Returns

the instance created from the data

Return type*BoundaryPair***Throws:**ValueError if *data* cannot be interpreted as a boundary pair**class** **BoundaryPeriodic** (*grid, axis, flip_sign=False*)Bases: *BoundaryPair*

represent a periodic axis

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **flip_sign** (*bool*) – Impose different signs on the two sides of the boundary

check_value_rank (*rank*)

check whether the values at the boundaries have the correct rank

Parameters

rank (*int*) – The tensorial rank of the field for this boundary condition

Return type

None

copy ()

return a copy of itself, but with a reference to the same grid

Return type

BoundaryPeriodic

property flip_sign

Whether different signs are imposed on the two sides of the boundary

Type

bool

get_boundary_axis (*grid, axis, data, rank=0*)

return object representing the boundary condition for a single axis

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **data** (*str or tuple or dict*) – Data describing the boundary conditions for this axis
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

Returns

Appropriate boundary condition for the axis

Return type

BoundaryAxisBase

pde.grids.boundaries.local module

This module contains classes for handling a single boundary of a non-periodic axis. Since an axis has two boundary, we simply distinguish them by a boolean flag *upper*, which is *True* for the side of the axis with the larger coordinate.

The module currently supports the following standard boundary conditions:

- *DirichletBC*: Imposing the value of a field at the boundary
- *NeumannBC*: Imposing the derivative of a field in the outward normal direction at the boundary
- *MixedBC*: Imposing the derivative of a field in the outward normal direction proportional to its value at the boundary
- *CurvatureBC*: Imposing the second derivative (curvature) of a field at the boundary

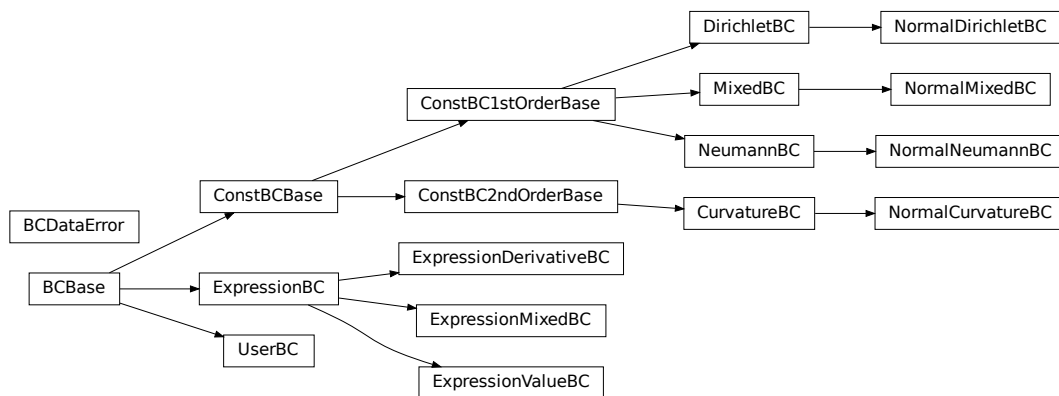
There are also variants of these boundary conditions that only affect the normal components of a vector or tensor field: *NormalDirichletBC*, *NormalNeumannBC*, *NormalMixedBC*, and *NormalCurvatureBC*.

Finally, there are more specialized classes, which offer greater flexibility, but might also require a slightly deeper understanding for proper use:

- *ExpressionValueBC*: Imposing the value of a field at the boundary based on a mathematical expression or a python function.
- *ExpressionDerivativeBC*: Imposing the derivative of a field in the outward normal direction at the boundary based on a mathematical expression or a python function.
- *ExpressionMixedBC*: Imposing a mixed (Robin) boundary condition using mathematical expressions or python functions.
- *UserBC*: Allows full control for setting virtual points, values, or derivatives. The boundary conditions are never enforced automatically. It is thus the user's responsibility to ensure virtual points are set correctly before operators are applied. To set boundary conditions a dictionary `{TARGET: value}` must be supplied as argument *args* to `set_ghost_cells()` or the numba equivalent. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Note that derivatives are generally given in the direction of the outward normal vector, such that positive derivatives correspond to a function that increases across the boundary.

Inheritance structure of the classes:



```
class BCBBase (grid, axis, upper, *, rank=0)
```

Bases: `object`

represents a single boundary in an `BoundaryPair` instance

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

```
property axis_coord: float
```

value of the coordinate that defines this boundary condition

Type

float

check_value_rank (*rank*)

check whether the values at the boundaries have the correct rank

Parameters**rank** (*int*) – The tensorial rank of the field for this boundary condition**Return type**

None

Throws:RuntimeError: if the value does not have rank *rank***copy** (*upper=None, rank=None*)**Parameters**

- **self** (*TBC*) –
- **upper** (*bool* | *None*) –
- **rank** (*int* | *None*) –

Return type*TBC***classmethod from_data** (*grid, axis, upper, data, *, rank=0*)

create boundary from some data

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Indicates whether this boundary condition is associated with the upper or lower side of the axis.
- **data** (*str* or *dict*) – Data that describes the boundary
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

Returns

the instance created from the data

Return type*BCBase***Throws:**ValueError if *data* cannot be interpreted as a boundary condition**classmethod from_dict** (*grid, axis, upper, data, *, rank=0*)

create boundary from data given in dictionary

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Indicates whether this boundary condition is associated with the upper or lower side of the axis.

- **data** (*dict*) – The dictionary defining the boundary condition
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

Return type

BCBase

classmethod from_str (*grid, axis, upper, condition, *, rank=0, **kwargs*)

creates boundary from a given string identifier

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Indicates whether this boundary condition is associated with the upper or lower side of the axis.
- **condition** (*str*) – Identifies the boundary condition
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- ****kwargs** – Additional arguments passed to the constructor

Return type

BCBase

classmethod get_help ()

Return information on how boundary conditions can be set

Return type

str

get_mathematical_representation (*field_name='C'*)

return mathematical representation of the boundary condition

Parameters**field_name** (*str*) –**Return type**

str

get_sparse_matrix_data (*idx*)**Parameters****idx** (*tuple[int, ...]*) –**Return type**

tuple[float, dict[int, float]]

get_virtual_point (*arr, idx=None*)**Parameters****idx** (*tuple[int, ...] | None*) –**Return type**

float

homogeneous: *bool*

determines whether the boundary condition depends on space

Type*bool*

make_adjacent_evaluator()

returns a function evaluating the value adjacent to a given point

Deprecated since version Since: 2023-12-19

Returns

A function with signature `(arr_1d, i_point, bc_idx)`, where *arr_1d* is the one-dimensional data array (the data points along the axis perpendicular to the boundary), *i_point* is the index into this array for the current point and *bc_idx* are the remaining indices of the current point, which indicate the location on the boundary plane. The result of the function is the data value at the adjacent point along the axis associated with this boundary condition in the upper (lower) direction when *upper* is True (False).

Return type

function

make_ghost_cell_sender()

return function that might `mpi_send` data to set ghost cells for this boundary

Return type

`GhostCellSetter`

make_ghost_cell_setter()

return function that sets the ghost cells for this boundary

Return type

`GhostCellSetter`

abstract make_virtual_point_evaluator()

returns a function evaluating the value at the virtual support point

Returns

A function that takes the data array and an index marking the current point, which is assumed to be a virtual point. The result is the data value at this point, which is calculated using the boundary condition.

Return type

function

names: list[str]

identifiers used to specify the given boundary class

Type

list

normal: bool = False

determines whether the boundary condition only affects normal components.

If this flag is *False*, boundary conditions must specify values for all components of the field. If *True*, only the normal components at the boundary are specified.

Type

bool

property periodic: bool

whether the boundary condition is periodic

Type

bool

abstract set_ghost_cells (*data_full*, *, *args=None*)

set the ghost cell values for this boundary

Parameters

- **data_full** (*ndarray*) – The full field data including ghost points
- **args** (*ndarray*) – Determines what boundary conditions are set. *args* should be set to {*TARGET*: *value*}. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Return type

None

to_subgrid (*subgrid*)

converts this boundary condition to one valid for a given subgrid

Parameters

- **subgrid** (*GridBase*) – Grid of the new boundary conditions
- **self** (*TBC*) –

Returns

Boundary conditions valid on the subgrid

Return type

BCBase

exception BCDataError

Bases: *ValueError*

exception that signals that incompatible data was supplied for the BC

class ConstBC1stOrderBase (*grid*, *axis*, *upper*, *, *rank=0*, *value=0*)

Bases: *ConstBCBase*

represents a single boundary in an *BoundaryPair* instance

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If *value* is a single value

(or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

get_sparse_matrix_data (*idx*)

sets the elements of the sparse representation of this condition

Parameters

idx (*tuple*) – The index of the point that must lie on the boundary condition

Returns

A constant value and a dictionary with indices and factors that can be used to calculate this virtual point

Return type

float, dict

get_virtual_point (*arr, idx=None*)

calculate the value of the virtual point outside the boundary

Parameters

- **arr** (*array*) – The data values associated with the grid
- **idx** (*tuple*) – The index of the point to evaluate. This is a tuple of length *grid.num_axes* with the either -1 or *dim* as the entry for the axis associated with this boundary condition. Here, *dim* is the dimension of the axis. The index is optional if *dim == 1*.

Returns

Value at the virtual support point

Return type

float

abstract get_virtual_point_data (*compiled=False*)

return data suitable for calculating virtual points

Parameters

compiled (*bool*) – Flag indicating whether a compiled version is required, which automatically takes updated values into account when it is used in numba-compiled code.

Returns

the data structure associated with this virtual point

Return type

tuple

make_adjacent_evaluator ()

returns a function evaluating the value adjacent to a given point

Deprecated since version Since: 2023-12-19

Returns

A function with signature (*arr_1d, i_point, bc_idx*), where *arr_1d* is the one-dimensional data array (the data points along the axis perpendicular to the boundary), *i_point* is the index into this array for the current point and *bc_idx* are the remaining indices of the current point, which indicate the location on the boundary plane. The result of the function is the data value at the adjacent point along the axis associated with this boundary condition in the upper (lower) direction when *upper* is True (False).

Return type

function

make_virtual_point_evaluator()

returns a function evaluating the value at the virtual support point

Returns

A function that takes the data array and an index marking the current point, which is assumed to be a virtual point. The result is the data value at this point, which is calculated using the boundary condition.

Return type

function

set_ghost_cells(*data_full*, *, *args=None*)

set the ghost cell values for this boundary

Parameters

- **data_full** (*ndarray*) – The full field data including ghost points
- **args** (*ndarray*) – Determines what boundary conditions are set. *args* should be set to {*TARGET*: *value*}. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Return type

None

class ConstBC2ndOrderBase(*grid*, *axis*, *upper*, *, *rank=0*, *value=0*)

Bases: *ConstBCBase*

abstract base class for boundary conditions of 2nd order

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If *value* is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

get_sparse_matrix_data(*idx*)

sets the elements of the sparse representation of this condition

Parameters

idx (*tuple*) – The index of the point that must lie on the boundary condition

Returns

A constant value and a dictionary with indices and factors that can be used to calculate this virtual point

Return type

float, dict

get_virtual_point (*arr, idx=None*)

calculate the value of the virtual point outside the boundary

Parameters

- **arr** (*array*) – The data values associated with the grid
- **idx** (*tuple*) – The index of the point to evaluate. This is a tuple of length *grid.num_axes* with the either -1 or *dim* as the entry for the axis associated with this boundary condition. Here, *dim* is the dimension of the axis. The index is optional if *dim == 1*.

Returns

Value at the virtual support point

Return type

float

abstract get_virtual_point_data ()

return data suitable for calculating virtual points

Returns

the data structure associated with this virtual point

Return type

tuple

make_adjacent_evaluator ()

returns a function evaluating the value adjacent to a given point

Deprecated since version Since: 2023-12-19

Returns

A function with signature (*arr_1d, i_point, bc_idx*), where *arr_1d* is the one-dimensional data array (the data points along the axis perpendicular to the boundary), *i_point* is the index into this array for the current point and *bc_idx* are the remaining indices of the current point, which indicate the location on the boundary plane. The result of the function is the data value at the adjacent point along the axis associated with this boundary condition in the upper (lower) direction when *upper* is True (False).

Return type

function

make_virtual_point_evaluator ()

returns a function evaluating the value at the virtual support point

Returns

A function that takes the data array and an index marking the current point, which is assumed to be a virtual point. The result is the data value at this point, which is calculated using the boundary condition.

Return type

function

set_ghost_cells (*data_full*, *, *args=None*)

set the ghost cell values for this boundary

Parameters

- **data_full** (*ndarray*) – The full field data including ghost points
- **args** (*ndarray*) – Determines what boundary conditions are set. *args* should be set to {*TARGET*: *value*}. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Return type

None

class ConstBCBase (*grid*, *axis*, *upper*, *, *rank=0*, *value=0*)

Bases: *BCBase*

base class representing a boundary whose virtual point is set from constants

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (*float* or *str* or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If *value* is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

copy (*upper=None*, *rank=None*, *value=None*)

return a copy of itself, but with a reference to the same grid

Parameters

- **self** (*ConstBCBase*) –
- **upper** (*bool* | *None*) –
- **rank** (*int* | *None*) –
- **value** (*float* | *ndarray* | *str* | *None*) –

Return type

ConstBCBase

link_value (*value*)

link value of this boundary condition to external array

Parameters

value (*ndarray*) –

to_subgrid (*subgrid*)

converts this boundary condition to one valid for a given subgrid

Parameters

- **subgrid** (*GridBase*) – Grid of the new boundary conditions
- **self** (*ConstBCBase*) –

Returns

Boundary conditions valid on the subgrid

Return type

ConstBCBase

property value: *ndarray*

value_is_linked: *bool*

flag that indicates whether the value associated with this boundary condition is linked to *ndarray* managed by external code.

Type

bool

class CurvatureBC (*grid, axis, upper, *, rank=0, value=0*)

Bases: *ConstBC2ndOrderBase*

represents a boundary condition imposing the 2nd normal derivative at the boundary

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If value is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

get_mathematical_representation (*field_name*='C')
 return mathematical representation of the boundary condition

Parameters

field_name (*str*) –

Return type

str

get_virtual_point_data ()
 return data suitable for calculating virtual points

Returns

the data structure associated with this virtual point

Return type

tuple

names: *list*[*str*] = ['curvature', 'second_derivative', 'extrapolate']
 identifiers used to specify the given boundary class

Type

list

class DirichletBC (*grid*, *axis*, *upper*, *, *rank*=0, *value*=0)

Bases: *ConstBC1stOrderBase*

represents a boundary condition imposing the value

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If value is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

get_mathematical_representation (*field_name*='C')
 return mathematical representation of the boundary condition

Parameters

field_name (*str*) –

Return type`str`**get_virtual_point_data** (*compiled=False*)

return data suitable for calculating virtual points

Parameters**compiled** (*bool*) – Flag indicating whether a compiled version is required, which automatically takes updated values into account when it is used in numba-compiled code.**Returns**

the data structure associated with this virtual point

Return type`tuple`**names:** `list[str]` = ['value', 'dirichlet']

identifiers used to specify the given boundary class

Type`list`**class ExpressionBC** (*grid, axis, upper, *, rank=0, value=0, const=0, target='virtual_point', user_funcs=None, value_cell=None*)Bases: *BCBase*

represents a boundary whose virtual point is calculated from an expression

The expression is given as a string and will be parsed by `sympy` or a function that is optionally compiled with `numba`. The expression can contain typical mathematical operators and may depend on the value at the last support point next to the boundary (*value*), spatial coordinates defined by the grid marking the boundary point (e.g., *x* or *r*), and time *t*.

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.**Parameters**

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **value** (*float or str or callable*) – An expression that determines the value of the boundary condition. Alternatively, this can be a function with signature (*value, dx, *coords, t*) that determines the value of *target* from the field value *value* (the value of the adjacent cell unless *value_cell* is specified), the spatial discretization *dx* in the direction perpendicular to the wall, the spatial coordinates of the wall point, and time *t*. Ideally, this function should be numba-compilable since simulations might otherwise be very slow.
- **const** (*float or str or callable*) – An expression similar to *value*, which is only used for mixed (Robin) boundary conditions. Note that the implementation currently does not support that one argument is given as a callable function while the other is defined via an expression, so both need to have the same type.

- **target** (*str*) – Selects which value is actually set. Possible choices include *value*, *derivative*, *mixed*, and *virtual_point*.
- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that can be used in expressions
- **value_cell** (*int*) – Determines which cells is read to determine the field value that is used as *value* in the expression or the function call. The default (*None*) specifies the adjacent cell.

copy (*upper=None*, *rank=None*)

return a copy of itself, but with a reference to the same grid

Parameters

- **self** (*ExpressionBC*) –
- **upper** (*bool* | *None*) –
- **rank** (*int* | *None*) –

Return type

ExpressionBC

get_mathematical_representation (*field_name='C'*)

return mathematical representation of the boundary condition

Parameters

field_name (*str*) –

Return type

str

get_sparse_matrix_data (*idx*)

Parameters

idx (*tuple[int, ...]*) –

Return type

tuple[float, dict[int, float]]

get_virtual_point (*arr*, *idx=None*)

Parameters

idx (*tuple[int, ...]* | *None*) –

Return type

float

make_adjacent_evaluator ()

returns a function evaluating the value adjacent to a given point

Deprecated since version Since: 2023-12-19

Returns

A function with signature (*arr_1d*, *i_point*, *bc_idx*), where *arr_1d* is the one-dimensional data array (the data points along the axis perpendicular to the boundary), *i_point* is the index into this array for the current point and *bc_idx* are the remaining indices of the current point, which indicate the location on the boundary plane. The result of the function is the data value at the adjacent point along the axis associated with this boundary condition in the upper (lower) direction when *upper* is True (False).

Return type

function

make_virtual_point_evaluator()

returns a function evaluating the value at the virtual support point

Returns

A function that takes the data array and an index marking the current point, which is assumed to be a virtual point. The result is the data value at this point, which is calculated using the boundary condition.

Return type

function

names: `list[str] = ['virtual_point']`

identifiers used to specify the given boundary class

Type

`list`

set_ghost_cells(*data_full*, *, *args=None*)

set the ghost cell values for this boundary

Parameters

- **data_full** (`ndarray`) – The full field data including ghost points
- **args** (`ndarray`) – Determines what boundary conditions are set. *args* should be set to `{TARGET: value}`. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Return type

`None`

to_subgrid(*subgrid*)

converts this boundary condition to one valid for a given subgrid

Parameters

- **subgrid** (`GridBase`) – Grid of the new boundary conditions
- **self** (`ExpressionBC`) –

Returns

Boundary conditions valid on the subgrid

Return type

`BCBase`

class ExpressionDerivativeBC(*grid*, *axis*, *upper*, *, *rank=0*, *value=0*, *target='derivative'*,
user_funcs=None, *value_cell=None*)

Bases: `ExpressionBC`

represents a boundary whose outward derivative is calculated from an expression

The expression is given as a string and will be parsed by `sympy`. The expression can contain typical mathematical operators and may depend on the value at the last support point next to the boundary (*value*), spatial coordinates defined by the grid marking the boundary point (e.g., *x* or *r*), and time *t*.

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **value** (*float or str or callable*) – An expression that determines the value of the boundary condition. Alternatively, this can be a function with signature (*value, dx, *coords, t*) that determines the value of *target* from the field value *value* (the value of the adjacent cell unless *value_cell* is specified), the spatial discretization *dx* in the direction perpendicular to the wall, the spatial coordinates of the wall point, and time *t*. Ideally, this function should be numba-compilable since simulations might otherwise be very slow.
- **const** (*float or str or callable*) – An expression similar to *value*, which is only used for mixed (Robin) boundary conditions. Note that the implementation currently does not support that one argument is given as a callable function while the other is defined via an expression, so both need to have the same type.
- **target** (*str*) – Selects which value is actually set. Possible choices include *value*, *derivative*, *mixed*, and *virtual_point*.
- **user_funcs** (*dict, optional*) – A dictionary with user defined functions that can be used in expressions
- **value_cell** (*int*) – Determines which cells is read to determine the field value that is used as *value* in the expression or the function call. The default (*None*) specifies the adjacent cell.

names: `list[str] = ['derivative_expression', 'derivative_expr']`

identifiers used to specify the given boundary class

Type

`list`

class ExpressionMixedBC (*grid, axis, upper, *, rank=0, value=0, const=0, target='mixed', user_funcs=None, value_cell=None*)

Bases: *ExpressionBC*

represents a boundary whose outward derivative is calculated from an expression

The expression is given as a string and will be parsed by `sympy`. The expression can contain typical mathematical operators and may depend on the value at the last support point next to the boundary (*value*), spatial coordinates defined by the grid marking the boundary point (e.g., *x* or *r*), and time *t*.

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated

- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **value** (*float or str or callable*) – An expression that determines the value of the boundary condition. Alternatively, this can be a function with signature (*value, dx, *coords, t*) that determines the value of *target* from the field value *value* (the value of the adjacent cell unless *value_cell* is specified), the spatial discretization *dx* in the direction perpendicular to the wall, the spatial coordinates of the wall point, and time *t*. Ideally, this function should be numba-compilable since simulations might otherwise be very slow.
- **const** (*float or str or callable*) – An expression similar to *value*, which is only used for mixed (Robin) boundary conditions. Note that the implementation currently does not support that one argument is given as a callable function while the other is defined via an expression, so both need to have the same type.
- **target** (*str*) – Selects which value is actually set. Possible choices include *value*, *derivative*, *mixed*, and *virtual_point*.
- **user_funcs** (*dict, optional*) – A dictionary with user defined functions that can be used in expressions
- **value_cell** (*int*) – Determines which cells is read to determine the field value that is used as *value* in the expression or the function call. The default (*None*) specifies the adjacent cell.

```
names: list[str] = ['mixed_expression', 'mixed_expr', 'robin_expression',  
                  'robin_expr']
```

identifiers used to specify the given boundary class

Type

`list`

```
class ExpressionValueBC (grid, axis, upper, *, rank=0, value=0, target='value', user_funcs=None,  
                        value_cell=None)
```

Bases: `ExpressionBC`

represents a boundary whose value is calculated from an expression

The expression is given as a string and will be parsed by `sympy`. The expression can contain typical mathematical operators and may depend on the value at the last support point next to the boundary (*value*), spatial coordinates defined by the grid marking the boundary point (e.g., *x* or *r*), and time *t*.

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

- **value** (*float or str or callable*) – An expression that determines the value of the boundary condition. Alternatively, this can be a function with signature (*value, dx, *coords, t*) that determines the value of *target* from the field value *value* (the value of the adjacent cell unless *value_cell* is specified), the spatial discretization *dx* in the direction perpendicular to the wall, the spatial coordinates of the wall point, and time *t*. Ideally, this function should be numba-compilable since simulations might otherwise be very slow.
- **const** (*float or str or callable*) – An expression similar to *value*, which is only used for mixed (Robin) boundary conditions. Note that the implementation currently does not support that one argument is given as a callable function while the other is defined via an expression, so both need to have the same type.
- **target** (*str*) – Selects which value is actually set. Possible choices include *value*, *derivative*, *mixed*, and *virtual_point*.
- **user_funcs** (*dict, optional*) – A dictionary with user defined functions that can be used in expressions
- **value_cell** (*int*) – Determines which cells is read to determine the field value that is used as *value* in the expression or the function call. The default (*None*) specifies the adjacent cell.

names: `list[str] = ['value_expression', 'value_expr']`

identifiers used to specify the given boundary class

Type

`list`

class MixedBC (*grid, axis, upper, *, rank=0, value=0, const=0*)

Bases: `ConstBC1stOrderBase`

represents a mixed (or Robin) boundary condition imposing a derivative in the outward normal direction of the boundary that is given by an affine function involving the actual value:

$$\partial_n c + \gamma c = \beta$$

Here, *c* is the field to which the condition is applied, γ quantifies the influence of the field and β is the constant term. Note that $\gamma = 0$ corresponds to Dirichlet conditions imposing β as the derivative. Conversely, $\gamma \rightarrow \infty$ corresponds to imposing a zero value on *c*.

This condition can be enforced by using one of the following variants

```
bc = {'mixed': VALUE}
bc = {'type': 'mixed', 'value': VALUE, 'const': CONST}
```

where *VALUE* corresponds to γ and *CONST* to β .

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **value** (*float or str or array*) – The parameter γ quantifying the influence of the field onto its normal derivative. If *value* is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are

possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

- **const** (float or `ndarray` or str) – The parameter β determining the constant term for the boundary condition. Supports the same input as *value*.

copy (*upper=None, rank=None, value=None, const=None*)

return a copy of itself, but with a reference to the same grid

Parameters

- **self** (`MixedBC`) –
- **upper** (`bool` | `None`) –
- **rank** (`int` | `None`) –
- **value** (`float` | `ndarray` | `str` | `None`) –
- **const** (`float` | `ndarray` | `str` | `None`) –

Return type

`MixedBC`

get_mathematical_representation (*field_name='C'*)

return mathematical representation of the boundary condition

Parameters

field_name (`str`) –

Return type

`str`

get_virtual_point_data (*compiled=False*)

return data suitable for calculating virtual points

Parameters

compiled (`bool`) – Flag indicating whether a compiled version is required, which automatically takes updated values into account when it is used in numba-compiled code.

Returns

the data structure associated with this virtual point

Return type

`tuple`

names: `list[str]` = `['mixed', 'robin']`

identifiers used to specify the given boundary class

Type

`list`

to_subgrid (*subgrid*)

converts this boundary condition to one valid for a given subgrid

Parameters

- **subgrid** (`GridBase`) – Grid of the new boundary conditions
- **self** (`MixedBC`) –

Returns

Boundary conditions valid on the subgrid

Return type*ConstBCBase***class NeumannBC** (*grid, axis, upper, *, rank=0, value=0*)Bases: *ConstBC1stOrderBase*

represents a boundary condition imposing the derivative in the outward normal direction of the boundary

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If value is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

get_mathematical_representation (*field_name='C'*)

return mathematical representation of the boundary condition

Parameters**field_name** (*str*) –**Return type***str***get_virtual_point_data** (*compiled=False*)

return data suitable for calculating virtual points

Parameters**compiled** (*bool*) – Flag indicating whether a compiled version is required, which automatically takes updated values into account when it is used in numba-compiled code.**Returns**

the data structure associated with this virtual point

Return type*tuple***names:** *list[str]* = ['derivative', 'neumann']

identifiers used to specify the given boundary class

Type*list*

```
class NormalCurvatureBC (grid, axis, upper, *, rank=0, value=0)
```

Bases: `CurvatureBC`

represents a boundary condition imposing the 2nd normal derivative onto the normal components at the boundary

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when `value` cannot be an arbitrary string.

Parameters

- **grid** (`GridBase`) – The grid for which the boundary conditions are defined
- **axis** (`int`) – The axis to which this boundary condition is associated
- **upper** (`bool`) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (`int`) – The tensorial rank of the field for this boundary condition
- **normal** (`bool`) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or `ndarray`) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If `value` is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

```
names: list[str] = ['normal_curvature']
```

identifiers used to specify the given boundary class

Type

`list`

```
normal: bool = True
```

determines whether the boundary condition only affects normal components.

If this flag is *False*, boundary conditions must specify values for all components of the field. If *True*, only the normal components at the boundary are specified.

Type

`bool`

```
class NormalDirichletBC (grid, axis, upper, *, rank=0, value=0)
```

Bases: `DirichletBC`

represents a boundary condition imposing the value on normal components

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when `value` cannot be an arbitrary string.

Parameters

- **grid** (`GridBase`) – The grid for which the boundary conditions are defined
- **axis** (`int`) – The axis to which this boundary condition is associated

- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (float or str or `ndarray`) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If value is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

```
names: list[str] = ['normal_value', 'normal_dirichlet',
'dirichlet_normal']
```

identifiers used to specify the given boundary class

Type
list

```
normal: bool = True
```

determines whether the boundary condition only affects normal components.

If this flag is *False*, boundary conditions must specify values for all components of the field. If *True*, only the normal components at the boundary are specified.

Type
bool

```
class NormalMixedBC (grid, axis, upper, *, rank=0, value=0, const=0)
```

Bases: *MixedBC*

represents a mixed (or Robin) boundary condition setting the derivative of the normal components in the outward normal direction of the boundary using an affine function involving the actual value:

$$\partial_n c + \gamma c = \beta$$

Here, c is the field to which the condition is applied, γ quantifies the influence of the field and β is the constant term. Note that $\gamma = 0$ corresponds to Dirichlet conditions imposing β as the derivative. Conversely, $\gamma \rightarrow \infty$ corresponds to imposing a zero value on c .

This condition can be enforced by using one of the following variants

```
bc = {'mixed': VALUE}
bc = {'type': 'mixed', 'value': VALUE, 'const': CONST}
```

where *VALUE* corresponds to γ and *CONST* to β .

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

- **value** (*float* or *str* or *array*) – The parameter γ quantifying the influence of the field onto its normal derivative. If *value* is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.
- **const** (*float* or *ndarray* or *str*) – The parameter β determining the constant term for the boundary condition. Supports the same input as *value*.

names: `list[str] = ['normal_mixed', 'normal_robin']`

identifiers used to specify the given boundary class

Type

`list`

normal: `bool = True`

determines whether the boundary condition only affects normal components.

If this flag is *False*, boundary conditions must specify values for all components of the field. If *True*, only the normal components at the boundary are specified.

Type

`bool`

class NormalNeumannBC (*grid*, *axis*, *upper*, *, *rank*=0, *value*=0)

Bases: *NeumannBC*

represents a boundary condition imposing the derivative of normal components in the outward normal direction of the boundary

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur. However, the function is safe when *value* cannot be an arbitrary string.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition
- **normal** (*bool*) – Flag indicating whether the condition is only applied in the normal direction.
- **value** (*float* or *str* or *ndarray*) – a value stored with the boundary condition. The interpretation of this value depends on the type of boundary condition. If *value* is a single value (or tensor in case of tensorial boundary conditions), the same value is applied to all points. Inhomogeneous boundary conditions are possible by supplying an expression as a string, which then may depend on the axes names of the respective grid.

names: `list[str] = ['normal_derivative', 'normal_neumann', 'neumann_normal']`

identifiers used to specify the given boundary class

Type
list

normal: `bool = True`

determines whether the boundary condition only affects normal components.

If this flag is *False*, boundary conditions must specify values for all components of the field. If *True*, only the normal components at the boundary are specified.

Type
bool

class UserBC (*grid*, *axis*, *upper*, *, *rank*=0)

Bases: *BCBase*

represents a boundary whose virtual point are set by the user.

Boundary conditions will only be set when a dictionary {*TARGET*: *value*} is supplied as argument *args* to *set_ghost_cells()* or the numba equivalent. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Warning: This implies that the boundary conditions are never enforced automatically, e.g., when evaluating an operator. It is thus the user's responsibility to ensure virtual points are set correctly before operators are applied.

Parameters

- **grid** (*GridBase*) – The grid for which the boundary conditions are defined
- **axis** (*int*) – The axis to which this boundary condition is associated
- **upper** (*bool*) – Flag indicating whether this boundary condition is associated with the upper side of an axis or not. In essence, this determines the direction of the local normal vector of the boundary.
- **rank** (*int*) – The tensorial rank of the field for this boundary condition

copy (*upper=None*, *rank=None*)

return a copy of itself, but with a reference to the same grid

Parameters

- **self** (*TBC*) –
- **upper** (*bool* | *None*) –
- **rank** (*int* | *None*) –

Return type

TBC

get_mathematical_representation (*field_name='C'*)

return mathematical representation of the boundary condition

Parameters

field_name (*str*) –

Return type

str

make_ghost_cell_setter()

return function that sets the ghost cells for this boundary

Return type

`GhostCellSetter`

make_virtual_point_evaluator()

returns a function evaluating the value at the virtual support point

Returns

A function that takes the data array and an index marking the current point, which is assumed to be a virtual point. The result is the data value at this point, which is calculated using the boundary condition.

Return type

function

names: `list[str] = ['user']`

identifiers used to specify the given boundary class

Type

`list`

set_ghost_cells(data_full, *, args=None)

set the ghost cell values for this boundary

Parameters

- **data_full** (`ndarray`) – The full field data including ghost points
- **args** (`ndarray`) – Determines what boundary conditions are set. *args* should be set to `{TARGET: value}`. Here, *TARGET* determines how the *value* is interpreted and what boundary condition is actually enforced: the value of the virtual points directly (*virtual_point*), the value of the field at the boundary (*value*) or the outward derivative of the field at the boundary (*derivative*).

Return type

`None`

to_subgrid(subgrid)

converts this boundary condition to one valid for a given subgrid

Parameters

- **subgrid** (`GridBase`) – Grid of the new boundary conditions
- **self** (`TBC`) –

Returns

Boundary conditions valid on the subgrid

Return type

`BCBase`

registered_boundary_condition_classes()

returns all boundary condition classes that are currently defined

Returns

a dictionary with the names of the boundary condition classes

Return type

`dict`

registered_boundary_condition_names()

returns all named boundary conditions that are currently defined

Returns

a dictionary with the names of the boundary conditions that can be used

Return type

dict

4.2.2 `pde.grids.coordinates` package

Package collecting classes representing orthonormal coordinate systems

<i>BipolarCoordinates</i>	2-dimensional bipolar coordinates
<i>BisphericalCoordinates</i>	3-dimensional bispherical coordinates
<i>CartesianCoordinates</i>	n-dimensional Cartesian coordinates
<i>CylindricalCoordinates</i>	n-dimensional Cartesian coordinates
<i>PolarCoordinates</i>	2-dimensional polar coordinates
<i>SphericalCoordinates</i>	3-dimensional spherical coordinates

`pde.grids.coordinates.base` module

class CoordinatesBase

Bases: `object`

Base class for orthonormal coordinate systems

axes: `list[str]`

name of each coordinate axis

Type

`list`

basis_rotation (*points*)

returns rotation matrix rotating basis vectors to Cartesian coordinates

Parameters

points (`ndarray`) – Coordinates of the point(s)

Returns

Rotation matrices for all points. The returned array has the shape $(dim, dim) + points_shape$, assuming *points* has the shape $points_shape + (dim,)$.

Return type

`ndarray`

cell_volume (*c_low*, *c_high*)

calculate the volume between coordinate lines

Parameters

- **c_low** (`ndarray`) – Lower values of the coordinate lines enclosing the volume
- **c_high** (`ndarray`) – Upper values of the coordinate lines enclosing the volume

Returns

Enclosed volumes for all given cells

Return type`ndarray`**coordinate_limits:** `list[tuple[float, float]]`

the limits of each coordinate axis

Type`list of tuple`**dim:** `int`

spatial dimension of the coordinate system

Type`int`**distance** (*p1*, *p2*)

Calculate the distance between two points

Parameters

- **p1** (`ndarray`) – First position
- **p2** (`ndarray`) – Second position

Returns

Distance between the two positions

Return type`float`**mapping_jacobian** (*points*)

returns the Jacobian matrix of the coordinate mapping

Parameters**points** (`ndarray`) – Coordinates of the point(s)**Returns**

The Jacobian

Return type`ndarray`**metric** (*points*)

calculate the metric tensor at coordinate points

Parameters**points** (`ndarray`) – The coordinates of the points**Returns**

Metric tensor at the points

Return type`ndarray`**pos_diff** (*p1*, *p2*)

return Cartesian vector(s) pointing from p1 to p2

Parameters

- **p1** (`ndarray`) – First point(s)
- **p2** (`ndarray`) – Second point(s)

Returns

The difference vectors between the points with periodic boundary conditions applied.

Return type

`ndarray`

pos_from_cart (*points*)

convert Cartesian coordinates to coordinates in this system

Parameters

points (`ndarray`) – Points given in Cartesian coordinates.

Returns

Points given in the coordinates of this system

Return type

`ndarray`

pos_to_cart (*points*)

convert coordinates to Cartesian coordinates

Parameters

points (`ndarray`) – The coordinates of points in the current coordinate system

Returns

Cartesian coordinates of the points

Return type

`ndarray`

scale_factors (*points*)

calculate the scale factors at various points

Parameters

points (`ndarray`) – The coordinates of the points

Returns

Scale factors at the points

Return type

`ndarray`

vec_to_cart (*points, components*)

convert the vectors at given points to a Cartesian basis

Parameters

- **points** (`ndarray`) – The coordinates of the point(s) where the vectors are specified.
- **components** (`ndarray`) – The components of the vectors at the given points

Returns

The vectors specified at the same position but with components given in Cartesian coordinates.

Return type

`ndarray`

volume_factor (*points*)

calculate the volume factors at various points

Parameters

points (`ndarray`) – Coordinates of the point(s)

Returns

Volume factors at the points

Return type

`ndarray`

exception DimensionError

Bases: `ValueError`

exception indicating that dimensions were inconsistent

pde.grids.coordinates.bipolar module**class BipolarCoordinates** (*scale_parameter=1*)

Bases: `CoordinatesBase`

2-dimensional bipolar coordinates

Parameters

scale_parameter (*float*) –

axes: `list[str]` = [' σ ', ' τ ']

name of each coordinate axis

Type

`list`

coordinate_limits: `list[tuple[float, float]]` = [(0, 6.283185307179586),
(-inf, inf)]

the limits of each coordinate axis

Type

`list of tuple`

dim: `int` = 2

spatial dimension of the coordinate system

Type

`int`

pde.grids.coordinates.bispherical module**class BisphericalCoordinates** (*scale_parameter=1*)

Bases: `CoordinatesBase`

3-dimensional bispherical coordinates

Parameters

scale_parameter (*float*) –

axes: `list[str]` = [' σ ', ' τ ', ' ψ ']

name of each coordinate axis

Type

`list`


```
coordinate_limits: list[tuple[float, float]] = [(0, 3.141592653589793),
(-inf, inf), (0, 6.283185307179586)]
```

the limits of each coordinate axis

Type

list of tuple

```
dim: int = 3
```

spatial dimension of the coordinate system

Type

int

pde.grids.coordinates.cartesian module

```
class CartesianCoordinates(dim)
```

Bases: *CoordinatesBase*

n-dimensional Cartesian coordinates

Parameters

dim (*int*) – Dimension of the Cartesian coordinate system

pde.grids.coordinates.cylindrical module

```
class CylindricalCoordinates
```

Bases: *CoordinatesBase*

n-dimensional Cartesian coordinates

```
axes: list[str] = ['r', 'φ', 'z']
```

name of each coordinate axis

Type

list

```
coordinate_limits: list[tuple[float, float]] = [(0, inf), (0,
6.283185307179586), (-inf, inf)]
```

the limits of each coordinate axis

Type

list of tuple

```
dim: int = 3
```

spatial dimension of the coordinate system

Type

int

pde.grids.coordinates.polar module

class PolarCoordinates

Bases: *CoordinatesBase*

2-dimensional polar coordinates

axes: `list[str]` = ['r', 'φ']

name of each coordinate axis

Type

`list`

coordinate_limits: `list[tuple[float, float]]` = [(0, inf), (0, 6.283185307179586)]

the limits of each coordinate axis

Type

`list of tuple`

dim: `int` = 2

spatial dimension of the coordinate system

Type

`int`

pde.grids.coordinates.spherical module

class SphericalCoordinates

Bases: *CoordinatesBase*

3-dimensional spherical coordinates

axes: `list[str]` = ['r', 'θ', 'φ']

name of each coordinate axis

Type

`list`

coordinate_limits: `list[tuple[float, float]]` = [(0, inf), (0, 3.141592653589793), (0, 6.283185307179586)]

the limits of each coordinate axis

Type

`list of tuple`

dim: `int` = 3

spatial dimension of the coordinate system

Type

`int`

major_axis = 0

4.2.3 `pde.grids.operators` package

Package collecting modules defining discretized operators for different grids.

These operators can either be used directly or they are imported by the respective methods defined on fields and grids.

<code>cartesian</code>	This module implements differential operators on Cartesian grids
<code>cylindrical_sym</code>	This module implements differential operators on cylindrical grids
<code>polar_sym</code>	This module implements differential operators on polar grids
<code>spherical_sym</code>	This module implements differential operators on spherical grids
<code>common.make_derivative</code>	make a derivative operator along a single axis using numba compilation
<code>common.make_derivative2</code>	make a second-order derivative operator along a single axis

`pde.grids.operators.cartesian` module

This module implements differential operators on Cartesian grids

<code>make_laplace</code>	make a Laplace operator on a Cartesian grid
<code>make_gradient</code>	make a gradient operator on a Cartesian grid
<code>make_divergence</code>	make a divergence operator on a Cartesian grid
<code>make_vector_gradient</code>	make a vector gradient operator on a Cartesian grid
<code>make_vector_laplace</code>	make a vector Laplacian on a Cartesian grid
<code>make_tensor_divergence</code>	make a tensor divergence operator on a Cartesian grid
<code>make_poisson_solver</code>	make an operator that solves Poisson's equation

`make_divergence` (*grid*, *backend*='auto')

make a divergence operator on a Cartesian grid

Parameters

- **`grid`** (*CartesianGrid*) – The grid for which the operator is created
- **`backend`** (*str*) – Backend used for calculating the divergence operator. If `backend`='auto', a suitable backend is chosen automatically.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

`make_gradient` (*grid*, *backend*='auto')

make a gradient operator on a Cartesian grid

Parameters

- **`grid`** (*CartesianGrid*) – The grid for which the operator is created
- **`backend`** (*str*) – Backend used for calculating the gradient operator. If `backend`='auto', a suitable backend is chosen automatically.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_laplace (*grid*, *backend*='auto')

make a Laplace operator on a Cartesian grid

Parameters

- **grid** (*CartesianGrid*) – The grid for which the operator is created
- **backend** (*str*) – Backend used for calculating the Laplace operator. If backend='auto', a suitable backend is chosen automatically.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_poisson_solver (*bcs*, *method*='auto')

make a operator that solves Poisson's equation

Parameters

- **bcs** (*Boundaries*) – {ARG_BOUNDARIES_INSTANCE}
- **method** (*str*) – Method used for calculating the tensor divergence operator. If method='auto', a suitable method is chosen automatically.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_tensor_divergence (*grid*, *backend*='numba')

make a tensor divergence operator on a Cartesian grid

Parameters

- **grid** (*CartesianGrid*) – The grid for which the operator is created
- **backend** (*str*) – Backend used for calculating the tensor divergence operator.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_vector_gradient (*grid*, *backend*='numba')

make a vector gradient operator on a Cartesian grid

Parameters

- **grid** (*CartesianGrid*) – The grid for which the operator is created
- **backend** (*str*) – Backend used for calculating the vector gradient operator.

Returns

A function that can be applied to an array of values

Return type`OperatorType`**make_vector_laplace** (*grid*, *backend*='numba')

make a vector Laplacian on a Cartesian grid

Parameters

- **grid** (`CartesianGrid`) – The grid for which the operator is created
- **backend** (`str`) – Backend used for calculating the vector Laplace operator.

Returns

A function that can be applied to an array of values

Return type`OperatorType`**pde.grids.operators.common module**

Common functions that are used by many operators

make_derivative (*grid*, *axis*=0, *method*='central')

make a derivative operator along a single axis using numba compilation

Parameters

- **grid** (`GridBase`) – The grid for which the operator is created
- **axis** (`int`) – The axis along which the derivative will be taken
- **method** (`str`) – The method for calculating the derivative. Possible values are 'central', 'forward', and 'backward'.

Returns

A function that can be applied to an full array of values including those at ghost cells. The result will be an array of the same shape containing the actual derivatives at the valid (interior) grid points.

Return type`OperatorType`**make_derivative2** (*grid*, *axis*=0)

make a second-order derivative operator along a single axis

Parameters

- **grid** (`GridBase`) – The grid for which the operator is created
- **axis** (`int`) – The axis along which the derivative will be taken

Returns

A function that can be applied to an full array of values including those at ghost cells. The result will be an array of the same shape containing the actual derivatives at the valid (interior) grid points.

Return type`OperatorType`**make_general_poisson_solver** (*matrix*, *vector*, *method*='auto')

make an operator that solves Poisson's problem

Parameters

- **matrix** – The (sparse) matrix representing the laplace operator on the given grid.

- **vector** – The constant part representing the boundary conditions of the Laplace operator.
- **method** (*str*) – The chosen method for implementing the operator

Returns

A function that can be applied to an array of values to obtain the solution to Poisson’s equation where the array is used as the right hand side

Return type

`OperatorType`

make_laplace_from_matrix (*matrix*, *vector*)

make a Laplace operator using matrix vector products

Parameters

- **matrix** – (Sparse) matrix representing the laplace operator on the given grid
- **vector** – Constant part representing the boundary conditions of the Laplace operator

Returns

A function that can be applied to an array of values to obtain the result of applying the linear operator *matrix* and the offset given by *vector*.

Return type

`Callable[[ndarray, ndarray | None], ndarray]`

uniform_discretization (*grid*)

returns the uniform discretization or raises `RuntimeError`

Parameters

grid (*GridBase*) – The grid whose discretization is tested

Raises

`RuntimeError` –

Returns

the common discretization of all axes

Return type

`float`

pde.grids.operators.cylindrical_sym module

This module implements differential operators on cylindrical grids

<code>make_laplace</code>	make a discretized laplace operator for a cylindrical grid
<code>make_gradient</code>	make a discretized gradient operator for a cylindrical grid
<code>make_divergence</code>	make a discretized divergence operator for a cylindrical grid
<code>make_vector_gradient</code>	make a discretized vector gradient operator for a cylindrical grid
<code>make_vector_laplace</code>	make a discretized vector laplace operator for a cylindrical grid
<code>make_tensor_divergence</code>	make a discretized tensor divergence operator for a cylindrical grid
<code>make_poisson_solver</code>	make an operator that solves Poisson's equation

make_divergence (*grid*)

make a discretized divergence operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

grid (*CylindricalSymGrid*) – The grid for which the operator is created

Returns

A function that can be applied to an array of values

Return type

OperatorType

make_gradient (*grid*)

make a discretized gradient operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

grid (*CylindricalSymGrid*) – The grid for which the operator is created

Returns

A function that can be applied to an array of values

Return type

OperatorType

make_gradient_squared (*grid*, *central=True*)

make a discretized gradient squared operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

- **grid** (*CylindricalSymGrid*) – The grid for which the operator is created
- **central** (*bool*) – Whether a central difference approximation is used for the gradient operator. If this is False, the squared gradient is calculated as the mean of the squared values of the forward and backward derivatives.

Returns

A function that can be applied to an array of values

Return type

OperatorType

make_laplace (*grid*)

make a discretized laplace operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

grid (*CylindricalSymGrid*) – The grid for which the operator is created

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_poisson_solver (*bcs*, *method*='auto')

make a operator that solves Poisson's equation

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

- **bcs** (*Boundaries*) – Specifies the boundary conditions applied to the field. This must be an instance of *Boundaries*, which can be created from various data formats using the class method `from_data()`.
- **method** (*str*) – The chosen method for implementing the operator

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_tensor_divergence (*grid*)

make a discretized tensor divergence operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

grid (*CylindricalSymGrid*) – The grid for which the operator is created

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_vector_gradient (*grid*)

make a discretized vector gradient operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

grid (*CylindricalSymGrid*) – The grid for which the operator is created

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_vector_laplace (*grid*)

make a discretized vector laplace operator for a cylindrical grid

The cylindrical grid assumes polar symmetry, so that fields only depend on the radial coordinate r and the axial coordinate z . Here, the first axis is along the radius, while the second axis is along the axis of the cylinder. The radial discretization is defined as $r_i = (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$.

Parameters

grid (*CylindricalSymGrid*) – The grid for which the operator is created

Returns

A function that can be applied to an array of values

Return type

OperatorType

pde.grids.operators.polar_sym module

This module implements differential operators on polar grids

<i>make_laplace</i>	make a discretized laplace operator for a polar grid
<i>make_gradient</i>	make a discretized gradient operator for a polar grid
<i>make_divergence</i>	make a discretized divergence operator for a polar grid
<i>make_vector_gradient</i>	make a discretized vector gradient operator for a polar grid
<i>make_tensor_divergence</i>	make a discretized tensor divergence operator for a polar grid
<i>make_poisson_solver</i>	make an operator that solves Poisson's equation

make_divergence (*grid*)

make a discretized divergence operator for a polar grid

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

grid (*PolarSymGrid*) – The polar grid for which this operator will be defined

Returns

A function that can be applied to an array of values

Return type

OperatorType

make_gradient (*grid*)

make a discretized gradient operator for a polar grid

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

grid (*PolarSymGrid*) – The polar grid for which this operator will be defined

Returns

A function that can be applied to an array of values

Return type

OperatorType

make_gradient_squared (*grid*, *central=True*)

make a discretized gradient squared operator for a polar grid

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **grid** (*PolarSymGrid*) – The polar grid for which this operator will be defined
- **central** (*bool*) – Whether a central difference approximation is used for the gradient operator. If this is False, the squared gradient is calculated as the mean of the squared values of the forward and backward derivatives.

Returns

A function that can be applied to an array of values

Return type*OperatorType***make_laplace** (*grid*)

make a discretized laplace operator for a polar grid

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters**grid** (*PolarSymGrid*) – The polar grid for which this operator will be defined**Returns**

A function that can be applied to an array of values

Return type*OperatorType***make_poisson_solver** (*bcs*, *method='auto'*)

make an operator that solves Poisson's equation

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **bcs** (*Boundaries*) – Specifies the boundary conditions applied to the field. This must be an instance of *Boundaries*, which can be created from various data formats using the class method *from_data()*.
- **method** (*str*) – The chosen method for implementing the operator

Returns

A function that can be applied to an array of values

Return type*OperatorType***make_tensor_divergence** (*grid*)

make a discretized tensor divergence operator for a polar grid

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r \Delta r$.

Parameters

grid (*PolarSymGrid*) – The polar grid for which this operator will be defined

Returns

A function that can be applied to an array of values

Return type

OperatorType

make_vector_gradient (*grid*)

make a discretized vector gradient operator for a polar grid

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r \Delta r$.

Parameters

grid (*PolarSymGrid*) – The polar grid for which this operator will be defined

Returns

A function that can be applied to an array of values

Return type

OperatorType

pde.grids.operators.spherical_sym module

This module implements differential operators on spherical grids

<i>make_laplace</i>	make a discretized laplace operator for a spherical grid
<i>make_gradient</i>	make a discretized gradient operator for a spherical grid
<i>make_divergence</i>	make a discretized divergence operator for a spherical grid
<i>make_vector_gradient</i>	make a discretized vector gradient operator for a spherical grid
<i>make_tensor_divergence</i>	make a discretized tensor divergence operator for a spherical grid
<i>make_poisson_solver</i>	make an operator that solves Poisson's equation

make_divergence (*grid*, *safe=True*, *conservative=True*)

make a discretized divergence operator for a spherical grid

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r \Delta r$.

Warning: This operator ignores the θ -component of the field when calculating the divergence. This is because the resulting scalar field could not be expressed on a *SphericalSymGrid*.

Parameters

- **grid** (*SphericalSymGrid*) – The polar grid for which this operator will be defined

- **safe** (*bool*) – Add extra checks for the validity of the input
- **conservative** (*bool*) – Flag indicating whether the operator should be conservative (which results in slightly slower computations). Conservative operators ensure mass conservation.

Returns

A function that can be applied to an array of values

Return type

[OperatorType](#)

make_gradient (*grid*)

make a discretized gradient operator for a spherical grid

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

grid ([SphericalSymGrid](#)) – The polar grid for which this operator will be defined

Returns

A function that can be applied to an array of values

Return type

[OperatorType](#)

make_gradient_squared (*grid*, *central=True*)

make a discretized gradient squared operator for a spherical grid

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **grid** ([SphericalSymGrid](#)) – The polar grid for which this operator will be defined
- **central** (*bool*) – Whether a central difference approximation is used for the gradient operator. If this is False, the squared gradient is calculated as the mean of the squared values of the forward and backward derivatives.

Returns

A function that can be applied to an array of values

Return type

[OperatorType](#)

make_laplace (*grid*, *conservative=True*)

make a discretized laplace operator for a spherical grid

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **grid** ([SphericalSymGrid](#)) – The polar grid for which this operator will be defined
- **conservative** (*bool*) – Flag indicating whether the laplace operator should be conservative (which results in slightly slower computations). Conservative operators ensure mass conservation.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_poisson_solver (*bcs*, *method*='auto')

make a operator that solves Poisson's equation

The polar grid assumes polar symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **bcs** (*Boundaries*) – Specifies the boundary conditions applied to the field. This must be an instance of *Boundaries*, which can be created from various data formats using the class method `from_data()`.
- **method** (*str*) – The chosen method for implementing the operator

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_tensor_divergence (*grid*, *safe*=*True*, *conservative*=*False*)

make a discretized tensor divergence operator for a spherical grid

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **grid** (*SphericalSymGrid*) – The polar grid for which this operator will be defined
- **safe** (*bool*) – Add extra checks for the validity of the input
- **conservative** (*bool*) – Flag indicating whether the operator should be conservative (which results in slightly slower computations). Conservative operators ensure mass conservation.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_tensor_double_divergence (*grid*, *safe*=*True*, *conservative*=*True*)

make a discretized tensor double divergence operator for a spherical grid

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **grid** (*SphericalSymGrid*) – The polar grid for which this operator will be defined
- **safe** (*bool*) – Add extra checks for the validity of the input

- **conservative** (*bool*) – Flag indicating whether the operator should be conservative (which results in slightly slower computations). Conservative operators ensure mass conservation.

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

make_vector_gradient (*grid*, *safe=True*)

make a discretized vector gradient operator for a spherical grid

Warning: This operator ignores the two angular components of the field when calculating the gradient. This is because the resulting field could not be expressed on a `SphericalSymGrid`.

The spherical grid assumes spherical symmetry, so that fields only depend on the radial coordinate r . The radial discretization is defined as $r_i = r_{\min} + (i + \frac{1}{2})\Delta r$ for $i = 0, \dots, N_r - 1$, where r_{\min} is the radius of the inner boundary, which is zero by default. Note that the radius of the outer boundary is given by $r_{\max} = r_{\min} + N_r\Delta r$.

Parameters

- **grid** (*SphericalSymGrid*) – The polar grid for which this operator will be defined
- **safe** (*bool*) – Add extra checks for the validity of the input

Returns

A function that can be applied to an array of values

Return type

`OperatorType`

4.2.4 pde.grids.base module

Defines the base class for all grids

exception DomainError

Bases: `ValueError`

exception indicating that point lies outside domain

class GridBase

Bases: `object`

Base class for all grids defining common methods and interfaces

initialize the grid

assert_grid_compatible (*other*)

checks whether *other* is compatible with the current grid

Parameters

other (*GridBase*) – The grid compared to this one

Raises

`ValueError` – if grids are not compatible

Return type

None

axes: `list[str]`

Names of all axes that are described by the grid

Type`list`**property axes_bounds:** `tuple[tuple[float, float], ...]`

lower and upper bounds of each axis

Type`tuple`**property axes_coords:** `tuple[ndarray, ...]`

coordinates of the cells for each axis

Type`tuple`**axes_symmetric:** `list[str] = []`

The names of the additional axes that the fields do not depend on, e.g. along which they are constant.

Type`list`**boundary_names:** `dict[str, tuple[int, bool]] = {}`

Names of boundaries to select them conveniently

Type`dict`**c:** `CoordinatesBase`

Coordinates of the grid

Type`CoordinatesBase`**cell_coords**

coordinate values for all axes of each cell

Type`ndarray`**cell_volume_data:** `Sequence[FloatNumerical] | None`

Information about the size of discretization cells

Type`list`**cell_volumes**

volume of each cell

Type`ndarray`**compatible_with** (*other*)

tests whether this grid is compatible with other grids.

Grids are compatible when they cover the same area with the same discretization. The difference to equality is that compatible grids do not need to have the same periodicity in their boundaries.

Parameters

other (*GridBase*) – The other grid to test against

Returns

Whether the grid is compatible

Return type

bool

contains_point (*points*, *, *coords*='cartesian', *full*=False)

check whether the point is contained in the grid

Parameters

- **point** (*ndarray*) – Coordinates of the point
- **coords** (*str*) – The coordinate system in which the points are given
- **full** (*bool*) – Indicates whether coordinates along symmetric axes are specified
- **points** (*ndarray*) –

Returns

A boolean array indicating which points lie within the grid

Return type

ndarray

coordinate_arrays

for each axes: coordinate values for all cells

Type

tuple

coordinate_constraints: *list*[*int*] = []

axes that not described explicitly

Type

list

copy ()

return a copy of the grid

Return type

GridBase

difference_vector (*p1*, *p2*, *, *coords*='grid')

return Cartesian vector(s) pointing from p1 to p2

In case of periodic boundary conditions, the shortest vector is returned.

Parameters

- **p1** (*ndarray*) – First point(s)
- **p2** (*ndarray*) – Second point(s)
- **coords** (*str*) – The coordinate system in which the points are specified. Valid values are *cartesian*, *cell*, and *grid*; see *transform()*.

Returns

The difference vectors between the points with periodic boundary conditions applied.

Return type

ndarray

difference_vector_real (*p1*, *p2*)

Parameters

- **p1** (*ndarray*) –
- **p2** (*ndarray*) –

Return type

ndarray

property dim: *int*

The spatial dimension in which the grid is embedded

Type

int

property discretization: *ndarray*

the linear size of a cell along each axis

Type

numpy.array

distance (*p1*, *p2*, *, *coords*='grid')

Calculate the distance between two points given in real coordinates

This takes periodic boundary conditions into account if necessary.

Parameters

- **p1** (*ndarray*) – First position
- **p2** (*ndarray*) – Second position
- **coords** (*str*) – The coordinate system in which the points are specified. Valid values are *cartesian*, *cell*, and *grid*; see *transform()*.

Returns

Distance between the two positions

Return type

float

distance_real (*p1*, *p2*)

Parameters

- **p1** (*ndarray*) –
- **p2** (*ndarray*) –

Return type

float

classmethod from_bounds (*bounds*, *shape*, *periodic*)

Parameters

- **bounds** (*Sequence[tuple[float, float]]*) –
- **shape** (*Sequence[int]*) –
- **periodic** (*Sequence[bool]*) –

Return type

GridBase

classmethod `from_state` (*state*)

create a field from a stored *state*.

Parameters

state (*str* or *dict*) – The state from which the grid is reconstructed. If *state* is a string, it is decoded as JSON, which should yield a *dict*.

Returns

Grid re-created from the state

Return type

GridBase

get_axis_index (*key*, *allow_symmetric=True*)

return the index belonging to an axis

Parameters

- **key** (*int* or *str*) – The index or name of an axis
- **allow_symmetric** (*bool*) – Whether axes with assumed symmetry are included

Returns

The index of the axis

Return type

int

get_boundary_conditions (*bc='auto_periodic_neumann'*, *rank=0*)

constructs boundary conditions from a flexible data format

Parameters

- **bc** (*str* or *list* or *tuple* or *dict*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by *{‘derivative’: DERIV}*) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **rank** (*int*) – The tensorial rank of the value associated with the boundary conditions.

Returns

The boundary conditions for all axes.

Return type

Boundaries

Raises

- **ValueError** – If the data given in *bc* cannot be read
- **PeriodicityError** – If the boundaries are not compatible with the periodic axes of the grid.

get_image_data (*data*)

return a 2d-image of the data

Parameters

data (`ndarray`) – The values at the grid points

Returns

A dictionary with information about the data convenient for plotting.

Return type

`dict`

get_line_data (*data*, *extract*='auto')

return a line cut through the grid

Parameters

- **data** (`ndarray`) – The values at the grid points
- **extract** (`str`) – Determines which cut is done through the grid. Possible choices depend on the actual grid.

Returns

A dictionary with information about the line cut, which is convenient for plotting.

Return type

`dict`

get_random_point (*, *boundary_distance*=0, *coords*='cartesian', *rng*=None)

return a random point within the grid

Parameters

- **boundary_distance** (`float`) – The minimal distance this point needs to have from all boundaries.
- **coords** (`str`) – Determines the coordinate system in which the point is specified. Valid values are *cartesian*, *cell*, and *grid*; see `transform()`.
- **rng** (`Generator`) – Random number generator (default: `default_rng()`)

Returns

The coordinates of the random point

Return type

`ndarray`

get_vector_data (*data*, ***kwargs*)

return data to visualize vector field

Parameters

- **data** (`ndarray`) – The vectorial values at the grid points
- ****kwargs** – Arguments forwarded to `get_image_data()`.

Returns

A dictionary with information about the data convenient for plotting.

Return type

`dict`

integrate (*data*, *axes*=None)

Integrates the discretized data over the grid

Parameters

- **data** (`ndarray`) – The values at the support points of the grid that need to be integrated.

- **axes** (*list of int, optional*) – The axes along which the integral is performed. If omitted, all axes are integrated over.

Returns

The values integrated over the entire grid

Return type

`ndarray`

iter_mirror_points (*point, with_self=False, only_periodic=True*)

generates all mirror points corresponding to *point*

Parameters

- **point** (`ndarray`) – The point within the grid
- **with_self** (`bool`) – Whether to include the point itself
- **only_periodic** (`bool`) – Whether to only mirror along periodic axes

Returns

A generator yielding the coordinates that correspond to mirrors

Return type

Generator

make_cell_volume_compiled (*flat_index=False*)

return a compiled function returning the volume of a grid cell

Parameters

flat_index (`bool`) – When True, cell_volumes are indexed by a single integer into the flattened array.

Returns

returning the volume of the chosen cell

Return type

function

make_inserter_compiled (*, *with_ghost_cells=False*)

return a compiled function to insert values at interpolated positions

Parameters

with_ghost_cells (`bool`) – Flag indicating that the interpolator should work on the full data array that includes values for the grid points. If this is the case, the boundaries are not checked and the coordinates are used as is.

Returns

A function with signature (data, position, amount), where *data* is the numpy array containing the field data, position is denotes the position in grid coordinates, and *amount* is the that is to be added to the field.

Return type

callable

make_integrator ()

return function that can be used to integrates discretized data over the grid

If this function is used in a multiprocessing run (using MPI), the integrals are performed on all subgrids and then accumulated. Each process then receives the same value representing the global integral.

Returns

A function that takes a numpy array and returns the integral with the correct weights given by the cell volumes.

Return type

callable

make_normalize_point_compiled (*reflect=True*)

return a compiled function that normalizes a point

Here, the point is assumed to be specified by the physical values along the non-symmetric axes of the grid. Normalizing points is useful to make sure they lie within the domain of the grid. This function respects periodic boundary conditions and can also reflect points off the boundary.

Parameters

reflect (*bool*) – Flag determining whether coordinates along non-periodic axes are reflected to lie in the valid range. If *False*, such coordinates are left unchanged and only periodic boundary conditions are enforced.

Returns

A function that takes a `ndarray` as an argument, which describes the coordinates of the points. This array is modified in-place!

Return type

callable

make_operator (*operator, bc, **kwargs*)

return a compiled function applying an operator with boundary conditions

The returned function takes the discretized data on the grid as an input and returns the data to which the operator *operator* has been applied. The function only takes the valid grid points and allocates memory for the ghost points internally to apply the boundary conditions specified as *bc*. Note that the function supports an optional argument *out*, which if given should provide space for the valid output array without the ghost cells. The result of the operator is then written into this output array. The function also accepts an optional parameter *args*, which is forwarded to *set_ghost_cells*.

Parameters

- **operator** (*str*) – Identifier for the operator. Some examples are ‘laplace’, ‘gradient’, or ‘divergence’. The registered operators for this grid can be obtained from the `operators` attribute.
- **bc** (*str or list or tuple or dict*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- ****kwargs** – Specifies extra arguments influencing how the operator is created.

Returns

the function that applies the operator. This function has the signature (*arr*: `np.ndarray`, *out*: `np.ndarray = None`, *args*=`None`).

Return type

callable

make_operator_no_bc (*operator*, ***kwargs*)

return a compiled function applying an operator without boundary conditions

A function that takes the discretized full data as an input and an array of valid data points to which the result of applying the operator is written.

Note: The resulting function does not check whether the ghost cells of the input array have been supplied with sensible values. It is the responsibility of the user to set the values of the ghost cells beforehand. Use this function only if you absolutely know what you're doing. In all other cases, `make_operator()` is probably the better choice.

Parameters

- **operator** (*str*) – Identifier for the operator. Some examples are 'laplace', 'gradient', or 'divergence'. The registered operators for this grid can be obtained from the `operators` attribute.
- ****kwargs** – Specifies extra arguments influencing how the operator is created.

Returns

the function that applies the operator. This function has the signature (`arr: np.ndarray, out: np.ndarray`), so they *out* array need to be supplied explicitly.

Return type

callable

normalize_point (*point*, ***, *reflect=False*)

normalize grid coordinates by applying periodic boundary conditions

Here, points are assumed to be specified by the physical values along the non-symmetric axes of the grid, e.g., by grid coordinates. Normalizing points is useful to make sure they lie within the domain of the grid. This function respects periodic boundary conditions and can also reflect points off the boundary if `reflect = True`.

Parameters

- **point** (*ndarray*) – Coordinates of a single point or an array of points, where the last axis denotes the point coordinates (e.g., a list of points).
- **reflect** (*bool*) – Flag determining whether coordinates along non-periodic axes are reflected to lie in the valid range. If *False*, such coordinates are left unchanged and only periodic boundary conditions are enforced.

Returns

The respective coordinates with periodic boundary conditions applied.

Return type

`ndarray`

num_axes: `int`

Number of axes that are *not* assumed symmetrically

Type

`int`

property num_cells: `int`

the number of cells in this grid

Type

`int`

property `numba_type: str`

represents type of the grid data in numba signatures

Type

`str`

operators: set[str] = {}

names of all operators defined for this grid

Type

`set`

property `periodic: list[bool]`

Flags that describe which axes are periodic

Type

`list`

plot()

visualize the grid

Return type

`None`

point_from_cartesian (*points*, *, *full=False*)

convert points given in Cartesian coordinates to grid coordinates

Parameters

- **points** (`ndarray`) – Points given in Cartesian coordinates.
- **full** (`bool`) – Indicates whether coordinates along symmetric axes are specified

Returns

Points given in the coordinates of the grid

Return type

`ndarray`

point_to_cartesian (*points*, *, *full=False*)

convert coordinates of a point in grid coordinates to Cartesian coordinates

Parameters

- **points** (`ndarray`) – The grid coordinates of the points
- **full** (`bool`) – Indicates whether coordinates along symmetric axes are specified

Returns

The Cartesian coordinates of the point

Return type

`ndarray`

classmethod `register_operator` (*name*, *factory_func=None*, *rank_in=0*, *rank_out=0*)

register an operator for this grid

Example

The method can either be used directly:

```
GridClass.register_operator("operator", make_operator)
```

or as a decorator for the factory function:

```
@GridClass.register_operator("operator")
def make_operator(grid: GridBase):
    ...
```

Parameters

- **name** (*str*) – The name of the operator to register
- **factory_func** (*callable*) – A function with signature `(grid: GridBase, **kwargs)`, which takes a grid object and optional keyword arguments and returns an implementation of the given operator. This implementation is a function that takes a `ndarray` of discretized values as arguments and returns the resulting discretized data in a `ndarray` after applying the operator.
- **rank_in** (*int*) – The rank of the input field for the operator
- **rank_out** (*int*) – The rank of the field that is returned by the operator

property **shape**: `tuple[int, ...]`

the number of support points of each axis

Type

`tuple of int`

slice (*indices*)

return a subgrid of only the specified axes

Parameters

indices (*list*) – Indices indicating the axes that are retained in the subgrid

Returns

The subgrid

Return type

`GridBase`

abstract property **state**: `dict[str, Any]`

all information required for reconstructing the grid

Type

`dict`

property **state_serialized**: `str`

JSON-serialized version of the state of this grid

Type

`str`

transform (*coordinates, source, target, *, full=False*)

converts coordinates from one coordinate system to another

Supported coordinate systems include the following:

- **cartesian:**
Cartesian coordinates where each point carries *dim* values. These are the true physical coordinates in space.
- **grid:**
Coordinates values in the coordinate system defined by the grid. A point is thus characterized by *grid.num_axes* values.
- **cell:**
Normalized grid coordinates based on indexing the discretization cells. A point is characterized by *grid.num_axes* values and the range of values for a given axis is between 0 and *N*, where *N* is the number of grid points. Consequently, the integral part of the cell coordinate denotes the cell, while the fractional part denotes the relative position within the cell. In particular, the cell center is located at $i + 0.5$ with $i = 0, \dots, N-1$.

Note: Some conversion might involve projections if the coordinate system imposes symmetries. For instance, converting 3d Cartesian coordinates to grid coordinates in a spherically symmetric grid will only return the radius from the origin. Conversely, converting these grid coordinates back to 3d Cartesian coordinates will only return coordinates along a particular ray originating at the origin.

Parameters

- **coordinates** (`ndarray`) – The coordinates to convert
- **source** (`str`) – The source coordinate system
- **target** (`str`) – The target coordinate system
- **full** (`bool`) – Indicates whether coordinates along symmetric axes are specified

Returns

The transformed coordinates

Return type

`ndarray`

property typical_discretization: `float`

the average side length of the cells

Type

`float`

uniform_cell_volumes

returns True if all cell volumes are the same

Type

`bool`

property volume: `float`

total volume of the grid

Type

`float`

class OperatorInfo (*factory, rank_in, rank_out, name=""*)

Bases: `NamedTuple`

stores information about an operator

Create new instance of `OperatorInfo(factory, rank_in, rank_out, name)`

Parameters

- **factory** (`OperatorFactory`) –
- **rank_in** (`int`) –
- **rank_out** (`int`) –
- **name** (`str`) –

factory: `OperatorFactory`

Alias for field number 0

name: `str`

Alias for field number 3

rank_in: `int`

Alias for field number 1

rank_out: `int`

Alias for field number 2

exception PeriodicityError

Bases: `RuntimeError`

exception indicating that the grid periodicity is inconsistent

discretize_interval (`x_min`, `x_max`, `num`)

construct a list of equidistantly placed intervals

The discretization is defined as

$$x_i = x_{\min} + \left(i + \frac{1}{2}\right) \Delta x \quad \text{for } i = 0, \dots, N - 1$$
$$\Delta x = \frac{x_{\max} - x_{\min}}{N}$$

where N is the number of intervals given by `num`.

Parameters

- **x_min** (`float`) – Minimal value of the axis
- **x_max** (`float`) – Maximal value of the axis
- **num** (`int`) – Number of intervals

Returns

(midpoints, dx): the midpoints of the intervals and the used discretization dx .

Return type

`tuple`

registered_operators ()

returns all operators that are currently defined

Returns

a dictionary with the names of the operators defined for each grid class

Return type

`dict`

4.2.5 `pde.grids.cartesian` module

Cartesian grids of arbitrary dimension.

class `CartesianGrid` (*bounds*, *shape*, *periodic=False*)

Bases: `GridBase`

d-dimensional Cartesian grid with uniform discretization for each axis

The grids can be thought of as a collection of n-dimensional boxes, called cells, of equal length in each dimension. The bounds then defined the total volume covered by these cells, while the cell coordinates give the location of the box centers. We index the boxes starting from 0 along each dimension. Consequently, the cell $i - \frac{1}{2}$ corresponds to the left edge of the covered interval and the index $i + \frac{1}{2}$ corresponds to the right edge, when the dimension is covered by d boxes.

In particular, the discretization along dimension k is defined as

$$x_i^{(k)} = x_{\min}^{(k)} + \left(i + \frac{1}{2}\right) \Delta x^{(k)} \quad \text{for } i = 0, \dots, N^{(k)} - 1$$

$$\Delta x^{(k)} = \frac{x_{\max}^{(k)} - x_{\min}^{(k)}}{N^{(k)}}$$

where $N^{(k)}$ is the number of cells along this dimension. Consequently, cells have dimension $\Delta x^{(k)}$ and cover the interval $[x_{\min}^{(k)}, x_{\max}^{(k)}]$.

Parameters

- **bounds** (*list of tuple*) – Give the coordinate range for each axis. This should be a tuple of two number (lower and upper bound) for each axis. The length of *bounds* thus determines the grid dimension.
- **shape** (*list*) – The number of support points for each axis. The length of *shape* needs to match the grid dimension.
- **periodic** (*bool or list*) – Specifies which axes possess periodic boundary conditions. This is either a list of booleans defining periodicity for each individual axis or a single boolean value specifying the same periodicity for all axes.

```
boundary_names: dict[str, tuple[int, bool]] = {'back': (2, False),
'bottom': (1, False), 'front': (2, True), 'left': (0, False), 'right':
(0, True), 'top': (1, True)}
```

Names of boundaries to select them conveniently

Type

`dict`

property `cell_volume_data`

size associated with each cell

cuboid: `Cuboid`

difference_vector (*p1*, *p2*, *, *coords='grid'*)

return Cartesian vector(s) pointing from p1 to p2

In case of periodic boundary conditions, the shortest vector is returned.

Parameters

- **p1** (`ndarray`) – First point(s)
- **p2** (`ndarray`) – Second point(s)

- **coords** (*str*) – The coordinate system in which the points are specified. Valid values are *cartesian*, *cell*, and *grid*; see *transform()*.

Returns

The difference vectors between the points with periodic boundary conditions applied.

Return type

ndarray

classmethod from_bounds (*bounds*, *shape*, *periodic*)

Parameters

- **bounds** (*tuple*) – Give the coordinate range for each axis. This should be a tuple of two number (lower and upper bound) for each axis. The length of *bounds* thus determines the grid dimension.
- **shape** (*tuple*) – The number of support points for each axis. The length of *shape* needs to match the grid dimension.
- **periodic** (*bool* or *list*) – Specifies which axes possess periodic boundary conditions. This is either a list of booleans defining periodicity for each individual axis or a single boolean value specifying the same periodicity for all axes.

Returns

representing the region chosen by bounds

Return type

CartesianGrid

classmethod from_state (*state*)

create a field from a stored *state*.

Parameters

state (*dict*) – The state from which the grid is reconstructed.

Returns

the grid re-created from the state data

Return type

CartesianGrid

get_image_data (*data*)

return a 2d-image of the data

Parameters

data (*ndarray*) – The values at the grid points

Returns

A dictionary with information about the data convenient for plotting.

Return type

dict

get_line_data (*data*, *extract*='auto')

return a line cut through the given data

Parameters

- **data** (*ndarray*) – The values at the grid points
- **extract** (*str*) – Determines which cut is done through the grid. Possible choices are (default is *cut_0*):

- *cut_#*: return values along the axis specified by # and use the mid point along all other axes.
- *project_#*: average values for all axes, except axis #.

Here, # can either be a zero-based index (from 0 to dim-1) or a letter denoting the axis.

Returns

A dictionary with information about the line cut, which is convenient for plotting.

Return type

`dict`

get_random_point (*, *boundary_distance*=0, *coords*='cartesian', *rng*=None)

return a random point within the grid

Parameters

- **boundary_distance** (*float*) – The minimal distance this point needs to have from all boundaries.
- **coords** (*str*) – Determines the coordinate system in which the point is specified. Valid values are *cartesian*, *cell*, and *grid*; see `transform()`.
- **rng** (*Generator*) – Random number generator (default: `default_rng()`)

Returns

The coordinates of the point

Return type

`ndarray`

get_vector_data (*data*, ***kwargs*)

return data to visualize vector field

Parameters

- **data** (`ndarray`) – The vectorial values at the grid points
- ****kwargs** – Arguments forwarded to `get_image_data()`.

Returns

A dictionary with information about the data convenient for plotting.

Return type

`dict`

iter_mirror_points (*point*, *with_self*=False, *only_periodic*=True)

generates all mirror points corresponding to *point*

Parameters

- **point** (`ndarray`) – The point within the grid
- **with_self** (*bool*) – Whether to include the point itself
- **only_periodic** (*bool*) – Whether to only mirror along periodic axes

Returns

A generator yielding the coordinates that correspond to mirrors

Return type

Generator

plot (*args, title=None, filename=None, action='auto', ax_style=None, fig_style=None, ax=None, **kwargs)
visualize the grid

Parameters

- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically.
- **filename** (*str*, *optional*) – If given, the plot is written to the specified file.
- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **ax_style** (*dict*) – Dictionary with properties that will be changed on the axis after the plot has been drawn by calling `matplotlib.pyplot.setp()`. A special item in this dictionary is *use_offset*, which is a flag that can be used to control whether offsets are shown along the axes of the plot.
- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.
- **ax** (`matplotlib.axes.Axes`) – Figure axes to be used for plotting. The special value “create” creates a new figure, while “reuse” attempts to reuse an existing figure, which is the default.
- ****kwargs** – Extra arguments are passed on to the matplotlib plotting routines, e.g., to set the color of the lines

slice (*indices*)

return a subgrid of only the specified axes

Parameters

indices (*list*) – Indices indicating the axes that are retained in the subgrid

Returns

The subgrid

Return type

CartesianGrid

property state: `dict[str, Any]`

the state of the grid

Type

`dict`

property volume: `float`

total volume of the grid

Type

`float`

class UnitGrid (*shape*, *periodic=False*)

Bases: *CartesianGrid*

d-dimensional Cartesian grid with unit discretization in all directions

The grids can be thought of as a collection of d-dimensional cells of unit length. The *shape* parameter determines how many boxes there are in each direction. The cells are enumerated starting with 0, so the last cell has index

$n - 1$ if there are n cells along a dimension. A given cell i extends from coordinates i to $i + 1$, so the midpoint is at $i + \frac{1}{2}$, which is the cell coordinate. Taken together, the cells covers the interval $[0, n]$ along this dimension.

Parameters

- **shape** (*list*) – The number of support points for each axis. The dimension of the grid is given by `len(shape)`.
- **periodic** (*bool or list*) – Specifies which axes possess periodic boundary conditions. This is either a list of booleans defining periodicity for each individual axis or a single boolean value specifying the same periodicity for all axes.

classmethod `from_state` (*state*)

create a field from a stored *state*.

Parameters

state (*dict*) – The state from which the grid is reconstructed.

Return type

UnitGrid

slice (*indices*)

return a subgrid of only the specified axes

Parameters

indices (*list*) – Indices indicating the axes that are retained in the subgrid

Returns

The subgrid

Return type

UnitGrid

property `state`: `dict[str, Any]`

the state of the grid

Type

`dict`

to_cartesian ()

convert unit grid to *CartesianGrid*

Returns

The equivalent cartesian grid

Return type

CartesianGrid

4.2.6 pde.grids.cylindrical module

Cylindrical grids with azimuthal symmetry

class `CylindricalSymGrid` (*radius, bounds_z, shape, periodic_z=False*)

Bases: *GridBase*

3-dimensional cylindrical grid assuming polar symmetry

The polar symmetry implies that states only depend on the radial and axial coordinates r and z , respectively. These are discretized uniformly as

$$\begin{aligned} r_i &= R_{\text{inner}} + \left(i + \frac{1}{2}\right) \Delta r & \text{for } i = 0, \dots, N_r - 1 & \quad \text{with } \Delta r = \frac{R_{\text{outer}} - R_{\text{inner}}}{N_r} \\ z_j &= z_{\text{min}} + \left(j + \frac{1}{2}\right) \Delta z & \text{for } j = 0, \dots, N_z - 1 & \quad \text{with } \Delta z = \frac{z_{\text{max}} - z_{\text{min}}}{N_z} \end{aligned}$$

where R_{outer} is the outer radius of the grid, R_{inner} corresponds to a possible inner radius (which is zero by default), and z_{min} and z_{max} denote the respective lower and upper bounds of the axial direction, so that $z_{\text{max}} - z_{\text{min}}$ is the total height. The two axes are discretized by N_r and N_z support points, respectively.

Warning: The order of components in the vector and tensor fields defined on this grid are still (r, ϕ, z) . To avoid any confusion it might thus be best to access components by name instead of index, e.g., use `field['z']` instead of `field[2]`.

Parameters

- **radius** (*float or tuple of floats*) – radius R_{outer} in case a simple float is given. If a tuple is supplied it is interpreted as the inner and outer radius, $(R_{\text{inner}}, R_{\text{outer}})$.
- **bounds_z** (*tuple*) – The lower and upper bound of the z-axis
- **shape** (*tuple*) – The number of support points in r and z direction, respectively. The same number is used for both if a single value is given.
- **periodic_z** (*bool*) – Determines whether the z-axis has periodic boundary conditions.

boundary_names: `dict[str, tuple[int, bool]] = {'bottom': (1, False), 'inner': (0, False), 'outer': (0, True), 'top': (1, True)}`

Names of boundaries to select them conveniently

Type

`dict`

c: `CoordinatesBase = CylindricalCoordinates()`

Coordinates of the grid

Type

`CoordinatesBase`

cell_volume_data: `Sequence[FloatNumerical] | None`

Information about the size of discretization cells

Type

`list`

coordinate_constraints: `list[int] = [0, 1]`

axes that not described explicitly

Type

`list`

difference_vector (*p1, p2, *, coords='grid'*)

return Cartesian vector(s) pointing from p1 to p2

In case of periodic boundary conditions, the shortest vector is returned.

Parameters

- **p1** (`ndarray`) – First point(s)
- **p2** (`ndarray`) – Second point(s)
- **coords** (`str`) – The coordinate system in which the points are specified. Valid values are *cartesian*, *cell*, and *grid*; see `transform()`.

Returns

The difference vectors between the points with periodic boundary conditions applied.

Return type

`ndarray`

classmethod `from_bounds` (*bounds*, *shape*, *periodic*)

Parameters

- **bounds** (`tuple`) – Give the coordinate range for each axis. This should be a tuple of two number (lower and upper bound) for each axis. The length of *bounds* must be 2.
- **shape** (`tuple`) – The number of support points for each axis. The length of *shape* needs to be 2.
- **periodic** (`bool` or `list`) – Specifies which axes possess periodic boundary conditions. The first entry is ignored.

Returns

grid representing the region chosen by bounds

Return type

`CylindricalSymGrid`

classmethod `from_state` (*state*)

create a field from a stored *state*.

Parameters

state (`dict`) – The state from which the grid is reconstructed.

Return type

`CylindricalSymGrid`

get_cartesian_grid (*mode*=`'valid'`)

return a Cartesian grid for this Cylindrical one

Parameters

mode (`str`) – Determines how the grid is determined. Setting it to `'valid'` only returns points that are fully resolved in the cylindrical grid, e.g., the cylinder is circumscribed. Conversely, `'full'` returns all data, so the cylinder is inscribed.

Returns

The requested grid

Return type

`pde.grids.cartesian.CartesianGrid`

get_image_data (*data*)

return a 2d-image of the data

Parameters

data (`ndarray`) – The values at the grid points

Returns

A dictionary with information about the image, which is convenient for plotting.

Return type`dict`**get_line_data** (*data*, *extract*='auto')

return a line cut for the cylindrical grid

Parameters

- **data** (`ndarray`) – The values at the grid points
- **extract** (`str`) – Determines which cut is done through the grid. Possible choices are (default is *cut_axial*):
 - *cut_z* or *cut_axial*: values along the axial coordinate for $r = 0$.
 - *project_z* or *project_axial*: average values for each axial position (radial average).
 - *project_r* or *project_radial*: average values for each radial position (axial average)

Returns

A dictionary with information about the line cut, which is convenient for plotting.

Return type`dict`**get_random_point** (*, *boundary_distance*=0, *avoid_center*=False, *coords*='cartesian', *rng*=None)

return a random point within the grid

Parameters

- **boundary_distance** (`float`) – The minimal distance this point needs to have from all boundaries.
- **avoid_center** (`bool`) – Determines whether the boundary distance should also be kept from the center, i.e., whether points close to the center are returned.
- **coords** (`str`) – Determines the coordinate system in which the point is specified. Valid values are *cartesian*, *cell*, and *grid*; see `transform()`.
- **rng** (`Generator`) – Random number generator (default: `default_rng()`)

Returns

The coordinates of the point

Return type`ndarray`**property has_hole:** `bool`

whether the inner radius is larger than zero

Type`bool`**iter_mirror_points** (*point*, *with_self*=False, *only_periodic*=True)generates all mirror points corresponding to *point***Parameters**

- **point** (`ndarray`) – The point within the grid
- **with_self** (`bool`) – Whether to include the point itself
- **only_periodic** (`bool`) – Whether to only mirror along periodic axes

Returns

A generator yielding the coordinates that correspond to mirrors

Return type*Generator***property length:** `float`

length of the cylinder

Type`float`**property radius:** `float | tuple[float, float]`

radius of the sphere

Type`float`**slice** (*indices*)

return a subgrid of only the specified axes

Parameters**indices** (*list*) – Indices indicating the axes that are retained in the subgrid**Returns***CartesianGrid* or *PolarSymGrid*: The subgrid**Return type***CartesianGrid* | *PolarSymGrid***property state:** `dict[str, Any]`

all information required for reconstructing the grid

Type`dict`**property volume:** `float`

total volume of the grid

Type`float`

4.2.7 `pde.grids.spherical` module

Spherically-symmetric grids in 2 and 3 dimensions. These are grids that only discretize the radial direction, assuming symmetry with respect to all angles. This choice implies that differential operators might not be applicable to all fields. For instance, the divergence of a vector field on a spherical grid can only be represented as a scalar field on the same grid if the θ -component of the vector field vanishes.

class `PolarSymGrid` (*radius, shape*)

Bases: *SphericalSymGridBase*

2-dimensional polar grid assuming angular symmetry

The angular symmetry implies that states only depend on the radial coordinate r , which is discretized uniformly as

$$r_i = R_{\text{inner}} + \left(i + \frac{1}{2}\right) \Delta r \quad \text{for } i = 0, \dots, N-1 \quad \text{with} \quad \Delta r = \frac{R_{\text{outer}} - R_{\text{inner}}}{N}$$

where R_{outer} is the outer radius of the grid and R_{inner} corresponds to a possible inner radius, which is zero by default. The radial direction is discretized by N support points.

Parameters

- **radius** (*float or tuple of floats*) – Radius R_{outer} in case a simple float is given. If a tuple is supplied it is interpreted as the inner and outer radius, $(R_{\text{inner}}, R_{\text{outer}})$.
- **shape** (*tuple or int*) – The number N of support points along the radial coordinate.

c: `CoordinatesBase = PolarCoordinates()`

Coordinates of the grid

Type

`CoordinatesBase`

coordinate_constraints: `list[int] = [0, 1]`

axes that not described explicitly

Type

`list`

class SphericalSymGrid (*radius, shape*)

Bases: `SphericalSymGridBase`

3-dimensional spherical grid assuming spherical symmetry

The symmetry implies that states only depend on the radial coordinate r , which is discretized as follows:

$$r_i = R_{\text{inner}} + \left(i + \frac{1}{2}\right) \Delta r \quad \text{for } i = 0, \dots, N-1 \quad \text{with} \quad \Delta r = \frac{R_{\text{outer}} - R_{\text{inner}}}{N}$$

where R_{outer} is the outer radius of the grid and R_{inner} corresponds to a possible inner radius, which is zero by default. The radial direction is discretized by N support points.

Warning: Not all results of differential operators on vectorial and tensorial fields can be expressed in terms of fields that only depend on the radial coordinate r . In particular, the gradient of a vector field can only be calculated if the azimuthal component of the vector field vanishes. Similarly, the divergence of a tensor field can only be taken in special situations.

Parameters

- **radius** (*float or tuple of floats*) – Radius R_{outer} in case a simple float is given. If a tuple is supplied it is interpreted as the inner and outer radius, $(R_{\text{inner}}, R_{\text{outer}})$.
- **shape** (*tuple or int*) – The number N of support points along the radial coordinate.

c: `CoordinatesBase = SphericalCoordinates()`

Coordinates of the grid

Type

`CoordinatesBase`

coordinate_constraints: `list[int] = [0, 1, 2]`

axes that not described explicitly

Type

`list`

class SphericalSymGridBase (*radius, shape*)

Bases: `GridBase`

Base class for d-dimensional spherical grids with angular symmetry

The angular symmetry implies that states only depend on the radial coordinate r , which is discretized uniformly as

$$r_i = R_{\text{inner}} + \left(i + \frac{1}{2}\right) \Delta r \quad \text{for } i = 0, \dots, N-1 \quad \text{with } \Delta r = \frac{R_{\text{outer}} - R_{\text{inner}}}{N}$$

where R_{outer} is the outer radius of the grid and R_{inner} corresponds to a possible inner radius, which is zero by default. The radial direction is discretized by N support points.

Parameters

- **radius** (*float or tuple of floats*) – Radius R_{outer} in case a simple float is given. If a tuple is supplied it is interpreted as the inner and outer radius, $(R_{\text{inner}}, R_{\text{outer}})$.
- **shape** (*tuple or int*) – The number N of support points along the radial coordinate.

boundary_names: `dict[str, tuple[int, bool]] = {'inner': (0, False), 'outer': (0, True)}`

Names of boundaries to select them conveniently

Type

`dict`

cell_volume_data: `Sequence[FloatNumerical] | None`

Information about the size of discretization cells

Type

`list`

classmethod from_bounds (*bounds, shape, periodic*)

Parameters

- **bounds** (*tuple*) – Give the coordinate range for the radial axis.
- **shape** (*tuple*) – The number of support points for the radial axis
- **periodic** (*tuple[bool]*) –

Returns

represents the region chosen by bounds

Return type

`SphericalGridBase`

classmethod from_state (*state*)

create a field from a stored *state*.

Parameters

state (*dict*) – The state from which the grid is reconstructed.

Return type

`SphericalSymGridBase`

get_cartesian_grid (*mode='valid', num=None*)

return a Cartesian grid for this spherical one

Parameters

- **mode** (*str*) – Determines how the grid is determined. Setting it to ‘valid’ (or ‘inscribed’) only returns points that are fully resolved in the spherical grid, e.g., the Cartesian grid is inscribed in the sphere. Conversely, ‘full’ (or ‘circumscribed’) returns all data, so the Cartesian grid is circumscribed.
- **num** (*int*) – Number of support points along each axis of the returned grid.

Returns

The requested grid

Return type

`pde.grids.cartesian.CartesianGrid`

get_image_data (*data*, *, *performance_goal*='speed', *fill_value*=0, *masked*=True)

return a 2d-image of the data

Parameters

- **data** (`ndarray`) – The values at the grid points
- **performance_goal** (`str`) – Determines the method chosen for interpolation. Possible options are *speed* and *quality*.
- **fill_value** (`float`) – The value assigned to invalid positions (those inside the hole or outside the region).
- **masked** (`bool`) – Whether a `numpy.ma.MaskedArray` is returned for the data instead of the normal `ndarray`.

Returns

dict: A dictionary with information about the image, which is convenient for plotting.

Return type

`dict[str, Any]`

get_line_data (*data*, *extract*='auto')

return a line cut along the radial axis

Parameters

- **data** (`ndarray`) – The values at the grid points
- **extract** (`str`) – Determines which cut is done through the grid. This parameter is mainly supplied for a consistent interface and has no effect for polar grids.

Returns

A dictionary with information about the line cut, which is convenient for plotting.

Return type

`dict[str, Any]`

get_random_point (*, *boundary_distance*=0, *avoid_center*=False, *coords*='cartesian', *rng*=None)

return a random point within the grid

Note that these points will be uniformly distributed in the volume, implying they are not uniformly distributed on the radial axis.

Parameters

- **boundary_distance** (`float`) – The minimal distance this point needs to have from all boundaries.
- **avoid_center** (`bool`) – Determines whether the boundary distance should also be kept from the center, i.e., whether points close to the center are returned.
- **coords** (`str`) – Determines the coordinate system in which the point is specified. Valid values are *cartesian*, *cell*, and *grid*; see `transform()`.
- **rng** (`Generator`) – Random number generator (default: `default_rng()`)

Returns

The coordinates of the point

Return type`ndarray`**property** `has_hole`: `bool`

returns whether the inner radius is larger than zero

plot (*args, title=None, filename=None, action='auto', ax_style=None, fig_style=None, ax=None, **kwargs)

visualize the spherically symmetric grid in two dimensions

Parameters

- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically.
- **filename** (*str*, *optional*) – If given, the plot is written to the specified file.
- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **ax_style** (*dict*) – Dictionary with properties that will be changed on the axis after the plot has been drawn by calling `matplotlib.pyplot.setp()`. A special item in this dictionary is *use_offset*, which is a flag that can be used to control whether offsets are shown along the axes of the plot.
- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.
- **ax** (`matplotlib.axes.Axes`) – Figure axes to be used for plotting. The special value “create” creates a new figure, while “reuse” attempts to reuse an existing figure, which is the default.
- ****kwargs** – Extra arguments are passed on to the matplotlib plotting routines, e.g., to set the color of the lines

property `radius`: `float` | `tuple[float, float]`

radius of the sphere

Type`float`**property** `state`: `dict[str, Any]`

the state of the grid

Type`state`**property** `volume`: `float`

total volume of the grid

Type`float`**volume_from_radius** (*radius*, *dim*)

Return the volume of a sphere with a given radius

Parameters

- **radius** (`float` or `ndarray`) – Radius of the sphere
- **dim** (*int*) – Dimension of the space

Returns

Volume of the sphere

Return typefloat or `ndarray`

4.3 pde.pdes package

Package that defines PDEs describing physical systems.

The examples in this package are often simple version of classical PDEs to demonstrate various aspects of the *py-pde* package. Clearly, not all extensions to these PDEs can be covered here, but this should serve as a starting point for custom investigations.

Publicly available methods should take fields with grid information and also only return such methods. There might be corresponding private methods that deal with raw data for faster simulations.

<i>PDE</i>	PDE defined by mathematical expressions
<i>AllenCahnPDE</i>	A simple Allen-Cahn equation
<i>CahnHilliardPDE</i>	A simple Cahn-Hilliard equation
<i>DiffusionPDE</i>	A simple diffusion equation
<i>KPZInterfacePDE</i>	The Kardar–Parisi–Zhang (KPZ) equation
<i>KuramotoSivashinskyPDE</i>	The Kuramoto-Sivashinsky equation
<i>SwiftHohenbergPDE</i>	The Swift-Hohenberg equation
<i>WavePDE</i>	A simple wave equation

Additionally, we offer two solvers for typical elliptical PDEs:

<i>solve_laplace_equation</i>	Solve Laplace's equation on a given grid.
<i>solve_poisson_equation</i>	Solve Laplace's equation on a given grid

4.3.1 pde.pdes.allen_cahn module

A Allen-Cahn equation

class `AllenCahnPDE` (*interface_width*=1, *bc*='auto_periodic_neumann')

Bases: `PDEBase`

A simple Allen-Cahn equation

The mathematical definition is

$$\partial_t c = \gamma \nabla^2 c - c^3 + c$$

where c is a scalar field and γ sets the (squared) interfacial width.

Parameters

- **interface_width** (*float*) – The diffusivity of the described species
- **bc** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end

(using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value `NUM` (specified by `{'value': NUM}`) and Neumann conditions enforcing the value `DERIV` for the derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).

evolution_rate (*state*, *t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (`ScalarField`) – The scalar field describing the concentration distribution
- **t** (`float`) – The current time point

Returns

Scalar field describing the evolution rate of the PDE

Return type

`ScalarField`

explicit_time_dependence: `bool | None = False`

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

`bool`

property expression: `str`

the expression of the right hand side of this PDE

Type

`str`

interface_width: `float`

4.3.2 pde.pdes.base module

Base class for defining partial differential equations

class PDEBase (*, *noise=0*, *rng=None*)

Bases: `object`

base class for defining partial differential equations (PDEs)

Custom PDEs can be implemented by subclassing `PDEBase` to specify the evolution rate. In the simple case of deterministic PDEs, the methods `PDEBase.evolution_rate()` and `PDEBase._make_pde_rhs_numba()` need to be overwritten for supporting the *numpy* and *numba* backend, respectively.

Parameters

- **noise** (`float` or `ndarray`) – Variance of the additive Gaussian white noise that is supported for all PDEs by default. If set to zero, a deterministic partial differential equation will be solved. Different noise magnitudes can be supplied for each field in coupled PDEs.
- **rng** (`Generator`) – Random number generator (default: `default_rng()`) used for stochastic simulations. Note that this random number generator is only used for *numpy* function, while compiled *numba* code uses the random number generator of *numba*. Moreover, in simulations using multiprocessing, setting the same generator in all processes might yield unintended correlations in the simulation results.

Note: If more complicated noise structures are required, the methods `PDEBase.noise_realization()` and `PDEBase._make_noise_realization_numba()` need to be overwritten for the *numpy* and *numba* backend, respectively.

cache_rhs: `bool = False`

Flag indicating whether the right hand side of the equation should be cached. If True, the same implementation is used in subsequent calls to *solve*. Note that the cache is only invalidated when the grid of the underlying state changes. Consequently, the simulation might lead to wrong results if the parameters of the PDE are changed after the first call. This option is thus disabled by default and should be used with care.

Type

`bool`

check_implementation: `bool = True`

Flag determining whether numba-compiled functions should be checked against their numpy counter-parts. This can help with implementing a correct compiled version for a PDE class.

Type

`bool`

check_rhs_consistency (*state*, *t=0*, *, *tol=1e-07*, *rhs_numba=None*, ***kwargs*)

check the numba compiled right hand side versus the numpy variant

Parameters

- **state** (*FieldBase*) – The state for which the evolution rates should be compared
- **t** (*float*) – The associated time point
- **tol** (*float*) – Acceptance tolerance. The check passes if the evolution rates differ by less than this value
- **rhs_numba** (*callable*) – The implementation of the numba variant that is to be checked. If omitted, an implementation is obtained by calling `PDEBase._make_pde_rhs_numba_cached()`.

Return type

`None`

complex_valued: `bool = False`

Flag indicating whether the right hand side is a complex-valued PDE, which requires all involved variables to have complex data type.

Type

`bool`

diagnostics: `dict[str, Any]`

Diagnostic information (available after the PDE has been solved)

Type

`dict`

abstract evolution_rate (*state*, *t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*FieldBase*) – The field at the current time point
- **t** (*float*) – The current time point

Returns

Field describing the evolution rate of the PDE

Return type

FieldBase

explicit_time_dependence: `bool` | `None` = `None`

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

`bool`

property is_sde: `bool`

flag indicating whether this is a stochastic differential equation

The `BasePDF` class supports additive Gaussian white noise, whose magnitude is controlled by the *noise* property. In this case, *is_sde* is *True* if *self.noise* != 0.

Type

`bool`

make_modify_after_step (*state*)

returns a function that can be called to modify a state

This function is applied to the state after each integration step when an explicit stepper is used. The default behavior is to not change the state.

Parameters

state (*FieldBase*) – An example for the state from which the grid and other information can be extracted

Returns

Function that can be applied to a state to modify it and which returns a measure for the corrections applied to the state

Return type

Callable[[*ndarray*], *float*]

make_pde_rhs (*state*, *backend*='auto', ***kwargs*)

return a function for evaluating the right hand side of the PDE

Parameters

- **state** (*FieldBase*) – An example for the state from which the grid and other information can be extracted.
- **backend** (*str*) – Determines how the function is created. Accepted values are 'numpy' and 'numba'. Alternatively, 'auto' lets the code pick the optimal backend.

Returns

Function determining the right hand side of the PDE

Return type

callable

make_sde_rhs (*state*, *backend*='auto', ***kwargs*)

return a function for evaluating the right hand side of the SDE

Parameters

- **state** (*FieldBase*) – An example for the state from which information can be extracted

- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code pick the optimal backend.

Returns

Function determining the deterministic part of the right hand side of the PDE together with a noise realization.

Return type

Callable[[*ndarray*, *float*], *tuple*[*ndarray*, *ndarray*]]

noise_realization (*state*, *t=0*, *, *label*=‘Noise realization’)

returns a realization for the noise

Parameters

- **state** (*ScalarField*) – The scalar field describing the concentration distribution
- **t** (*float*) – The current time point
- **label** (*str*) – The label for the returned field

Returns

Scalar field describing the evolution rate of the PDE

Return type

ScalarField

solve (*state*, *t_range*, *dt=None*, *tracker*=‘auto’, *, *solver*=‘explicit’, *ret_info=False*, ***kwargs*)

solves the partial differential equation

The method constructs a suitable solver (*SolverBase*) and controller (*Controller*) to advance the state over the temporal range specified by *t_range*. This method only exposes the most common functions, so explicit construction of these classes might offer more flexibility.

Parameters

- **state** (*FieldBase*) – The initial state (which also defines the spatial grid).
- **t_range** (*float or tuple*) – Sets the time range for which the PDE is solved. This should typically be a tuple of two numbers, (*t_start*, *t_end*), specifying the initial and final time of the simulation. If only a single value is given, it is interpreted as *t_end* and the time range is (*0*, *t_end*).
- **dt** (*float*) – Time step of the chosen stepping scheme. If *None*, a default value based on the stepper will be chosen. If an adaptive stepper is used (supported by *ScipySolver* and *ExplicitSolver*), *dt* sets the initial time step.
- **tracker** (*TrackerCollectionDataType*) – Defines trackers that process the state of the simulation at specified times. A tracker is either an instance of *TrackerBase* or a string identifying a tracker (possible identifiers can be obtained by calling *get_named_trackers()*). Multiple trackers can be specified as a list. The default value *auto* checks the state for consistency (tracker ‘consistency’) and displays a progress bar (tracker ‘progress’) when *tqdm* is installed. More general trackers are defined in *trackers*, where all options are explained in detail. In particular, the time points where the tracker analyzes data can be chosen when creating a tracker object explicitly.
- **solver** (*SolverBase* or *str*) – Specifies the method for solving the differential equation. This can either be an instance of *SolverBase* or a descriptive name like ‘explicit’ or ‘scipy’. The valid names are given by *pde.solvers.registered_solvers()*. Details of the solvers and additional features (like adaptive time steps) are explained in *solvers*.

- **ret_info** (*bool*) – Flag determining whether diagnostic information about the solver process should be returned. Note that the same information is also available as the *diagnostics* attribute.
- ****kwargs** – Additional keyword arguments are forwarded to the solver class chosen with the *solver* argument. In particular, *ExplicitSolver* supports several *schemes* and an adaptive stepper can be enabled using *adaptive=True*. Conversely, *ScipySolver* accepts the additional arguments of *scipy.integrate.solve_ivp()*.

Returns

The state at the final time point. If *ret_info == True*, a tuple with the final state and a dictionary with additional information is returned. Note that *None* instead of a field is returned in multiprocessing simulations if the current node is not the main MPI node.

Return type

FieldBase

expr_prod (*factor, expression*)

helper function for building an expression with an (optional) pre-factor

Parameters

- **factor** (*float*) – The value of the prefactor
- **expression** (*str*) – The remaining expression

Returns

The expression with the factor appended if necessary

Return type

str

4.3.3 pde.pdes.cahn_hilliard module

A Cahn-Hilliard equation

```
class CahnHilliardPDE (interface_width=1, bc_c='auto_periodic_neumann',
                      bc_mu='auto_periodic_neumann')
```

Bases: *PDEBase*

A simple Cahn-Hilliard equation

The mathematical definition is

$$\partial_t c = \nabla^2 (c^3 - c - \gamma \nabla^2 c)$$

where *c* is a scalar field taking values on the interval $[-1, 1]$ and γ sets the (squared) interfacial width.

Parameters

- **interface_width** (*float*) – The width of the interface between the separated phases. This defines a characteristic length in the simulation. The grid needs to resolve this length of a stable simulation.
- **bc_c** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by *{‘value’: NUM}*) and Neumann conditions enforcing the value *DERIV* for the

derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).

- **bc_mu** (*BoundariesData*) – The boundary conditions applied to the chemical potential associated with the scalar field *c*. Supports the same options as *bc_c*.

evolution_rate (*state*, *t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*ScalarField*) – The scalar field describing the concentration distribution
- **t** (*float*) – The current time point

Returns

Scalar field describing the evolution rate of the PDE

Return type

ScalarField

explicit_time_dependence: *bool* | *None* = *False*

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

bool

property expression: *str*

the expression of the right hand side of this PDE

Type

str

4.3.4 `pde.pdes.diffusion` module

A simple diffusion equation

class `DiffusionPDE` (*diffusivity=1*, *, *bc='auto_periodic_neumann'*, *noise=0*, *rng=None*)

Bases: *PDEBase*

A simple diffusion equation

The mathematical definition is

$$\partial_t c = D \nabla^2 c$$

where *c* is a scalar field and *D* denotes the diffusivity.

Parameters

- **diffusivity** (*float*) – The diffusivity of the described species
- **bc** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by 'periodic' and 'anti-periodic'). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{'value': NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note

that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).

- **noise** (*float*) – Variance of the (additive) noise term
- **rng** (*Generator*) – Random number generator (default: `default_rng()`) used for stochastic simulations. Note that this random number generator is only used for numpy function, while compiled numba code uses the random number generator of numba. Moreover, in simulations using multiprocessing, setting the same generator in all processes might yield unintended correlations in the simulation results.

evolution_rate (*state*, *t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*ScalarField*) – The scalar field describing the concentration distribution
- **t** (*float*) – The current time point

Returns

Scalar field describing the evolution rate of the PDE

Return type

ScalarField

explicit_time_dependence: *bool* | *None* = *False*

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

bool

property expression: *str*

the expression of the right hand side of this PDE

Type

str

4.3.5 `pde.pdes.kpz_interface` module

The Kardar–Parisi–Zhang (KPZ) equation describing the evolution of an interface

class `KPZInterfacePDE` (*nu=0.5*, *lmbda=1*, ***, *bc='auto_periodic_neumann'*, *noise=0*, *rng=None*)

Bases: *PDEBase*

The Kardar–Parisi–Zhang (KPZ) equation

The mathematical definition is

$$\partial_t h = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(\mathbf{r}, t)$$

where h is the height of the interface in Monge parameterization. The dynamics are governed by the two parameters ν and λ , while η is Gaussian white noise, whose strength is controlled by the *noise* argument.

Parameters

- **nu** (*float*) – Parameter ν for the strength of the diffusive term
- **lmbda** (*float*) – Parameter λ for the strenth of the gradient term

- **bc** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **noise** (*float*) – Variance of the (additive) noise term
- **rng** (*Generator*) – Random number generator (default: `default_rng()`) used for stochastic simulations. Note that this random number generator is only used for numpy function, while compiled numba code uses the random number generator of numba. Moreover, in simulations using multiprocessing, setting the same generator in all processes might yield unintended correlations in the simulation results.

evolution_rate (*state*, *t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*ScalarField*) – The scalar field describing the concentration distribution
- **t** (*float*) – The current time point

Returns

Scalar field describing the evolution rate of the PDE

Return type

ScalarField

explicit_time_dependence: `bool | None = False`

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

`bool`

property expression: `str`

the expression of the right hand side of this PDE

Type

`str`

4.3.6 pde.pdes.kuramoto_sivashinsky module

The Kardar–Parisi–Zhang (KPZ) equation describing the evolution of an interface

class KuramotoSivashinskyPDE (*nu=1*, ***, *bc='auto_periodic_neumann'*, *bc_lap=None*, *noise=0*, *rng=None*)

Bases: *PDEBase*

The Kuramoto-Sivashinsky equation

The mathematical definition is

$$\partial_t u = -\nu \nabla^4 u - \nabla^2 u - \frac{1}{2} (\nabla h)^2 + \eta(\mathbf{r}, t)$$

where u is the height of the interface in Monge parameterization. The dynamics are governed by the parameters ν , while η is Gaussian white noise, whose strength is controlled by the *noise* argument.

Parameters

- **nu** (*float*) – Parameter ν for the strength of the fourth-order term
- **bc** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **bc_lap** (*BoundariesData* | *None*) – The boundary conditions applied to the second derivative of the scalar field c . If *None*, the same boundary condition as *bc* is chosen. Otherwise, this supports the same options as *bc*.
- **noise** (*float*) – Variance of the (additive) noise term
- **rng** (*Generator*) – Random number generator (default: `default_rng()`) used for stochastic simulations. Note that this random number generator is only used for numpy function, while compiled numba code uses the random number generator of numba. Moreover, in simulations using multiprocessing, setting the same generator in all processes might yield unintended correlations in the simulation results.

evolution_rate (*state*, *t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*ScalarField*) – The scalar field describing the concentration distribution
- **t** (*float*) – The current time point

Returns

Scalar field describing the evolution rate of the PDE

Return type

ScalarField

explicit_time_dependence: *bool* | *None* = *False*

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

bool

property expression: *str*

the expression of the right hand side of this PDE

Type

str

4.3.7 `pde.pdes.laplace` module

Solvers for Poisson's and Laplace's equation

`solve_laplace_equation` (*grid*, *bc*, *label*="Solution to Laplace's equation")

Solve Laplace's equation on a given grid.

This is implemented by calling `solve_poisson_equation()` with a vanishing right hand side.

Parameters

- **`grid`** (*GridBase*) – The grid on which the equation is solved
- **`bc`** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by 'periodic' and 'anti-periodic'). For non- periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value *NUM* (specified by `{'value': NUM}`) and Neumann conditions enforcing the value *DERIV* for the derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **`label`** (*str*) – The label of the returned field.

Returns

The field that solves the equation. This field will be defined on the given *grid*.

Return type

ScalarField

`solve_poisson_equation` (*rhs*, *bc*, *label*="Solution to Poisson's equation", ***kwargs*)

Solve Laplace's equation on a given grid

Denoting the current field by *u*, we thus solve for *f*, defined by the equation

$$\nabla^2 u(\mathbf{r}) = -f(\mathbf{r})$$

with boundary conditions specified by *bc*.

Note: In case of periodic or Neumann boundary conditions, the right hand side $f(\mathbf{r})$ needs to satisfy the following condition

$$\int f \, dV = \oint g \, dS ,$$

where *g* denotes the function specifying the outwards derivative for Neumann conditions. Note that for periodic boundaries *g* vanishes, so that this condition implies that the integral over *f* must vanish for neutral Neumann or periodic conditions.

Parameters

- **`rhs`** (*ScalarField*) – The scalar field *f* describing the right hand side
- **`bc`** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by 'periodic' and 'anti-periodic'). For non- periodic axes, different boundary conditions can be specified for the lower and upper end

(using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value `NUM` (specified by `{'value': NUM}`) and Neumann conditions enforcing the value `DERIV` for the derivative in the normal direction (specified by `{'derivative': DERIV}`) are supported. Note that the special value 'natural' imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).

- **label** (*str*) – The label of the returned field.

Returns

The field u that solves the equation. This field will be defined on the same grid as *rhs*.

Return type

ScalarField

4.3.8 `pde.pdes.pde` module

Defines a PDE class whose right hand side is given as a string

```
class PDE (rhs, *, bc='auto_periodic_neumann', bc_ops=None, user_funcs=None, consts=None, noise=0,
           rng=None)
```

Bases: *PDEBase*

PDE defined by mathematical expressions

variables

The name of the variables (i.e., fields) in the order they are expected to appear in the *state*.

Type

tuple

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **rhs** (*dict*) – The expressions defining the evolution rate. The dictionary keys define the name of the fields whose evolution is considered, while the values specify their evolution rate as a string that can be parsed by *sympy*. These expression may contain variables (i.e., the fields themselves, spatial coordinates of the grid, and t for the time), standard local mathematical operators defined by *sympy*, and the operators defined in the *pde* package. Note that operators need to be specified with their full name, i.e., *laplace* for a scalar Laplacian and *vector_laplace* for a Laplacian operating on a vector field. Moreover, the dot product between two vector fields can be denoted by using *dot(field1, field2)* in the expression, an outer product is calculated using *outer(field1, field2)*, and *integral(field)* denotes an integral over a field. More information can be found in the [expression documentation](#).
- **bc** (*BoundariesData*) – Boundary conditions for the operators used in the expression. The conditions here are applied to all operators that do not have a specialized condition given in *bc_ops*. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by 'periodic' and 'anti-periodic'). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value `NUM` (specified by `{'value': NUM}`) and Neumann conditions enforcing the value `DERIV` for the derivative in the normal direction (specified by `{'derivative': DERIV}`)

are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).

- **bc_ops** (*dict*) – Special boundary conditions for some operators. The keys in this dictionary specify where the boundary condition will be applied. The keys follow the format “VARIABLE:OPERATOR”, where VARIABLE specifies the expression in *rhs* where the boundary condition is applied to the operator specified by OPERATOR. For both identifiers, the wildcard symbol “*” denotes that all fields and operators are affected, respectively. For instance, the identifier “c:*” allows specifying a condition for all operators of the field named *c*.
- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that can be used in the expressions in *rhs*.
- **consts** (*dict*, *optional*) – A dictionary with user defined constants that can be used in the expression. These can be either scalar numbers or fields defined on the same grid as the actual simulation.
- **noise** (float or *ndarray*) – Variance of additive Gaussian white noise. The default value of zero implies deterministic partial differential equations will be solved. Different noise magnitudes can be supplied for each field in coupled PDEs by either specifying a sequence of numbers or a dictionary with values for each field.
- **rng** (*Generator*) – Random number generator (default: `default_rng()`) used for stochastic simulations. Note that this random number generator is only used for numpy function, while compiled numba code uses the random number generator of numba. Moreover, in simulations using multiprocessing, setting the same generator in all processes might yield unintended correlations in the simulation results.

Note: The order in which the fields are given in *rhs* defines the order in which they need to appear in the *state* variable when the evolution rate is calculated. Note that *dict* keep the insertion order since Python version 3.7, so a normal dictionary can be used to define the equations.

evolution_rate (*state*, *t=0.0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*FieldBase*) – The field describing the state of the PDE
- **t** (*float*) – The current time point

Returns

Field describing the evolution rate of the PDE

Return type

FieldBase

property expressions: `dict[str, str]`

show the expressions of the PDE

4.3.9 `pde.pdes.swift_hohenberg` module

The Swift-Hohenberg equation

```
class SwiftHohenbergPDE (rate=0.1, kc2=1.0, delta=1.0, *, bc='auto_periodic_neumann', bc_lap=None)
```

Bases: `PDEBase`

The Swift-Hohenberg equation

The mathematical definition is

$$\partial_t c = \left[\epsilon - (k_c^2 + \nabla^2)^2 \right] c + \delta c^2 - c^3$$

where c is a scalar field and ϵ , k_c^2 , and δ are parameters of the equation.

Parameters

- **rate** (*float*) – The bifurcation parameter ϵ
- **kc2** (*float*) – Squared wave vector k_c^2 of the linear instability
- **delta** (*float*) – Parameter δ of the non-linearity
- **bc** (*BoundariesData*) – The boundary conditions applied to the field. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **bc_lap** (*BoundariesData | None*) – The boundary conditions applied to the second derivative of the scalar field c . If *None*, the same boundary condition as *bc* is chosen. Otherwise, this supports the same options as *bc*.

```
evolution_rate (state, t=0)
```

evaluate the right hand side of the PDE

Parameters

- **state** (*ScalarField*) – The scalar field describing the concentration distribution
- **t** (*float*) – The current time point

Returns

Scalar field describing the evolution rate of the PDE

Return type

`ScalarField`

```
explicit_time_dependence: bool | None = False
```

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type

`bool`

```
property expression: str
```

the expression of the right hand side of this PDE

Type
str

4.3.10 pde.pdes.wave module

A simple wave equation

class **WavePDE** (*speed=1, bc='auto_periodic_neumann'*)

Bases: *PDEBase*

A simple wave equation

The mathematical definition, $\partial_t^2 u = c^2 \nabla^2 u$, is implemented as two first-order equations,

$$\begin{aligned}\partial_t u &= v \\ \partial_t v &= c^2 \nabla^2 u\end{aligned}$$

where c sets the wave speed and v is an auxiliary field. Note that the class expects an initial condition specifying both fields, which can be created using the `WavePDE.get_initial_condition()` method. The result will also return two fields.

Parameters

- **speed** (*float*) – The speed c of the wave
- **bc** (*BoundariesData*) – The boundary conditions applied to the field u . Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non-periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value NUM (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value DERIV for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).

evolution_rate (*state, t=0*)

evaluate the right hand side of the PDE

Parameters

- **state** (*FieldCollection*) – The fields u and v
- **t** (*float*) – The current time point

Returns

Fields describing the evolution rates of the PDE

Return type

FieldCollection

explicit_time_dependence: *bool* | *None* = *False*

Flag indicating whether the right hand side of the PDE has an explicit time dependence.

Type
bool

property expressions: *dict[str, str]*

the expressions of the right hand side of this PDE

Type

dict

get_initial_condition (*u*, *v=None*)

create a suitable initial condition

Parameters

- **u** (*ScalarField*) – The initial density on the grid
- **v** (*ScalarField*, optional) – The initial rate of change. This is assumed to be zero if the value is omitted.

ReturnsThe combined fields *u* and *v*, suitable for the simulation**Return type**

FieldCollection

4.4 pde.solvers package

Solvers define how a PDE is solved, i.e., how the initial state is advanced in time.

<i>Controller</i>	class controlling a simulation
<i>ExplicitSolver</i>	various explicit PDE solvers
<i>ExplicitMPSolver</i>	various explicit PDE solve using MPI
<i>ImplicitSolver</i>	implicit (backward) Euler PDE solver
<i>CrankNicolsonSolver</i>	Crank-Nicolson solver
<i>AdamsBashforthSolver</i>	explicit Adams-Bashforth multi-step solver
<i>ScipySolver</i>	PDE solver using <code>scipy.integrate.solve_ivp()</code> .
<i>registered_solvers</i>	returns all solvers that are currently registered

class AdamsBashforthSolver (*pde*, *, *backend='auto'*)

Bases: *SolverBase*

explicit Adams-Bashforth multi-step solver

Parameters

- **pde** (*PDEBase*) – The partial differential equation that should be solved
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.

name = 'adams-bashforth'

class Controller (*solver*, *t_range*, *tracker='auto'*)

Bases: *object*

class controlling a simulation

The controller calls a solver to advance the simulation into the future and it takes care of trackers that analyze and modify the state periodically.

Parameters

- **solver** (*SolverBase*) – Solver instance that is used to advance the simulation in time

- **t_range** (*float or tuple*) – Sets the time range for which the simulation is run. If only a single value *t_end* is given, the time range is assumed to be $[0, t_{end}]$.
- **tracker** (*TrackerCollectionDataType*) – Defines trackers that process the state of the simulation at specified times. A tracker is either an instance of *TrackerBase* or a string identifying a tracker (possible identifiers can be obtained by calling *get_named_trackers()*). Multiple trackers can be specified as a list. The default value *auto* checks the state for consistency (tracker ‘consistency’) and displays a progress bar (tracker ‘progress’) when *tqdm* is installed. More general trackers are defined in *trackers*, where all options are explained in detail. In particular, the time points where the tracker analyzes data can be chosen when creating a tracker object explicitly.

diagnostics: `dict[str, Any]`

diagnostic information (available after simulation finished)

Type

`dict`

run (*initial_state, dt=None*)

run the simulation

Diagnostic information about the solver are available in the *diagnostics* property after this function has been called.

Parameters

- **initial_state** (*FieldBase*) – The initial state of the simulation. This state will be copied and thus not modified by the simulation. Instead, the final state will be returned and trackers can be used to record intermediate states.
- **dt** (*float*) – Time step of the chosen stepping scheme. If *None*, a default value based on the stepper will be chosen.

Returns

The state at the final time point. If multiprocessing is used, only the main node will return the state. All other nodes return *None*.

Return type

TState | *None*

property t_range: `tuple[float, float]`

start and end time of the simulation

Type

`tuple`

class CrankNicolsonSolver (*pde, *, maxiter=100, maxerror=0.0001, explicit_fraction=0, backend='auto'*)

Bases: *SolverBase*

Crank-Nicolson solver

Parameters

- **pde** (*PDEBase*) – The instance describing the pde that needs to be solved
- **maxiter** (*int*) – The maximal number of iterations per step
- **maxerror** (*float*) – The maximal error that is permitted in each step
- **explicit_fraction** (*float*) – Hyperparameter determining the fraction of explicit time stepping in the implicit step. *explicit_fraction == 0* is the simple Crank-Nicolson scheme, while *explicit_fraction == 1* reduces to the explicit Euler method. Intermediate values can improve convergence.

- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.

name = 'crank-nicolson'

class ExplicitSolver (*pde, scheme='euler', *, backend='auto', adaptive=False, tolerance=0.0001*)

Bases: *AdaptiveSolverBase*

various explicit PDE solvers

Parameters

- **pde** (*PDEBase*) – The instance describing the pde that needs to be solved
- **scheme** (*str*) – Defines the explicit scheme to use. Supported values are ‘euler’ and ‘runge-kutta’ (or ‘rk’ for short).
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.
- **adaptive** (*bool*) – When enabled, the time step is adjusted during the simulation using the error tolerance set with *tolerance*.
- **tolerance** (*float*) – The error tolerance used in adaptive time stepping. This is used in adaptive time stepping to choose a time step which is small enough so the truncation error of a single step is below *tolerance*.

name = 'explicit'

class ImplicitSolver (*pde, maxiter=100, maxerror=0.0001, backend='auto'*)

Bases: *SolverBase*

implicit (backward) Euler PDE solver

Parameters

- **pde** (*PDEBase*) – The instance describing the pde that needs to be solved
- **maxiter** (*int*) – The maximal number of iterations per step
- **maxerror** (*float*) – The maximal error that is permitted in each step
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.

name = 'implicit'

class ScipySolver (*pde, backend='auto', **kwargs*)

Bases: *SolverBase*

PDE solver using `scipy.integrate.solve_ivp()`.

This class is a thin wrapper around `scipy.integrate.solve_ivp()`. In particular, it supports all the methods implemented by this function and exposes its arguments, so details can be controlled.

Parameters

- **pde** (*PDEBase*) – The instance describing the pde that needs to be solved
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.
- ****kwargs** – All extra arguments are forwarded to `scipy.integrate.solve_ivp()`.

make_stepper (*state*, *dt=None*)

return a stepper function

Parameters

- **state** (`FieldBase`) – An example for the state from which the grid and other information can be extracted.
- **dt** (`float`) – Initial time step for the simulation. If *None*, the solver will choose a suitable initial value.

Returns

Function that can be called to advance the *state* from time *t_start* to time *t_end*.

Return type

`Callable[[FieldBase, float, float], float]`

name = 'scipy'

registered_solvers ()

returns all solvers that are currently registered

Returns

List with the names of the solvers

Return type

list of `str`

4.4.1 `pde.solvers.adams_bashforth` module

Defines an explicit Adams-Bashforth solver

class `AdamsBashforthSolver` (*pde*, *, *backend='auto'*)

Bases: `SolverBase`

explicit Adams-Bashforth multi-step solver

Parameters

- **pde** (`PDEBase`) – The partial differential equation that should be solved
- **backend** (`str`) – Determines how the function is created. Accepted values are 'numpy' and 'numba'. Alternatively, 'auto' lets the code decide for the most optimal backend.

info: `dict[str, Any]`

name = 'adams-bashforth'

4.4.2 `pde.solvers.base` module

Package that contains base classes for solvers.

Beside the abstract base class defining the interfaces, we also provide `AdaptiveSolverBase`, which contains methods for implementing adaptive solvers.

class `AdaptiveSolverBase` (*pde*, *, *backend='auto'*, *adaptive=True*, *tolerance=0.0001*)

Bases: `SolverBase`

base class for adaptive time steppers

Parameters

- **pde** (*PDEBase*) – The instance describing the pde that needs to be solved
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.
- **adaptive** (*bool*) – When enabled, the time step is adjusted during the simulation using the error tolerance set with *tolerance*.
- **tolerance** (*float*) – The error tolerance used in adaptive time stepping. This is used in adaptive time stepping to choose a time step which is small enough so the truncation error of a single step is below *tolerance*.

dt_max: *float* = 10000000000.0

maximal time step that the adaptive solver will use

Type

float

dt_min: *float* = 1e-10

minimal time step that the adaptive solver will use

Type

float

make_stepper (*state*, *dt=None*)

return a stepper function using an explicit scheme

Parameters

- **state** (*FieldBase*) – An example for the state from which the grid and other information can be extracted
- **dt** (*float*) – Time step used (Uses *SolverBase.dt_default* if *None*). This sets the initial time step for adaptive solvers.

Returns

Function that can be called to advance the *state* from time *t_start* to time *t_end*. The function call signature is (*state: numpy.ndarray*, *t_start: float*, *t_end: float*)

Return type

Callable[[*FieldBase*, *float*, *float*], *float*]

exception ConvergenceError

Bases: *RuntimeError*

indicates that an implicit step did not converge

class SolverBase (*pde*, *, *backend='auto'*)

Bases: *object*

base class for PDE solvers

Parameters

- **pde** (*PDEBase*) – The partial differential equation that should be solved
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.

dt_default: `float` = 0.001

default time step used if no time step was specified

Type

`float`

classmethod from_name (*name*, *pde*, ***kwargs*)

create solver class based on its name

Solver classes are automatically registered when they inherit from `SolverBase`. Note that this also requires that the respective python module containing the solver has been loaded before it is attempted to be used.

Parameters

- **name** (*str*) – The name of the solver to construct
- **pde** (*PDEBase*) – The partial differential equation that should be solved
- ****kwargs** – Additional arguments for the constructor of the solver

Returns

An instance of a subclass of `SolverBase`

Return type

`SolverBase`

make_stepper (*state*, *dt=None*)

return a stepper function using an explicit scheme

Parameters

- **state** (*FieldBase*) – An example for the state from which the grid and other information can be extracted
- **dt** (*float*) – Time step used (Uses `SolverBase.dt_default` if *None*)

Returns

Function that can be called to advance the *state* from time *t_start* to time *t_end*. The function call signature is (*state: numpy.ndarray*, *t_start: float*, *t_end: float*)

Return type

`Callable[[FieldBase, float, float], float]`

```
registered_solvers = ['AdamsBashforthSolver', 'AdaptiveSolverBase',
                      'CrankNicolsonSolver', 'ExplicitMPSolver', 'ExplicitSolver',
                      'ImplicitSolver', 'ScipySolver', 'adams-bashforth', 'crank-nicolson',
                      'explicit', 'explicit_mpi', 'implicit', 'scipy']
```

4.4.3 pde.solvers.controller module

Defines a class controlling the simulations of PDEs

class Controller (*solver*, *t_range*, *tracker='auto'*)

Bases: `object`

class controlling a simulation

The controller calls a solver to advance the simulation into the future and it takes care of trackers that analyze and modify the state periodically.

Parameters

- **solver** (*SolverBase*) – Solver instance that is used to advance the simulation in time
- **t_range** (*float or tuple*) – Sets the time range for which the simulation is run. If only a single value *t_end* is given, the time range is assumed to be *[0, t_end]*.
- **tracker** (*TrackerCollectionDataType*) – Defines trackers that process the state of the simulation at specified times. A tracker is either an instance of *TrackerBase* or a string identifying a tracker (possible identifiers can be obtained by calling *get_named_trackers()*). Multiple trackers can be specified as a list. The default value *auto* checks the state for consistency (tracker ‘consistency’) and displays a progress bar (tracker ‘progress’) when *tqdm* is installed. More general trackers are defined in *trackers*, where all options are explained in detail. In particular, the time points where the tracker analyzes data can be chosen when creating a tracker object explicitly.

diagnostics: *dict[str, Any]*

diagnostic information (available after simulation finished)

Type

dict

info: *dict[str, Any]*

run (*initial_state, dt=None*)

run the simulation

Diagnostic information about the solver are available in the *diagnostics* property after this function has been called.

Parameters

- **initial_state** (*FieldBase*) – The initial state of the simulation. This state will be copied and thus not modified by the simulation. Instead, the final state will be returned and trackers can be used to record intermediate states.
- **dt** (*float*) – Time step of the chosen stepping scheme. If *None*, a default value based on the stepper will be chosen.

Returns

The state at the final time point. If multiprocessing is used, only the main node will return the state. All other nodes return *None*.

Return type

TState | *None*

property t_range: *tuple[float, float]*

start and end time of the simulation

Type

tuple

4.4.4 `pde.solvers.crank_nicolson` module

Defines a Crank-Nicolson solver

```
class CrankNicolsonSolver(pde, *, maxiter=100, maxerror=0.0001, explicit_fraction=0, backend='auto')
```

Bases: `SolverBase`

Crank-Nicolson solver

Parameters

- **pde** (`PDEBase`) – The instance describing the pde that needs to be solved
- **maxiter** (`int`) – The maximal number of iterations per step
- **maxerror** (`float`) – The maximal error that is permitted in each step
- **explicit_fraction** (`float`) – Hyperparameter determining the fraction of explicit time stepping in the implicit step. `explicit_fraction == 0` is the simple Crank-Nicolson scheme, while `explicit_fraction == 1` reduces to the explicit Euler method. Intermediate values can improve convergence.
- **backend** (`str`) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.

info: `dict[str, Any]`

name = ‘crank-nicolson’

4.4.5 `pde.solvers.explicit` module

Defines an explicit solver supporting various methods

```
class ExplicitSolver(pde, scheme='euler', *, backend='auto', adaptive=False, tolerance=0.0001)
```

Bases: `AdaptiveSolverBase`

various explicit PDE solvers

Parameters

- **pde** (`PDEBase`) – The instance describing the pde that needs to be solved
- **scheme** (`str`) – Defines the explicit scheme to use. Supported values are ‘euler’ and ‘runge-kutta’ (or ‘rk’ for short).
- **backend** (`str`) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.
- **adaptive** (`bool`) – When enabled, the time step is adjusted during the simulation using the error tolerance set with *tolerance*.
- **tolerance** (`float`) – The error tolerance used in adaptive time stepping. This is used in adaptive time stepping to choose a time step which is small enough so the truncation error of a single step is below *tolerance*.

info: `dict[str, Any]`

name = ‘explicit’

4.4.6 `pde.solvers.explicit_mpi` module

Defines an explicit solver using multiprocessing via MPI

```
class ExplicitMPISolver (pde, scheme='euler', decomposition=-1, *, backend='auto', adaptive=False, tolerance=0.0001)
```

Bases: `ExplicitSolver`

various explicit PDE solve using MPI

Warning: This solver can only be used if MPI is properly installed. In particular, python scripts then need to be started using `mpirun` or `mpiexec`. Please refer to the documentation of your MPI distribution for details.

The main idea of the solver is to take the full initial state in the main node (ID 0) and split the grid into roughly equal subgrids. The main node then distributes these subfields to all other nodes and each node creates the right hand side of the PDE for itself (and independently). Each node then advances the PDE independently, ensuring proper coupling to neighboring nodes via special boundary conditions, which exchange field values between sub grids. This is implemented by the `get_boundary_conditions()` method of the sub grids, which takes the boundary conditions for the full grid and creates conditions suitable for the specific sub grid on the given node. The trackers (and thus all input and output) are only handled on the main node.

Warning: The function providing the right hand side of the PDE needs to support MPI. This is automatically the case for local evaluations (which only use the field value at the current position), for the differential operators provided by `pde`, and integration of fields. Similarly, `modify_after_step` can only be used to do local modifications since the field data supplied to the function is local to each MPI node.

Example

A minimal example using the MPI solver is

```
from pde import DiffusionPDE, ScalarField, UnitGrid

grid = UnitGrid([64, 64])
state = ScalarField.random_uniform(grid, 0.2, 0.3)

eq = DiffusionPDE(diffusivity=0.1)
result = eq.solve(state, t_range=10, dt=0.1, method="explicit_mpi")

if result is not None: # restrict the output to the main node
    result.plot()
```

Saving this script as `multiprocessing.py`, a parallel simulation is started by

```
mpiexec -n 2 python3 multiprocessing.py
```

Here, the number 2 determines the number of cores that will be used. Note that macOS might require an additional hint on how to connect the processes even when they are run on the same machine (e.g., your workstation). It might help to run `mpiexec -n 2 -host localhost python3 multiprocessing.py` in this case

Parameters

- `pde` (`PDEBase`) – The instance describing the pde that needs to be solved

- **scheme** (*str*) – Defines the explicit scheme to use. Supported values are ‘euler’ and ‘runge-kutta’ (or ‘rk’ for short).
- **decomposition** (*list of ints*) – Number of subdivision in each direction. Should be a list of length *grid.num_axes* specifying the number of nodes along this axis. If one value is *-1*, its value will be determined from the number of available nodes. The default value decomposed the first axis using all available nodes.
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.
- **adaptive** (*bool*) – When enabled, the time step is adjusted during the simulation using the error tolerance set with *tolerance*.
- **tolerance** (*float*) – The error tolerance used in adaptive time stepping. This is used in adaptive time stepping to choose a time step which is small enough so the truncation error of a single step is below *tolerance*.

make_stepper (*state*, *dt=None*)

return a stepper function using an explicit scheme

Parameters

- **state** (*FieldBase*) – An example for the state from which the grid and other information can be extracted
- **dt** (*float*) – Time step of the explicit stepping. If *None*, this solver specifies 1e-3 as a default value.

Returns

Function that can be called to advance the *state* from time *t_start* to time *t_end*. The function call signature is (*state: numpy.ndarray*, *t_start: float*, *t_end: float*)

Return type

Callable[[*FieldBase*, *float*, *float*], *float*]

name = 'explicit_mpi'

4.4.7 pde.solvers.implicit module

Defines an implicit Euler solver

class ImplicitSolver (*pde*, *maxiter=100*, *maxerror=0.0001*, *backend='auto'*)

Bases: *SolverBase*

implicit (backward) Euler PDE solver

Parameters

- **pde** (*PDEBase*) – The instance describing the pde that needs to be solved
- **maxiter** (*int*) – The maximal number of iterations per step
- **maxerror** (*float*) – The maximal error that is permitted in each step
- **backend** (*str*) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.

info: *dict*[*str*, *Any*]

name = 'implicit'

4.4.8 `pde.solvers.scipy` module

Defines a solver using `scipy.integrate`

class `ScipySolver` (*pde*, *backend*='auto', ***kwargs*)

Bases: `SolverBase`

PDE solver using `scipy.integrate.solve_ivp()`.

This class is a thin wrapper around `scipy.integrate.solve_ivp()`. In particular, it supports all the methods implemented by this function and exposes its arguments, so details can be controlled.

Parameters

- **pde** (`PDEBase`) – The instance describing the pde that needs to be solved
- **backend** (`str`) – Determines how the function is created. Accepted values are ‘numpy’ and ‘numba’. Alternatively, ‘auto’ lets the code decide for the most optimal backend.
- ****kwargs** – All extra arguments are forwarded to `scipy.integrate.solve_ivp()`.

info: `dict[str, Any]`

make_stepper (*state*, *dt*=None)

return a stepper function

Parameters

- **state** (`FieldBase`) – An example for the state from which the grid and other information can be extracted.
- **dt** (`float`) – Initial time step for the simulation. If *None*, the solver will choose a suitable initial value.

Returns

Function that can be called to advance the *state* from time *t_start* to time *t_end*.

Return type

`Callable[[FieldBase, float, float], float]`

name = 'scipy'

4.5 `pde.storage` package

Module defining classes for storing simulation data.

<code>get_memory_storage</code>	a context manager that can be used to create a MemoryStorage
<code>MemoryStorage</code>	store discretized fields in memory
<code>FileStorage</code>	store discretized fields in a hdf5 file
<code>MovieStorage</code>	store discretized fields in a movie file

4.5.1 `pde.storage.base` module

Base classes for storing data

class `StorageBase` (*info=None*, *write_mode='truncate_once'*)

Bases: `object`

base class for storing time series of discretized fields

These classes store time series of `FieldBase`, i.e., they store the values of the fields at particular time points. Iterating of the storage will return the fields in order and individual time points can also be accessed.

Parameters

- **info** (*dict*) – Supplies extra information that is stored in the storage
- **write_mode** (*str*) – Determines how new data is added to already existing one. Possible values are: ‘append’ (data is always appended), ‘truncate’ (data is cleared every time this storage is used for writing), or ‘truncate_once’ (data is cleared for the first writing, but subsequent data using the same instances are appended). Alternatively, specifying ‘readonly’ will disable writing completely.

append (*field*, *time=None*)

add field to the storage

Parameters

- **field** (*FieldBase*) – The field that is added to the storage
- **time** (*float*, *optional*) – The time point

Return type

`None`

apply (*func*, *out=None*, ***, *progress=False*)

applies function to each field in a storage

Parameters

- **func** (*callable*) – The function to apply to each stored field. The function must either take as a single argument the field or as two arguments the field and the associated time point. In both cases, it should return a field.
- **out** (*StorageBase*) – Storage to which the output is written. If omitted, a new `MemoryStorage` is used and returned
- **progress** (*bool*) – Flag indicating whether the progress is shown during the calculation

Returns

The new storage that contains the data after the function *func* has been applied

Return type

`StorageBase`

clear (*clear_data_shape=False*)

truncate the storage by removing all stored data.

Parameters

- **clear_data_shape** (*bool*) – Flag determining whether the data shape is also deleted.

Return type

`None`

copy (*out=None, *, progress=False*)

copies all fields in a storage to a new one

Parameters

- **out** (*StorageBase*) – Storage to which the output is written. If omitted, a new *MemoStorage* is used and returned
- **progress** (*bool*) – Flag indicating whether the progress is shown during the calculation

Returns

The new storage that contains the copied data

Return type

StorageBase

data: *Any*

property data_shape: *tuple[int, ...]*

the current data shape.

Raises

RuntimeError – if *data_shape* was not set

property dtype: *dtype[Any] | None | type[Any] | _SupportsDType[dtype[Any]] | str | tuple[Any, int] | tuple[Any, SupportsIndex] | Sequence[SupportsIndex] | list[Any] | _DTypeDict | tuple[Any, Any]*

the current data type.

Raises

RuntimeError – if *data_type* was not set

end_writing ()

finalize the storage after writing

Return type

None

extract_field (*field_id, label=None*)

extract the time course of a single field from a collection

This method makes a copy of the underlying data.

Parameters

- **field_id** (*int or str*) – The index into the field collection. This determines which field of the collection is returned. Instead of a numerical index, the field label can also be supplied. If there are multiple fields with the same label, only the first field is returned.
- **label** (*str*) – The label of the returned field. If omitted, the stored label is used.

Returns

a storage instance that contains the data for the single field

Return type

MemoryStorage

extract_time_range (*t_range=None*)

extract a particular time interval

Note: This might return a view into the original data, so modifying the returned data can also change the underlying original data.

Parameters

t_range (*float or tuple*) – Determines the range of time points included in the result. If only a single number is given, all data up to this time point are included.

Returns

a storage instance that contains the extracted data.

Return type

MemoryStorage

property grid: *GridBase* | *None*

the grid associated with this storage

This returns *None* if grid was not stored in *self.info*.

Type

GridBase

property has_collection: *bool*

whether the storage is storing a collection

Type

bool

items ()

iterate over all times and stored fields, returning pairs

Return type

Iterator[*tuple*[*float*, *FieldBase*]]

property shape: *tuple*[*int*, ...] | *None*

the shape of the stored data

start_writing (*field*, *info=None*)

initialize the storage for writing data

Parameters

- **field** (*FieldBase*) – An example of the data that will be written to extract the grid and the data_shape
- **info** (*dict*) – Supplies extra information that is stored in the storage

Return type

None

times: *Sequence*[*float*]

tracker (*interrupts=1*, ***, *transformation=None*, *interval=None*)

create object that can be used as a tracker to fill this storage

Parameters

- **interrupts** (*InterruptsBase* | *float* | *str* | *Sequence*[*float*] | *ndarray*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string

is interpreted as a duration in real time assuming the format 'hh:mm:ss'. A list of numbers is taken as explicit simulation time points. More fine-grained control is possible by passing an instance of classes defined in *interrupts*.

- **transformation** (*callable*, *optional*) – A function that transforms the current state into a new field or field collection, which is then stored. This allows to store derived quantities of the field during calculations. The argument needs to be a callable function taking 1 or 2 arguments. The first argument always is the current field, while the optional second argument is the associated time.

Returns

The tracker that fills the current storage

Return type

StorageTracker

Example

The *transformation* argument allows storing additional fields:

```
def add_to_state(state):
    transformed_field = state.smooth(1)
    return field.append(transformed_field)

storage = pde.MemoryStorage()
tracker = storage.tracker(1, transformation=add_to_state)
eq.solve(..., tracker=tracker)
```

In this example, *storage* will contain a trajectory of the fields of the simulation as well as the smoothed fields. Other transformations are possible by defining appropriate *add_to_state*()

view_field (*field_id*)

returns a view into this storage focusing on a particular field

Note: Modifying data returned by the view will modify the underlying storage

Parameters

field_id (*int* or *str*) – The index into the field collection. This determines which field of the collection is returned. Instead of a numerical index, the field label can also be supplied. If there are multiple fields with the same label, only the first field is returned.

Returns

A view into the storage only returning a single field

Return type

StorageView

write_mode: `Literal['append', 'readonly', 'truncate', 'truncate_once']`

class StorageTracker (*storage*, *interrupts=1*, *, *transformation=None*, *interval=None*)

Bases: *TrackerBase*

Tracker that stores data in special storage classes

storage

The underlying storage class through which the data can be accessed

Type

StorageBase

Parameters

- **storage** (*StorageBase*) – Storage instance to which the data is written
- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.
- **transformation** (*callable, optional*) – A function that transforms the current state into a new field or field collection, which is then stored. This allows to store derived quantities of the field during calculations. The argument needs to be a callable function taking 1 or 2 arguments. The first argument always is the current field, while the optional second argument is the associated time.

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

info (*dict*) – Extra information from the simulation

Return type

None

handle (*field, t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

initialize (*field, info=None*)

Parameters

- **field** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

class StorageView (*storage, *, field*)

Bases: *object*

represents a view into a storage that extracts a particular field

Parameters

- **storage** (*StorageBase*) – The storage providing the basic data
- **field** (*int* or *str*) – The index into the field collection determining which field of the collection is returned. Instead of a numerical index, the field label can also be supplied. If there are multiple fields with the same label, only the first field is returned.

property `grid`: *GridBase* | *None*

has_collection: *bool* = *False*

items ()

iterate over all times and stored fields, returning pairs

Return type

Iterator[*tuple*[*float*, *DataFieldBase*]]

property `times`: *Sequence*[*float*]

4.5.2 pde.storage.file module

Defines a class storing data on the file system using the hierarchical data format (hdf)

class `FileStorage` (*filename*, *, *info*=*None*, *write_mode*='truncate_once', *max_length*=*None*, *compression*=*True*, *keep_opened*=*True*, *check_mpi*=*True*)

Bases: *StorageBase*

store discretized fields in a hdf5 file

Parameters

- **filename** (*str*) – The path to the hdf5-file where the data is stored
- **info** (*dict*) – Supplies extra information that is stored in the storage
- **write_mode** (*str*) – Determines how new data is added to already existing data. Possible values are: 'append' (data is always appended), 'truncate' (data is cleared every time this storage is used for writing), or 'truncate_once' (data is cleared for the first writing, but appended subsequently). Alternatively, specifying 'readonly' will disable writing completely.
- **max_length** (*int*, *optional*) – Maximal number of entries that will be stored in the file. This can be used to preallocate data, which can lead to smaller files, but is also less flexible. Giving *max_length* = *None*, allows for arbitrarily large data, which might lead to larger files.
- **compression** (*bool*) – Whether to store the data in compressed form. Automatically enabled chunked storage.
- **keep_opened** (*bool*) – Flag indicating whether the file should be kept opened after each writing. If *False*, the file will be closed after writing a dataset. This keeps the file in a consistent state, but also requires more work before data can be written.
- **check_mpi** (*bool*) – If *True*, files will only be opened in the main node for an parallel simulation using MPI. This flag has no effect in serial code.

clear (*clear_data_shape*=*False*)

truncate the storage by removing all stored data.

Parameters

clear_data_shape (*bool*) – Flag determining whether the data shape is also deleted.

close()

close the currently opened file

Return type

None

property data

The actual data for all time

Type

`ndarray`

end_writing()

finalize the storage after writing.

This makes sure the data is actually written to a file when `self.keep_opened == False`

Return type

None

start_writing(*field*, *info=None*)

initialize the storage for writing data

Parameters

- **field** (`FieldBase`) – An example of the data that will be written to extract the grid and the `data_shape`
- **info** (`dict`) – Supplies extra information that is stored in the storage

Return type

None

property times

The times at which data is available

Type

`ndarray`

4.5.3 `pde.storage.memory` module

Defines a class storing data in memory.

class `MemoryStorage` (*times=None*, *data=None*, *, *info=None*, *field_obj=None*, *write_mode='truncate_once'*)

Bases: `StorageBase`

store discretized fields in memory

Parameters

- **times** (`ndarray`) – Sequence of times for which data is known
- **data** (list of `ndarray`) – The field data at the given times
- **field_obj** (`FieldBase`) – An instance of the field class store data for a single time point.
- **info** (`dict`) – Supplies extra information that is stored in the storage
- **write_mode** (`str`) – Determines how new data is added to already existing data. Possible values are: ‘append’ (data is always appended), ‘truncate’ (data is cleared every time this storage is used for writing), or ‘truncate_once’ (data is cleared for the first writing, but appended subsequently). Alternatively, specifying ‘readonly’ will disable writing completely.

clear (*clear_data_shape=False*)

truncate the storage by removing all stored data.

Parameters

clear_data_shape (*bool*) – Flag determining whether the data shape is also deleted.

Return type

None

classmethod from_collection (*storages, label=None, *, rtol=1e-05, atol=1e-08*)

combine multiple memory storages into one

This method can be used to combine multiple time series of different fields into a single representation. This requires that all time series contain data at the same time points.

Parameters

- **storages** (*list*) – A collection of instances of *StorageBase* whose data will be concatenated into a single *MemoryStorage*
- **label** (*str, optional*) – The label of the instances of *FieldCollection* that represent the concatenated data
- **rtol** (*float*) – Relative tolerance used when checking times for merging
- **atol** (*float*) – Absolute tolerance used when checking times for merging

Returns

Storage containing all the data.

Return type

MemoryStorage

classmethod from_fields (*times=None, fields=None, info=None, write_mode='truncate_once'*)

create *MemoryStorage* from a list of fields

Parameters

- **times** (*ndarray*) – Sequence of times for which data is known
- **fields** (list of *FieldBase*) – The fields at all given time points
- **info** (*dict*) – Supplies extra information that is stored in the storage
- **write_mode** (*str*) – Determines how new data is added to already existing data. Possible values are: ‘append’ (data is always appended), ‘truncate’ (data is cleared every time this storage is used for writing), or ‘truncate_once’ (data is cleared for the first writing, but appended subsequently). Alternatively, specifying ‘readonly’ will disable writing completely.

Return type

MemoryStorage

start_writing (*field, info=None*)

initialize the storage for writing data

Parameters

- **field** (*FieldBase*) – An instance of the field class store data for a single time point.
- **info** (*dict*) – Supplies extra information that is stored in the storage

Return type

None

get_memory_storage (*field*, *info=None*)

a context manager that can be used to create a `MemoryStorage`

Example

This can be used to quickly store data:

```
with get_memory_storage(field_class) as storage:
    storage.append(numpy_array0, 0)
    storage.append(numpy_array1, 1)

# use storage thereafter
```

Parameters

- **field** (`FieldBase`) – An instance of the field class store data for a single time point.
- **info** (`dict`) – Supplies extra information that is stored in the storage

Yields

`MemoryStorage`

4.5.4 `pde.storage.movie` module

Defines a class storing data on the file system as a compressed movie

This package requires the optional `ffmpeg-python` package to use `FFmpeg` for reading and writing movies.

class MovieStorage (*filename*, *, *vmin=0*, *vmax=1*, *bits_per_channel=8*, *video_format='auto'*, *bitrate=-1*, *info=None*, *write_mode='truncate_once'*, *write_times=False*, *loglevel='warning'*)

Bases: `StorageBase`

store discretized fields in a movie file

This storage only works when the `ffmpeg` program and `ffmpeg` is installed. The default codec is `FFV1`, which supports lossless compression for various configurations. Not all video players support this codec, but `VLC` usually works quite well.

Note that important metainformation is stored as a comment in the movie, so this data must not be deleted or altered if the video should be read again.

Warning: This storage potentially compresses data and can thus lead to loss of some information. The data quality depends on many parameters, but most important are the bits per channel of the video format and the range that is encoded (determined by *vmin* and *vmax*).

Note also that selecting individual time points might be quite slow since the video needs to be read from the beginning each time. Instead, it is much more efficient to process entire videos (by iterating over them or using `items()`).

Parameters

- **filename** (`str`) – The path where the movie is stored. The file extension determines the container format of the movie. The standard codec `FFV1` plays well with the “.avi”, “.mkv”, and “.mov” container format.

- **vmin** (*float* or *array*) – Lowest values that are encoded (per field). Smaller values are clipped to this value.
- **vmax** (*float* or *array*) – Highest values that are encoded (per field). Larger values are clipped to this value.
- **bits_per_channel** (*int*) – The number of bits used per color channel. Typical values are 8 and 16. The relative accuracy of stored values is 0.01 and 0.0001, respectively.
- **video_format** (*str*) – Identifier for a video format from *formats*, which determines the number of channels, the bit depth of individual colors, and the codec. The special value *auto* tries to find a suitable format automatically, taking *bits_per_channel* into account.
- **bitrate** (*float*) – The bitrate of the movie (in kilobits per second). The default value of -1 let's the encoder choose an appropriate bit rate.
- **info** (*dict*) – Supplies extra information that is stored in the storage alongside additional information necessary to reconstruct fields and grids.
- **write_mode** (*str*) – Determines how new data is added to already existing data. Possible values are: 'append' (data is always appended), 'truncate' (data is cleared every time this storage is used for writing), or 'truncate_once' (data is cleared for the first writing, but appended subsequently). Alternatively, specifying 'readonly' will disable writing completely.
- **write_times** (*bool*) – Flag determining whether timestamps are written to a file. If True, a separate file with name `filename + ".times"` is created where the times are written as plain text. Without these timestamps, the time information might be inaccurate.
- **loglevel** (*str*) – FFmpeg log level determining the amount of data sent to stdout. The default only emits warnings and errors, but setting this to "info" can be useful to get additional information about the encoding.

clear()

truncate the storage by removing all stored data.

close()

close the currently opened file

Return type

None

property data

The actual data for all time

Type

ndarray

end_writing()

finalize the storage after writing

Return type

None

items()

iterate over all times and stored fields, returning pairs

Return type

Iterator[*tuple*[*float*, *FieldBase*]]

start_writing (*field*, *info=None*)

initialize the storage for writing data

Parameters

- **field** (*FieldBase*) – An example of the data that will be written to extract the grid and the *data_shape*
- **info** (*dict*) – Supplies extra information that is stored in the storage

Return type

None

times: **Sequence**[**float**]

The times at which data is available

Type

ndarray

tracker (*interrupts=1*, ***, *transformation=None*)

create object that can be used as a tracker to fill this storage

Parameters

- **interrupts** (*InterruptsBase* / *float* / *str* / *Sequence*[*float*] / *ndarray*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.
- **transformation** (*callable*, *optional*) – A function that transforms the current state into a new field or field collection, which is then stored. This allows to store derived quantities of the field during calculations. The argument needs to be a callable function taking 1 or 2 arguments. The first argument always is the current field, while the optional second argument is the associated time.

Returns

The tracker that fills the current storage

Return type

StorageTracker

Example

The *transformation* argument allows storing additional fields:

```
def add_to_state(state):
    transformed_field = state.smooth(1)
    return field.append(transformed_field)

storage = pde.MemoryStorage()
tracker = storage.tracker(1, transformation=add_to_state)
eq.solve(..., tracker=tracker)
```

In this example, *storage* will contain a trajectory of the fields of the simulation as well as the smoothed fields. Other transformations are possible by defining appropriate *add_to_state()*

4.6 pde.tools package

Package containing several tools required in py-pde

<i>cache</i>	Functions, classes, and decorators for managing caches
<i>config</i>	Handles configuration variables of the package
<i>cuboid</i>	An n-dimensional, axes-aligned cuboid
<i>docstrings</i>	Methods for automatic transformation of docstrings
<i>expressions</i>	Handling mathematical expressions with sympy
<i>ffmpeg</i>	Functions for interacting with FFmpeg
<i>math</i>	Auxiliary mathematical functions
<i>misc</i>	Miscellaneous python functions
<i>mpi</i>	Auxillary functions and variables for dealing with MPI multiprocessing
<i>numba</i>	Helper functions for just-in-time compilation with numba
<i>output</i>	Python functions for handling output
<i>parameters</i>	Infrastructure for managing classes with parameters
<i>parse_duration</i>	Parsing time durations from strings
<i>plotting</i>	Tools for plotting and controlling plot output using context managers
<i>spectral</i>	Functions making use of spectral decompositions
<i>typing</i>	Provides support for mypy type checking of the package

4.6.1 pde.tools.cache module

Functions, classes, and decorators for managing caches

<i>cached_property</i>	Decorator to use a method as a cached property
<i>cached_method</i>	Decorator to enable caching of a method
<i>hash_mutable</i>	return hash also for (nested) mutable objects.
<i>hash_readable</i>	return human readable hash also for (nested) mutable objects.
<i>make_serializer</i>	returns a function that serialize data with the given method.
<i>make_unserializer</i>	returns a function that unserialize data with the given method
<i>DictFiniteCapacity</i>	cache with a limited number of items
<i>SerializedDict</i>	a key value database which is stored on the disk

```
class DictFiniteCapacity(*args, **kwargs)
```

Bases: `OrderedDict`

cache with a limited number of items

```
check_length()
```

ensures that the dictionary does not grow beyond its capacity

```
default_capacity: int = 100
```

update ($[E,]**F$) \rightarrow None. Update D from dict/iterable E and F.

If E is present and has a `.keys()` method, then does: for k in E: D[k] = E[k] If E is present and lacks a `.keys()` method, then does: for k, v in E: D[k] = v In either case, this is followed by: for k in F: D[k] = F[k]

class SerializedDict (*key_serialization='pickle', value_serialization='pickle', storage_dict=None*)

Bases: `MutableMapping`

a key value database which is stored on the disk

This class provides hooks for converting arbitrary keys and values to strings, which are then stored in the database. provides a dictionary whose keys and values are serialized

Parameters

- **key_serialization** (*str*) – Determines the serialization method for keys
- **value_serialization** (*str*) – Determines the serialization method for values
- **storage_dict** (*dict*) – Can be used to chose a different dictionary for the underlying storage mechanism, e.g., `storage_dict = PersistentDict()`

class cached_method (*factory=None, extra_args=None, ignore_args=None, hash_function='hash_mutable', doc=None, name=None*)

Bases: `_class_cache`

Decorator to enable caching of a method

The function is only called the first time and each successive call returns the cached result of the first call.

Example

The decorator can be used like so:

```
class Foo:

    @cached_method
    def bar(self):
        return "Cached"

foo = Foo()
result = foo.bar()
```

The data is stored in a dictionary named `_cache_methods` attached to the instance of each object. The cache can thus be cleared by setting `self._cache_methods = {}`. The cache of specific property can be cleared using `self._cache_methods[property_name] = {}`, where *property_name* is the name of the property.

decorator that caches calls in a dictionary attached to the instances. This can be used with most classes

Example

An example for using the class is:

```
class Foo():

    @cached_property()
    def property(self):
        return "Cached property"
```

(continues on next page)

(continued from previous page)

```

@cached_method()
def method(self):
    return "Cached method"

foo = Foo()
foo.property
foo.method()

```

The cache can be cleared by setting `foo._cache_methods = {}` if the cache factory is a simple dict, i.e. if `factory == None`. Alternatively, each cached method has a `clear_cache_of_obj()` method, which clears the cache of this particular method. In the example above we could thus call `foo.bar.clear_cache_of_obj(foo)` to clear the cache.

Note that the object instance has to be passed as a parameter, since the method `bar()` is defined on the class, not the instance, i.e., we could also call `Foo.bar.clear_cache_of_obj(foo)`. To clear the cache from within a method, one can thus call `self.method_name.clear_cache_of_obj(self)`, where *method_name* is the name of the method whose cache is cleared

Example

An advanced example is:

```

class Foo():

    def get_cache(self, name):
        # `name` is the name of the method to cache
        return DictFiniteCapacity()

    @cached_method(factory='get_cache')
    def foo(self):
        return "Cached"

```

Parameters

- **factory** (*callable*) – Function/class creating an empty cache. *dict* by default. This can be used with user-supplied storage backends by. The cache factory should return a dict-like object that handles the cache for the given method.
- **extra_args** (*list*) – List of attributes of the class that are included in the cache key. They are then treated as if they are supplied as arguments to the method. This is important to include when the result of a method depends not only on method arguments but also on instance attributes.
- **ignore_args** (*list*) – List of keyword arguments that are not included in the cache key. These should be arguments that do not influence the result of a method, e.g., because they only affect how intermediate results are displayed.
- **hash_function** (*str*) – An identifier determining what hash function is used on the arguments
- **doc** (*str*) – Optional string giving the docstring of the decorated method
- **name** (*str*) – Optional string giving the name of the decorated method

```
class cached_property (factory=None, extra_args=None, ignore_args=None, hash_function='hash_mutable',
                        doc=None, name=None)
```

Bases: `_class_cache`

Decorator to use a method as a cached property

The function is only called the first time and each successive call returns the cached result of the first call.

Example

Here is an example for how to use the decorator:

```
class Foo():

    @cached_property
    def bar(self):
        return "Cached"

foo = Foo()
result = foo.bar
```

The data is stored in a dictionary named `_cache_methods` attached to the instance of each object. The cache can thus be cleared by setting `self._cache_methods = {}`. The cache of specific property can be cleared using `self._cache_methods[property_name] = {}`, where *property_name* is the name of the property.

Adapted from <<https://wiki.python.org/moin/PythonDecoratorLibrary>>.

decorator that caches calls in a dictionary attached to the instances. This can be used with most classes

Example

An example for using the class is:

```
class Foo():

    @cached_property()
    def property(self):
        return "Cached property"

    @cached_method()
    def method(self):
        return "Cached method"

foo = Foo()
foo.property
foo.method()
```

The cache can be cleared by setting `foo._cache_methods = {}` if the cache factory is a simple dict, i.e. if `factory == None`. Alternatively, each cached method has a `clear_cache_of_obj()` method, which clears the cache of this particular method. In the example above we could thus call `foo.bar.clear_cache_of_obj(foo)` to clear the cache.

Note that the object instance has to be passed as a parameter, since the method `bar()` is defined on the class, not the instance, i.e., we could also call `Foo.bar.clear_cache_of_obj(foo)`. To clear the cache from within

a method, one can thus call `self.method_name.clear_cache_of_obj(self)`, where *method_name* is the name of the method whose cache is cleared

Example

An advanced example is:

```
class Foo():

    def get_cache(self, name):
        # `name` is the name of the method to cache
        return DictFiniteCapacity()

    @cached_method(factory='get_cache')
    def foo(self):
        return "Cached"
```

Parameters

- **factory** (*callable*) – Function/class creating an empty cache. *dict* by default. This can be used with user-supplied storage backends by. The cache factory should return a dict-like object that handles the cache for the given method.
- **extra_args** (*list*) – List of attributes of the class that are included in the cache key. They are then treated as if they are supplied as arguments to the method. This is important to include when the result of a method depends not only on method arguments but also on instance attributes.
- **ignore_args** (*list*) – List of keyword arguments that are not included in the cache key. These should be arguments that do not influence the result of a method, e.g., because they only affect how intermediate results are displayed.
- **hash_function** (*str*) – An identifier determining what hash function is used on the arguments
- **doc** (*str*) – Optional string giving the docstring of the decorated method
- **name** (*str*) – Optional string giving the name of the decorated method

hash_mutable (*obj*)

return hash also for (nested) mutable objects.

Notes

This function might be a bit slow, since it iterates over all containers and hashes objects recursively. Moreover, the returned value might change with each run of the python interpreter, since the hash values of some basic objects, like *None*, change with each instance of the interpreter.

Parameters

obj – A general python object

Returns

A hash value associated with the data of *obj*

Return type

`int`

hash_readable (*obj*)

return human readable hash also for (nested) mutable objects.

This function returns a JSON-like representation of the object. The function might be a bit slow, since it iterates over all containers and hashes objects recursively. Note that this hash function tries to return the same value for equivalent objects, but it does not ensure that the objects can be reconstructed from this data.

Parameters

obj – A general python object

Returns

A hash value associated with the data of *obj*

Return type

`str`

make_serializer (*method*)

returns a function that serialize data with the given method. Note that some of the methods destroy information and cannot be reverted.

Parameters

method (`str`) – An identifier determining the serializer that will be returned

Returns

A function that serializes objects

Return type

callable

make_unserializer (*method*)

returns a function that unserialize data with the given method

This is the inverse function of `make_serializer()`.

Parameters

method (`str`) – An identifier determining the unserializer that will be returned

Returns

A function that serializes objects

Return type

callable

objects_equal (*a*, *b*)

compares two objects to see whether they are equal

In particular, this uses `numpy.array_equal()` to check for numpy arrays

Parameters

- **a** – The first object
- **b** – The second object

Returns

Whether the two objects are considered equal

Return type

`bool`

4.6.2 pde.tools.config module

Handles configuration variables of the package

<code>Config</code>	class handling the package configuration
<code>get_package_versions</code>	tries to load certain python packages and returns their version
<code>parse_version_str</code>	helper function converting a version string into a list of integers
<code>check_package_version</code>	checks whether a package has a sufficient version
<code>packages_from_requirements</code>	read package names from a requirements file
<code>environment</code>	obtain information about the compute environment

class Config (*items=None, mode='update'*)

Bases: `UserDict`

class handling the package configuration

Parameters

- **items** (*dict, optional*) – Configuration values that should be added or overwritten to initialize the configuration.
- **mode** (*str*) – Defines the mode in which the configuration is used. Possible values are
 - *insert*: any new configuration key can be inserted
 - *update*: only the values of pre-existing items can be updated
 - *locked*: no values can be changed

Note that the items specified by *items* will always be inserted, independent of the *mode*.

to_dict ()

convert the configuration to a simple dictionary

Returns

A representation of the configuration in a normal `dict`.

Return type

`dict`

check_package_version (*package_name, min_version*)

checks whether a package has a sufficient version

Parameters

- **package_name** (*str*) –
- **min_version** (*str*) –

environment ()

obtain information about the compute environment

Returns

information about the python installation and packages

Return type

`dict`

get_package_versions (*packages*, *, *na_str*='not available')

tries to load certain python packages and returns their version

Parameters

- **packages** (*list*) – The names of all packages
- **na_str** (*str*) – Text to return if package is not available

Returns

Dictionary with version for each package name

Return type

`dict`

packages_from_requirements (*requirements_file*)

read package names from a requirements file

Parameters

requirements_file (*str* or `Path`) – The file from which everything is read

Returns

list of package names

Return type

`list[str]`

parse_version_str (*ver_str*)

helper function converting a version string into a list of integers

Parameters

ver_str (*str*) –

Return type

`list[int]`

4.6.3 pde.tools.cuboid module

An n-dimensional, axes-aligned cuboid

This module defines the `Cuboid` class, which represents an n-dimensional cuboid that is aligned with the axes of a Cartesian coordinate system.

class Cuboid (*pos*, *size*, *mutable*=`True`)

Bases: `object`

class that represents a cuboid in *n* dimensions

defines a cuboid from a position and a size vector

Parameters

- **pos** (*list*) – The position of the lower left corner. The length of this list determines the dimensionality of space
- **size** (*list*) – The size of the cuboid along each dimension.
- **mutable** (*bool*) – Flag determining whether the cuboid parameters can be changed

property bounds: `tuple[tuple[float, float], ...]`

buffer (*amount=0, inplace=False*)

dilate the cuboid by a certain amount in all directions

Parameters

amount (*float* | *ndarray*) –

Return type

Cuboid

property centroid

contains_point (*points*)

returns a True when *points* are within the Cuboid

Parameters

points (*ndarray*) – List of point coordinates

Returns

list of booleans indicating which points are inside

Return type

ndarray

copy ()

Return type

Cuboid

property corners: *tuple*[*ndarray*, *ndarray*]

return coordinates of two extreme corners defining the cuboid

property diagonal: *float*

returns the length of the diagonal

property dim: *int*

classmethod from_bounds (*bounds, **kwargs*)

create cuboid from bounds

Parameters

bounds (*list*) – Two dimensional array of axes bounds

Returns

cuboid with positive size

Return type

Cuboid

classmethod from_centerpoint (*centerpoint, size, **kwargs*)

create cuboid from two points

Parameters

- **centerpoint** (*list*) – Coordinates of the center
- **size** (*list*) – Size of the cuboid

Returns

cuboid with positive size

Return type

Cuboid

classmethod `from_points` (*p1*, *p2*, ***kwargs*)

create cuboid from two points

Parameters

- **p1** (*list*) – Coordinates of first corner point
- **p2** (*list*) – Coordinates of second corner point

Returns

cuboid with positive size

Return type

Cuboid

property `mutable`: `bool`

property `size`: `ndarray`

property `surface_area`: `float`

surface area of a cuboid in n dimensions.

The surface area is the volume of the $(n - 1)$ -dimensional hypercubes that bound the current cuboid:

- $n = 1$: the number of end points (2)
- $n = 2$: the perimeter of the rectangle
- $n = 3$: the surface area of the cuboid

property `vertices`: `list[list[float]]`

return the coordinates of all the corners

property `volume`: `float`

asanyarray_flags (*data*, *dtype=None*, *writeable=True*)

turns data into an array and sets the respective flags.

A copy is only made if necessary

Parameters

- **data** (`ndarray`) – numpy array that whose flags are adjusted
- **dtype** (`dtype[Any]` | `None` | `type[Any]` | `_SupportsDType[dtype[Any]]` | `str` | `tuple[Any, int]` | `tuple[Any, SupportsIndex]` | `Sequence[SupportsIndex]` | `list[Any]` | `_DTypeDict` | `tuple[Any, Any]`) – the resultant dtype
- **writeable** (`bool`) – Flag determining whether the results is writable

Returns

array with same data as *data* but with flags adjusted.

Return type

`ndarray`

4.6.4 `pde.tools.docstrings` module

Methods for automatic transformation of docstrings

<code>get_text_block</code>	return a single text block
<code>replace_in_docstring</code>	replace a text in a docstring using the correct indentation
<code>fill_in_docstring</code>	decorator that replaces text in the docstring of a function

`fill_in_docstring(f)`

decorator that replaces text in the docstring of a function

Parameters

`f` (*TFunc*) –

Return type

TFunc

`get_text_block(identifier)`

return a single text block

Parameters

`identifier` (*str*) – The name of the text block

Returns

the text block as one long line.

Return type

str

`replace_in_docstring(f, token, value, docstring=None)`

replace a text in a docstring using the correct indentation

Parameters

- **`f`** (*callable*) – The function with the docstring to handle
- **`token`** (*str*) – The token to search for
- **`value`** (*str*) – The replacement string
- **`docstring`** (*str*) – A docstring that should be used instead of `f.__doc__`

Returns

The function with the modified docstring

Return type

callable

4.6.5 `pde.tools.expressions` module

Handling mathematical expressions with sympy

This module provides classes representing expressions that can be provided as human-readable strings and are converted to `numpy` and `numba` representations using `sympy`.

<code>parse_number</code>	return a number compiled from an expression
<code>ScalarExpression</code>	describes a mathematical expression of a scalar quantity
<code>TensorExpression</code>	describes a mathematical expression of a tensorial quantity
<code>evaluate</code>	evaluate an expression involving fields

class ExpressionBase (*expression*, *signature=None*, *, *user_funcs=None*, *consts=None*, *repl=None*)

Bases: `object`

abstract base class for handling expressions

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **expression** (`sympy.core.basic.Basic`) – A sympy expression or array. This could for instance be an instance of `Expr` or `NDimArray`.
- **signature** (*list of str*, *optional*) – The signature defines which variables are expected in the expression. This is typically a list of strings identifying the variable names. Individual names can be specified as list, in which case any of these names can be used. The first item in such a list is the definite name and if another name of the list is used, the associated variable is renamed to the definite name. If signature is *None*, all variables in *expressions* are allowed.
- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that used in the expression.
- **consts** (*dict*, *optional*) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or `ndarray`.
- **repl** (*dict*, *optional*) – Replacements that are applied to symbols before turning the expression into a python equivalent.

property complex: `bool`

whether the expression contains the imaginary unit I

Type

`bool`

property constant: `bool`

whether the expression is a constant

Type

`bool`

depends_on (*variable*)

determine whether the expression depends on *variable*

Parameters

variable (*str*) – the name of the variable to check for

Returns

whether the variable appears in the expression

Return type`bool`**property expression:** `str`

the expression in string form

Type`str`**get_compiled** (*single_arg=False*)

return numba function evaluating expression

Parameters**single_arg** (*bool*) – Determines whether the function takes all variables in a single argument as an array or whether all variables need to be supplied separately.**Returns**

the compiled function

Return type

function

property rank: `int`

the rank of the expression

Type`int`**abstract property shape:** `tuple[int, ...]`

the shape of the tensor

Type`tuple`**class ScalarExpression** (*expression=0, signature=None, *, user_funcs=None, consts=None, repl=None, explicit_symbols=None, allow_indexed=False*)Bases: [*ExpressionBase*](#)

describes a mathematical expression of a scalar quantity

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.**Parameters**

- **expression** (*str or float*) – The expression, either a number or a string that sympy can parse.
- **signature** (*list of str*) – The signature defines which variables are expected in the expression. This is typically a list of strings identifying the variable names. Individual names can be specified as lists, in which case any of these names can be used. The first item in such a list is the definite name and if another name of the list is used, the associated variable is renamed to the definite name. If signature is *None*, all variables in *expressions* are allowed.
- **user_funcs** (*dict, optional*) – A dictionary with user defined functions that used in the expression.
- **consts** (*dict, optional*) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or `ndarray`.

- **repl** (*dict*, *optional*) – Replacements that are applied to symbols before turning the expression into a python equivalent.
- **explicit_symbols** (*list of str*) – List of symbols that need to be interpreted as general sympy symbols
- **allow_indexed** (*bool*) – Whether to allow indexing of variables. If enabled, array variables are allowed to be indexed using square bracket notation.

copy ()

return a copy of the current expression

Return type

`ScalarExpression`

derivatives

differentiate the expression with respect to all variables

differentiate (*var*)

return the expression differentiated with respect to var

Parameters

var (*str*) –

Return type

`ScalarExpression`

property is_zero: `bool`

returns whether the expression is zero

Type

`bool`

shape: `tuple[int, ...]` = ()

property value: `int | float | complex`

the value for a constant expression

Type

`float`

class TensorExpression (*expression*, *signature=None*, *, *user_funcs=None*, *consts=None*, *repl=None*, *explicit_symbols=None*)

Bases: `ExpressionBase`

describes a mathematical expression of a tensorial quantity

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **expression** (*str or float*) – The expression, either a number or a string that sympy can parse.
- **signature** (*list of str*) – The signature defines which variables are expected in the expression. This is typically a list of strings identifying the variable names. Individual names can be specified as list, in which case any of these names can be used. The first item in such

a list is the definite name and if another name of the list is used, the associated variable is renamed to the definite name. If signature is *None*, all variables in *expressions* are allowed.

- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that used in the expression.
- **consts** (*dict*, *optional*) – A dictionary with user defined constants that can be used in the expression. The values of these constants should either be numbers or `ndarray`.
- **repl** (*dict*, *optional*) – Replacements that are applied to symbols before turning the expression into a python equivalent.
- **explicit_symbols** (*list of str*) – List of symbols that need to be interpreted as general sympy symbols

derivatives

differentiate the expression with respect to all variables

differentiate (*var*)

return the expression differentiated with respect to var

Parameters

var (*str*) –

Return type

`TensorExpression`

get_compiled_array (*single_arg=True*)

compile the tensor expression such that a numpy array is returned

Parameters

single_arg (*bool*) – Whether the compiled function expects all arguments as a single array or whether they are supplied individually.

Return type

`Callable[[ndarray, ndarray | None], ndarray]`

property rank: `int`

rank of the tensor expression

Type

`int`

property shape: `tuple[int, ...]`

the shape of the tensor

Type

`tuple`

property value

the value for a constant expression

evaluate (*expression*, *fields*, *, *bc*='auto_periodic_neumann', *bc_ops*=*None*, *user_funcs*=*None*, *consts*=*None*, *label*=*None*)

evaluate an expression involving fields

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **expression** (*str*) – The expression, which is parsed by `sympy`. The expression may contain variables (i.e., fields and spatial coordinates of the grid), standard local mathematical operators defined by `sympy`, and the operators defined in the `pde` package. Note that operators need to be specified with their full name, i.e., `laplace` for a scalar Laplacian and `vector_laplace` for a Laplacian operating on a vector field. Moreover, the dot product between two vector fields can be denoted by using `dot(field1, field2)` in the expression, and `outer(field1, field2)` calculates an outer product. More information can be found in the [expression documentation](#).
- **fields** (dict or *FieldCollection*) – Dictionary of the fields involved in the expression. The dictionary keys specify the field names allowed in *expression*. Alternatively, *fields* can be a *FieldCollection* with unique labels.
- **bc** (*BoundariesData*) – Boundary conditions for the operators used in the expression. The conditions here are applied to all operators that do not have a specialized condition given in *bc_ops*. Boundary conditions are generally given as a list with one condition for each axis. For periodic axes, only periodic boundary conditions are allowed (indicated by ‘periodic’ and ‘anti-periodic’). For non- periodic axes, different boundary conditions can be specified for the lower and upper end (using a tuple of two conditions). For instance, Dirichlet conditions enforcing a value `NUM` (specified by `{‘value’: NUM}`) and Neumann conditions enforcing the value `DERIV` for the derivative in the normal direction (specified by `{‘derivative’: DERIV}`) are supported. Note that the special value ‘natural’ imposes periodic boundary conditions for periodic axis and a vanishing derivative otherwise. More information can be found in the [boundaries documentation](#).
- **bc_ops** (*dict*) – Special boundary conditions for some operators. The keys in this dictionary specify the operator to which the boundary condition will be applied.
- **user_funcs** (*dict*, *optional*) – A dictionary with user defined functions that can be used in the expressions in *rhs*.
- **consts** (*dict*, *optional*) – A dictionary with user defined constants that can be used in the expression. These can be either scalar numbers or fields defined on the same grid as the actual simulation.
- **label** (*str*) – Name of the field that is returned.

Returns

The resulting field. The rank of the returned field (and thus the precise class) is determined automatically.

Return type

`pde.fields.base.DataFieldBase`

parse_number (*expression*, *variables=None*)

return a number compiled from an expression

Warning: This implementation uses `exec()` and should therefore not be used in a context where malicious input could occur.

Parameters

- **expression** (*str* or *Number*) – An expression that can be interpreted as a number
- **variables** (*dict*) – A dictionary of values that replace variables in the expression

Returns
the calculated value

Return type
Number

4.6.6 pde.tools.ffmpeg module

Functions for interacting with FFmpeg

<i>FFmpegFormat</i>	defines a FFmpeg format used for storing field data in a video
<i>formats</i>	dict of pre-defined <i>FFmpegFormat</i> formats
<i>find_format</i>	find a defined FFmpegFormat that satisfies the requirements

class FFmpegFormat (*pix_fmt_file, pix_fmt_data, channels, bits_per_channel, dtype, codec='ffv1'*)

Bases: `object`

defines a FFmpeg format used for storing field data in a video

Note: All pixel formats supported by FFmpeg can be obtained by running `ffmpeg -pix_fmts`. However, not all pixel formats are supported by all codecs. Supported pixel formats are listed in the output of `ffmpeg -h encoder=<ENCODER>`, where `<ENCODER>` is one of the encoders listed in `ffmpeg -codecs`.

Parameters

- **pix_fmt_file** (*str*) –
- **pix_fmt_data** (*str*) –
- **channels** (*int*) –
- **bits_per_channel** (*int*) –
- **dtype** (*dtype[Any] | None | type[Any] | _SupportsDType[dtype[Any]] | str | tuple[Any, int] | tuple[Any, SupportsIndex] | Sequence[SupportsIndex] | list[Any] | _DTypeDict | tuple[Any, Any]*) –
- **codec** (*str*) –

bits_per_channel: `int`
number of bits per color channel in this pixel format

Type
`int`

property bytes_per_channel: `int`
number of bytes per color channel

Type
`int`

channels: `int`

number of color channels in this pixel format

Type

`int`

codec: `str = 'ffv1'`

name of the codec that supports this pixel format

Type

`str`

data_from_frame (*frame_data*)

converts data stored in a color channel to normalized data

Parameters

frame_data (*ndarray*) –

data_to_frame (*normalized_data*)

converts normalized data to data being stored in a color channel

Parameters

normalized_data (*ndarray*) –

Return type

ndarray

dtype: `dtype[Any] | None | type[Any] | _SupportsDType[dtype[Any]] | str | tuple[Any, int] | tuple[Any, SupportsIndex] | Sequence[SupportsIndex] | list[Any] | _DTypeDict | tuple[Any, Any]`

numpy dtype corresponding to the data of a single channel

property max_value: `float | int`

maximal value stored in a color channel

pix_fmt_data: `str`

name of the pixel format used in the frame data

Type

`str`

pix_fmt_file: `str`

name of the pixel format used in the codec

Type

`str`

find_format (*channels*, *bits_per_channel=8*)

find a defined FFmpegFormat that satisfies the requirements

Parameters

- **channels** (*int*) – Minimal number of color channels
- **bits_per_channel** (*int*) – Minimal number of bits per channel

Returns

Identifier for a format that satisfies the requirements (but might have more channels or more bits per channel than requested. *None* is returned if no format can be identified.

Return type

`str`

```

formats = {'gbrap16le': FFmpegFormat(pix_fmt_file='gbrap16le',
pix_fmt_data='gbrap16le', channels=4, bits_per_channel=16,
dtype=dtype('uint16'), codec='ffv1'), 'gbrp16le':
FFmpegFormat(pix_fmt_file='gbrp16le', pix_fmt_data='gbrp16le', channels=3,
bits_per_channel=16, dtype=dtype('uint16'), codec='ffv1'), 'gray':
FFmpegFormat(pix_fmt_file='gray', pix_fmt_data='gray', channels=1,
bits_per_channel=8, dtype=<class 'numpy.uint8'>, codec='ffv1'), 'gray16le':
FFmpegFormat(pix_fmt_file='gray16le', pix_fmt_data='gray16le', channels=1,
bits_per_channel=16, dtype=dtype('uint16'), codec='ffv1'), 'rgb24':
FFmpegFormat(pix_fmt_file='rgb24', pix_fmt_data='rgb24', channels=3,
bits_per_channel=8, dtype=<class 'numpy.uint8'>, codec='ffv1'), 'rgb32':
FFmpegFormat(pix_fmt_file='rgb32', pix_fmt_data='rgb32', channels=4,
bits_per_channel=8, dtype=<class 'numpy.uint8'>, codec='ffv1')}

```

dict of pre-defined *FFmpegFormat* formats

4.6.7 `pde.tools.math` module

Auxiliary mathematical functions

class `OnlineStatistics` (*args, **kwargs)

Bases: *OnlineStatistics*

class for using an online algorithm for calculating statistics

```

class_type = jitclass.OnlineStatistics#7f3ffc1e4a90<min:float64,
max:float64,mean:float64,_mean2:float64,count:uint64>

```

count: `int`

recorded number of items

Type

`int`

mean: `float`

recorded mean

Type

`float`

class `SmoothData1D` (x, y, sigma=None)

Bases: *object*

allows smoothing data in 1d using a Gaussian kernel of defined width

The data is given a pairs of x and y , the assumption being that there is an underlying relation $y = f(x)$.

initialize with data

Parameters

- **x** – List of x values
- **y** – List of y values
- **sigma** (*float*) – The size of the smoothing window in units of x . If omitted, the average distance of x values multiplied by *sigma_auto_scale* is used.

property bounds: `tuple[float, float]`

return minimal and maximal x values

derivative (*xs*)

return the derivative of the smoothed values for the positions *xs*

Note that this value

Parameters

xs (list of `ndarray`) – the x-values

Returns

The associated values of the derivative

Return type

`ndarray`

sigma_auto_scale: `float` = 10

scale for setting automatic values for sigma

Type

`float`

4.6.8 `pde.tools.misc` module

Miscellaneous python functions

<code>module_available</code>	check whether a python module is available
<code>ensure_directory_exists</code>	creates a folder if it not already exists
<code>preserve_scalars</code>	decorator that makes vectorized methods work with scalars
<code>decorator_arguments</code>	make a decorator usable with and without arguments:
<code>import_class</code>	import a class or module given an identifier
<code>classproperty</code>	decorator that can be used to define read-only properties for classes.
<code>hybridmethod</code>	descriptor that can be used as a decorator to allow calling a method both as a classmethod and an instance method
<code>estimate_computation_speed</code>	estimates the computation speed of a function
<code>hdf_write_attributes</code>	write (JSON-serialized) attributes to a hdf file
<code>number</code>	convert a value into a float or complex number
<code>get_common_dtype</code>	returns a dtype in which all arguments can be represented
<code>number_array</code>	convert an array with arbitrary dtype either to <code>np.double</code> or <code>np.cdouble</code>

class `classproperty` (*fget=None, doc=None*)

Bases: `property`

decorator that can be used to define read-only properties for classes.

This is inspired by the implementation of `astropy`, see astropy.org.

Example

The decorator can be used much like the `property` decorator:

```
class Test():
    item: str = 'World'
```

(continues on next page)

(continued from previous page)

```

@classproperty
def message(cls):
    return 'Hello ' + cls.item

print(Test.message)

```

deleter (*fdel*)

Descriptor to obtain a copy of the property with a different deleter.

getter (*fget*)

Descriptor to obtain a copy of the property with a different getter.

setter (*fset*)

Descriptor to obtain a copy of the property with a different setter.

decorator_arguments (*decorator*)

make a decorator usable with and without arguments:

The resulting decorator can be used like `@decorator` or `@decorator(*args, **kwargs)`Inspired by <https://stackoverflow.com/a/14412901/932593>**Parameters****decorator** (*Callable*) – the decorator that needs to be modified**Returns**

the decorated function

Return type*Callable***ensure_directory_exists** (*folder*)

creates a folder if it not already exists

Parameters**folder** (*str*) – path of the new folder**estimate_computation_speed** (*func*, **args*, ***kwargs*)

estimates the computation speed of a function

Parameters**func** (*callable*) – The function to call**Returns**

the number of times the function can be calculated in one second. The inverse is thus the runtime in seconds per function call

Return type*float***get_common_dtype** (**args*)

returns a dtype in which all arguments can be represented

Parameters***args** – All items (arrays, scalars, etc) to be checked

Returns: numpy.cdouble if any entry is complex, otherwise np.double

hdf_write_attributes (*hdf_path*, *attributes=None*, *raise_serialization_error=False*)

write (JSON-serialized) attributes to a hdf file

Parameters

- **hdf_path** – Path to a group or dataset in an open HDF file
- **attributes** (*dict*) – Dictionary with values written as attributes
- **raise_serialization_error** (*bool*) – Flag indicating whether serialization errors are raised or silently ignored

Return type

None

class hybridmethod (*fclass*, *finstance=None*, *doc=None*)

Bases: *object*

descriptor that can be used as a decorator to allow calling a method both as a classmethod and an instance method

Adapted from <https://stackoverflow.com/a/28238047>

classmethod (*fclass*)

instancemethod (*finstance*)

import_class (*identifier*)

import a class or module given an identifier

Parameters

identifier (*str*) – The identifier can be a module or a class. For instance, calling the function with the string *identifier* == *'numpy.linalg.norm'* is roughly equivalent to running *from numpy.linalg import norm* and would return a reference to *norm*.

module_available (*module_name*)

check whether a python module is available

Parameters

module_name (*str*) – The name of the module

Returns

True if the module can be imported and *False* otherwise

Return type

bool

number (*value*)

convert a value into a float or complex number

Parameters

value (*Number or str*) – The value which needs to be converted

Return type

int | float | complex

Result:

Number: A complex number or a float if the imaginary part vanishes

number_array (*data*, *dtype=None*, *copy=True*)

convert an array with arbitrary dtype either to *np.double* or *np.cdouble*

Parameters

- **data** (`ndarray`) – The data that needs to be converted to a float array. This can also be any iterable of numbers.
- **dtype** (`numpy dtype`) – The data type of the field. All the numpy dtypes are supported. If omitted, it will be determined from *data* automatically.
- **copy** (`bool`) – Whether the data must be copied (in which case the original array is left untouched). Note that data will always be copied when changing the dtype.

Returns

An array with the correct dtype

Return type

`ndarray`

preserve_scalars (*method*)

decorator that makes vectorized methods work with scalars

This decorator allows to call functions that are written to work on numpy arrays to also accept python scalars, like *int* and *float*. Essentially, this wrapper turns them into an array and unboxes the result.

Parameters

method (*TFunc*) – The method being decorated

Returns

The decorated method

Return type

TFunc

skipUnlessModule (*module_names*)

decorator that skips a test when a module is not available

Parameters

module_names (*str*) – The name of the required module(s)

Returns

A function, so this can be used as a decorator

Return type

Callable[[*TFunc*], *TFunc*]

4.6.9 `pde.tools.mpi` module

Auxillary functions and variables for dealing with MPI multiprocessing

Warning: These functions are mostly no-ops unless MPI is properly installed and python code was started using `mpirun` or `mpiexec`. Please refer to the documentation of your MPI distribution for details.

<code>mpi_send</code>	send data to another MPI node
<code>mpi_recv</code>	receive data from another MPI node
<code>mpi_allreduce</code>	combines data from all MPI nodes

initialized: `bool = False`

Flag determining whether mpi was initialized (and is available)

Type`bool`**is_main:** `bool = True`

Flag indicating whether the current process is the main process (with ID 0)

Type`bool`**mpi_allreduce** (*data*, *operator=None*)

combines data from all MPI nodes

Note that complex datatypes and user-defined functions are not properly supported.

Parameters

- **data** – Data being send from this node to all others
- **operator** (*int* | *str* | *None*) – The operator used to combine all data. Possible options are summarized in the `IntEnum numba_mpi.Operator`.

Returns

The accumulated data

mpi_recv (*data*, *source*, *tag*)

receive data from another MPI node

Parameters

- **data** – A buffer into which the received data is written
- **dest** (*int*) – The ID of the sending node
- **tag** (*int*) – A numeric tag identifying the message

Return type

None

mpi_send (*data*, *dest*, *tag*)

send data to another MPI node

Parameters

- **data** – The data being send
- **dest** (*int*) – The ID of the receiving node
- **tag** (*int*) – A numeric tag identifying the message

Return type

None

ol_mpi_allreduce (*data*, *operator=None*)overload the *mpi_allreduce* function**Parameters****operator** (*int* | *str* | *None*) –**ol_mpi_recv** (*data*, *source*, *tag*)overload the *mpi_recv* function**Parameters**

- **source** (*int*) –
- **tag** (*int*) –

`ol_mpi_send(data, dest, tag)`

overload the `mpi_send` function

Parameters

- `dest(int)` –
- `tag(int)` –

`parallel_run: bool = False`

Flag indicating whether the current run is using multiprocessing

Type

`bool`

`rank: int = 0`

ID of the current process

Type

`int`

`size: int = 1`

Total process count

Type

`int`

4.6.10 `pde.tools.numba` module

Helper functions for just-in-time compilation with numba

`class Counter(value=0)`

Bases: `object`

helper class for implementing JIT_COUNT

We cannot use a simple integer for this, since integers are immutable, so if one imports `JIT_COUNT` from this module it would always stay at the fixed value it had when it was first imported. The workaround would be to import the symbol every time the counter is read, but this is error-prone. Instead, we implement a thin wrapper class around an int, which only supports reading and incrementing the value. Since this object is now mutable it can be used easily. A disadvantage is that the object needs to be converted to int before it can be used in most expressions.

Parameters

`value(int)` –

`increment()`

`flat_idx(arr, i)`

helper function allowing indexing of scalars as if they arrays

Parameters

- `arr(ndarray)` –
- `i(int)` –

Return type

`int | float | complex`

get_common_numba_dtype (*args)

returns a numba numerical type in which all arrays can be represented

Parameters

***args** – All items to be tested

Returns: numba.complex128 if any entry is complex, otherwise numba.double

jit (function, signature=None, parallel=False, **kwargs)

apply nb.jit with predefined arguments

Parameters

- **function** (*TFunc*) – The function which is jitted
- **signature** – Signature of the function to compile
- **parallel** (*bool*) – Allow parallel compilation of the function
- ****kwargs** – Additional arguments to *nb.jit*

Returns

Function that will be compiled using numba

Return type

TFunc

make_array_constructor (arr)

returns an array within a jitted function using basic information

Parameters

arr (*ndarray*) – The array that should be accessible within jit

Return type

Callable[[*ndarray*]

Warning: A reference to the array needs to be retained outside the numba code to prevent garbage collection from removing the array

numba_dict (data=None)

converts a python dictionary to a numba typed dictionary

Parameters

data (*dict*[*str*, *Any*] | *None*) –

Return type

Dict | *None*

numba_environment ()

return information about the numba setup used

Returns

(dict) information about the numba setup

Return type

dict[*str*, *Any*]

ol_flat_idx (arr, i)

helper function allowing indexing of scalars as if they arrays

random_seed (*seed=0*)

sets the seed of the random number generator of numpy and numba

Parameters

seed (*int*) – Sets random seed

Return type

None

4.6.11 pde.tools.output module

Python functions for handling output

<code>get_progress_bar_class</code>	returns a class that behaves as progress bar.
<code>display_progress</code>	displays a progress bar when iterating
<code>in_jupyter_notebook</code>	checks whether we are in a jupyter notebook
<code>BasicOutput</code>	class that writes text line to stdout
<code>JupyterOutput</code>	class that writes text lines as html in a jupyter cell

class BasicOutput (*stream=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='utf-8'>*)

Bases: `OutputBase`

class that writes text line to stdout

Parameters

stream – The stream where the lines are written

show ()

shows the actual text

class JupyterOutput (*header="", footer=""*)

Bases: `OutputBase`

class that writes text lines as html in a jupyter cell

Parameters

- **header** (*str*) – The html code written before all lines
- **footer** (*str*) – The html code written after all lines

show ()

shows the actual text

class OutputBase

Bases: `object`

base class for output management

abstract show ()

shows the actual text

display_progress (*iterator, total=None, enabled=True, **kwargs*)

displays a progress bar when iterating

Parameters

- **iterator** (*iter*) – The iterator

- **total** (*int*) – Total number of steps
- **enabled** (*bool*) – Flag determining whether the progress is display
- ****kwargs** – All extra arguments are forwarded to the progress bar class

Returns

A class that behaves as the original iterator, but shows the progress alongside iteration.

get_progress_bar_class (*fancy=True*)

returns a class that behaves as progress bar.

This either uses classes from the optional *tqdm* package or a simple version that writes dots to stderr, if the class is not available.

Parameters

fancy (*bool*) – Flag determining whether a fancy progress bar should be used in jupyter notebooks (if *ipywidgets* is installed)

in_jupyter_notebook ()

checks whether we are in a jupyter notebook

Return type

bool

4.6.12 `pde.tools.parameters` module

Infrastructure for managing classes with parameters

One aim is to allow easy management of inheritance of parameters.

<i>Parameter</i>	class representing a single parameter
<i>DeprecatedParameter</i>	a parameter that can still be used normally but is deprecated
<i>HideParameter</i>	a helper class that allows hiding parameters of the parent classes
<i>Parameterized</i>	a mixin that manages the parameters of a class
<i>get_all_parameters</i>	get a dictionary with all parameters of all registered classes

class **DeprecatedParameter** (*name*, *default_value=None*, *cls=<class 'object'>*, *description=""*, *hidden=False*, *extra=None*)

Bases: *Parameter*

a parameter that can still be used normally but is deprecated

initialize a parameter

Parameters

- **name** (*str*) – The name of the parameter
- **default_value** – The default value
- **cls** – The type of the parameter, which is used for conversion
- **description** (*str*) – A string describing the impact of this parameter. This description appears in the parameter help
- **hidden** (*bool*) – Whether the parameter is hidden in the description summary

- **extra** (*dict*) – Extra arguments that are stored with the parameter

class HideParameter (*name*)

Bases: `object`

a helper class that allows hiding parameters of the parent classes

Parameters

name (*str*) – The name of the parameter

class Parameter (*name, default_value=None, cls=<class 'object'>, description="", hidden=False, extra=None*)

Bases: `object`

class representing a single parameter

initialize a parameter

Parameters

- **name** (*str*) – The name of the parameter
- **default_value** – The default value
- **cls** – The type of the parameter, which is used for conversion
- **description** (*str*) – A string describing the impact of this parameter. This description appears in the parameter help
- **hidden** (*bool*) – Whether the parameter is hidden in the description summary
- **extra** (*dict*) – Extra arguments that are stored with the parameter

convert (*value=None*)

converts a *value* into the correct type for this parameter. If *value* is not given, the default value is converted.

Note that this does not make a copy of the values, which could lead to unexpected effects where the default value is changed by an instance.

Parameters

value – The value to convert

Returns

The converted value, which is of type *self.cls*

class Parameterized (*parameters=None*)

Bases: `object`

a mixin that manages the parameters of a class

initialize the parameters of the object

Parameters

parameters (*dict*) – A dictionary of parameters to change the defaults. The allowed parameters can be obtained from `get_parameters()` or displayed by calling `show_parameters()`.

get_parameter_default (*name*)

return the default value for the parameter with *name*

Parameters

name (*str*) – The parameter name

classmethod `get_parameters` (*include_hidden=False, include_deprecated=False, sort=True*)

return a dictionary of parameters that the class supports

Parameters

- **include_hidden** (*bool*) – Include hidden parameters
- **include_deprecated** (*bool*) – Include deprecated parameters
- **sort** (*bool*) – Return ordered dictionary with sorted keys

Returns

a dictionary of instance of *Parameter* with their names as keys.

Return type

dict

parameters_default: *Sequence[Parameter | HideParameter]* = []

show_parameters (*description=None, sort=False, show_hidden=False, show_deprecated=False*)

show all parameters in human readable format

Parameters

- **description** (*bool*) – Flag determining whether the parameter description is shown. The default is to show the description only when we are in a jupyter notebook environment.
- **sort** (*bool*) – Flag determining whether the parameters are sorted
- **show_hidden** (*bool*) – Flag determining whether hidden parameters are shown
- **show_deprecated** (*bool*) – Flag determining whether deprecated parameters are shown
- **default_value** (*bool*) – Flag determining whether the default values or the current values are shown

All flags default to *False*.

get_all_parameters (*data='name'*)

get a dictionary with all parameters of all registered classes

Parameters

data (*str*) – Determines what data is returned. Possible values are 'name', 'value', or 'description', to return the respective information about the parameters.

Return type

dict[str, Any]

sphinx_display_parameters (*app, what, name, obj, options, lines*)

helper function to display parameters in sphinx documentation

Example

This function should be connected to the 'autodoc-process-docstring' event like so:

```
app.connect('autodoc-process-docstring', sphinx_display_parameters)
```

4.6.13 pde.tools.parse_duration module

Parsing time durations from strings

This module provides a function that parses time durations from strings. It has been copied from the django software, which comes with the following notes:

Copyright (c) Django Software Foundation and individual contributors. All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

1. Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
3. Neither the name of Django nor the names of its contributors may be used to endorse or promote products derived from this software without specific prior written permission.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS “AS IS” AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT OWNER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

parse_duration (*value*)

Parse a duration string and return a `datetime.timedelta`.

Parameters

value (*str*) – A time duration given as text. The preferred format for durations is ‘%d %H:%M:%S.%f’. This function also supports ISO 8601 representation and PostgreSQL’s day-time interval format.

Returns

An instance representing the duration.

Return type

`datetime.timedelta`

4.6.14 pde.tools.plotting module

Tools for plotting and controlling plot output using context managers

<code>add_scaled_colorbar</code>	add a vertical color bar to an image plot
<code>disable_interactive</code>	context manager disabling the interactive mode of matplotlib
<code>plot_on_axes</code>	decorator for a plot method or function that uses a single axes
<code>plot_on_figure</code>	decorator for a plot method or function that fills an entire figure
<code>PlotReference</code>	contains all information to update a plot element
<code>BasicPlottingContext</code>	basic plotting using just matplotlib
<code>JupyterPlottingContext</code>	plotting in a jupyter widget using the <i>inline</i> backend
<code>get_plotting_context</code>	returns a suitable plotting context
<code>napari_add_layers</code>	adds layers to a napari viewer

class BasicPlottingContext (*fig_or_ax=None, title=None, show=True*)

Bases: *PlottingContextBase*

basic plotting using just matplotlib

Parameters

- **fig_or_ax** – If axes are given, they are used. If a figure is given, it is set as active.
- **title** (*str*) – The shown in the plot
- **show** (*bool*) – Flag determining whether plots are actually shown

class JupyterPlottingContext (*title=None, show=True*)

Bases: *PlottingContextBase*

plotting in a jupyter widget using the *inline* backend

Parameters

- **title** (*str*) – The shown in the plot
- **show** (*bool*) – Flag determining whether plots are actually shown

close()

close the plot

supports_update: **bool = False**

flag indicating whether the context supports that plots can be updated with out redrawing the entire plot. The jupyter backend (*inline*) requires replotting of the entire figure, so an update is not supported.

class PlotReference (*ax, element, parameters=None*)

Bases: *object*

contains all information to update a plot element

Parameters

- **ax** (*matplotlib.axes.Axes*) – The axes of the element
- **element** (*matplotlib.artist.Artist*) – The actual element
- **parameters** (*dict*) – Parameters to recreate the plot element

ax

element

parameters

class `PlottingContextBase` (*title=None, show=True*)

Bases: `object`

base class of the plotting contexts

Example

The context wraps calls to the `matplotlib.pyplot` interface:

```
context = PlottingContext()
with context:
    plt.plot(...)
    plt.xlabel(...)
```

Parameters

- **title** (*str*) – The shown in the plot
- **show** (*bool*) – Flag determining whether plots are actually shown

close ()

close the plot

fig: `mpl_figure.Figure` | `None`

supports_update: `bool` = `True`

flag indicating whether the context supports that plots can be updated with out redrawing the entire plot

add_scaled_colorbar (*axes_image, ax=None, aspect=20, pad_fraction=0.5, label="", **kwargs*)

add a vertical color bar to an image plot

The height of the colorbar is now adjusted to the plot, so that the width determined by *aspect* is now given relative to the height. Moreover, the gap between the colorbar and the plot is now given in units of the fraction of the width by *pad_fraction*.

Inspired by <https://stackoverflow.com/a/33505522/932593>

Parameters

- **axes_image** (`matplotlib.cm.ScalarMappable`) – Mappable object, e.g., returned from `matplotlib.pyplot.imshow()`
- **ax** (`matplotlib.axes.Axes`) – The current figure axes from which space is taken for the colorbar. If omitted, the axes in which the *axes_image* is shown is taken.
- **aspect** (*float*) – The target aspect ratio of the colorbar
- **pad_fraction** (*float*) – Width of the gap between colorbar and image
- **label** (*str*) – Set a label for the colorbar
- ****kwargs** – Additional parameters are passed to colorbar call

Returns

The resulting Colorbar object

Return type

`Colorbar`

disable_interactive()

context manager disabling the interactive mode of matplotlib

This context manager restores the previous state after it is done. Details of the interactive mode are described in `matplotlib.interactive()`.

get_plotting_context (*context=None, title=None, show=True*)

returns a suitable plotting context

Parameters

- **context** – An instance of `PlottingContextBase` or an instance of `matplotlib.axes.Axes` or `matplotlib.figure.Figure` to determine where the plotting will happen. If omitted, the context is determined automatically.
- **title** (*str*) – The title shown in the plot
- **show** (*bool*) – Determines whether the plot is shown while the simulation is running. If *False*, the files are created in the background.

Returns

The plotting context

Return type

`PlottingContextBase`

in_ipython()

try to detect whether we are in an ipython shell, e.g., a jupyter notebook

Return type

`bool`

napari_add_layers (*viewer, layers_data*)

adds layers to a `napari` viewer

Parameters

- **viewer** (`napari.viewer.Viewer`) – The napari application
- **layers_data** (*dict*) – Data for all layers that will be added.

napari_viewer (*grid, run=None, close=False, **kwargs*)

creates an napari viewer for interactive plotting

Parameters

- **grid** (`pde.grids.base.GridBase`) – The grid defining the space
- **run** (*bool*) – Whether to run the event loop of napari.
- **close** (*bool*) – Whether to close the viewer immediately (e.g. for testing)
- ****kwargs** – Extra arguments are passed to `napari.Viewer`

Return type

`Generator[napari.viewer.Viewer, None, None]`

class nested_plotting_check

Bases: `object`

context manager that checks whether it is the root plotting call

Example

The context manager can be used in plotting calls to check for nested plotting calls:

```
with nested_plotting_check() as is_outermost_plot_call:
    make_plot(...) # could potentially call other plotting methods
    if is_outermost_plot_call:
        plt.show()
```

plot_on_axes (*wrapped=None, update_method=None*)

decorator for a plot method or function that uses a single axes

This decorator adds typical options for creating plots that fill a single axes. These options are available via keyword arguments. To avoid redundancy in describing these options in the docstring, the placeholder *{PLOT_ARGS}* can be added to the docstring of the wrapped function or method and will be replaced by the appropriate text. Note that the decorator can be used on both functions and methods.

Example

The following example illustrates how this decorator can be used to implement plotting for a given class. In particular, supplying the *update_method* will allow efficient dynamical plotting:

```
class State:
    def __init__(self) -> None:
        self.data = np.arange(8)

    def _update_plot(self, reference):
        reference.element.set_ydata(self.data)

    @plot_on_axes(update_method='_update_plot')
    def plot(self, ax):
        line, = ax.plot(np.arange(8), self.data)
        return PlotReference(ax, line)

@plot_on_axes
def make_plot(ax):
    ax.plot(...)
```

When *update_method* is absent, the method can still be used for plotting, but dynamic updating, e.g., by `pde.trackers.PlotTracker`, is not possible.

Parameters

- **wrapped** (*callable*) – Function to be wrapped
- **update_method** (*callable or str*) – Method to call to update the plot. The argument of the new method will be the result of the initial call of the wrapped method.

plot_on_figure (*wrapped=None, update_method=None*)

decorator for a plot method or function that fills an entire figure

This decorator adds typical options for creating plots that fill an entire figure. This decorator adds typical options for creating plots that fill a single axes. These options are available via keyword arguments. To avoid redundancy in describing these options in the docstring, the placeholder *{PLOT_ARGS}* can be added to the docstring of the

wrapped function or method and will be replaced by the appropriate text. Note that the decorator can be used on both functions and methods.

Example

The following example illustrates how this decorator can be used to implement plotting for a given class. In particular, supplying the `update_method` will allow efficient dynamical plotting:

```
class State:
    def __init__(self) -> None:
        self.data = np.random.random((2, 8))

    def _update_plot(self, reference):
        ref1, ref2 = reference
        ref1.element.set_ydata(self.data[0])
        ref2.element.set_ydata(self.data[1])

    @plot_on_figure(update_method='_update_plot')
    def plot(self, fig):
        ax1, ax2 = fig.subplots(1, 2)
        l1, = ax1.plot(np.arange(8), self.data[0])
        l2, = ax2.plot(np.arange(8), self.data[1])
        return [PlotReference(ax1, l1), PlotReference(ax2, l2)]

@plot_on_figure
def make_plot(fig):
    ...
```

When `update_method` is not supplied, the method can still be used for plotting, but dynamic updating, e.g., by `pde.trackers.PlotTracker`, is not possible.

Parameters

- **wrapped** (*callable*) – Function to be wrapped
- **update_method** (*callable or str*) – Method to call to update the plot. The argument of the new method will be the result of the initial call of the wrapped method.

4.6.15 pde.tools.spectral module

Functions making use of spectral decompositions

`make_colored_noise`

Return a function creating an array of random values that obey

make_colored_noise (*shape, dx=1.0, exponent=0, scale=1, rng=None*)

Return a function creating an array of random values that obey

$$\langle c(\mathbf{k})c(\mathbf{k}') \rangle = \Gamma^2 |\mathbf{k}|^\nu \delta(\mathbf{k} - \mathbf{k}')$$

in spectral space on a Cartesian grid. The special case $\nu = 0$ corresponds to white noise. For simplicity, the correlations respect periodic boundary conditions.

Parameters

- **shape** (*tuple of ints*) – Number of supports points in each spatial dimension. The number of the list defines the spatial dimension.
- **dx** (*float or list of floats*) – Discretization along each dimension. A uniform discretization in each direction can be indicated by a single number.
- **exponent** (*float*) – Exponent ν of the power spectrum
- **scale** (*float*) – Scaling factor Γ determining noise strength
- **rng** (*Generator*) – Random number generator (default: `default_rng()`)

Returns

a function returning a random realization

Return type

callable

4.6.16 `pde.tools.typing` module

Provides support for mypy type checking of the package

class `AdjacentEvaluator` (**args, **kwargs*)

Bases: `Protocol`

class `CellVolume` (**args, **kwargs*)

Bases: `Protocol`

class `GhostCellSetter` (**args, **kwargs*)

Bases: `Protocol`

class `OperatorFactory` (**args, **kwargs*)

Bases: `Protocol`

a factory function that creates an operator for a particular grid

class `OperatorType` (**args, **kwargs*)

Bases: `Protocol`

an operator that acts on an array

class `VirtualPointEvaluator` (**args, **kwargs*)

Bases: `Protocol`

4.7 `pde.trackers` package

Classes for tracking simulation results in controlled interrupts

Trackers are classes that periodically receive the state of the simulation to analyze, store, or output it. The trackers defined in this module are:

<code>CallbackTracker</code>	Tracker calling a function periodically
<code>ProgressTracker</code>	Tracker showing the progress of the simulation
<code>PrintTracker</code>	Tracker printing data to a stream (default: stdout)
<code>PlotTracker</code>	Tracker plotting data on screen, to files, or writes a movie
<code>LivePlotTracker</code>	PlotTracker with defaults for live plotting
<code>DataTracker</code>	Tracker storing custom data obtained by calling a function
<code>SteadyStateTracker</code>	Tracker aborting the simulation once steady state is reached
<code>RuntimeTracker</code>	Tracker interrupting the simulation once a duration has passed
<code>ConsistencyTracker</code>	Tracker interrupting the simulation when the state is not finite
<code>InteractivePlotTracker</code>	Tracker showing the state interactively in napari

Some trackers can also be referenced by name for convenience when using them in simulations. The list of supported names is returned by `get_named_trackers()`.

Multiple trackers can be collected in a `TrackerCollection`, which provides methods for handling them efficiently. Moreover, custom trackers can be implemented by deriving from `TrackerBase`. Note that trackers generally receive a view into the current state, implying that they can adjust the state by modifying it in-place. Moreover, trackers can abort the simulation by raising the special exception `StopIteration`.

For each tracker, the time at which the simulation is interrupted can be decided using one of the following classes:

<code>FixedInterrupts</code>	class representing a list of interrupt times
<code>ConstantInterrupts</code>	class representing equidistantly spaced time interrupts
<code>LogarithmicInterrupts</code>	class representing logarithmically spaced time interrupts
<code>RealtimeInterrupts</code>	class representing time interrupts spaced equidistantly in real time

In particular, interrupts can be specified conveniently using `parse_interrupt()`.

4.7.1 `pde.trackers.base` module

Base classes for trackers

exception `FinishedSimulation`

Bases: `StopIteration`

exception for signaling that simulation finished successfully

class `TrackerBase` (`interrupts=1, *, interval=None`)

Bases: `object`

base class for implementing trackers

Parameters

interrupts (`InterruptData`) – Determines when the tracker interrupts the simulation. A single number determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine-grained control is possible by passing an instance of classes defined in `interrupts`.

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

info (*dict*) – Extra information from the simulation

Return type

None

classmethod from_data (*data, **kwargs*)

create tracker class from given data

Parameters

data (*str* or *TrackerBase*) – Data describing the tracker

Returns

An instance representing the tracker

Return type

TrackerBase

abstract handle (*field, t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

initialize (*field, info=None*)

initialize the tracker with information about the simulation

Parameters

- **field** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

class TrackerCollection (*trackers=None*)

Bases: *object*

List of trackers providing methods to handle them efficiently

trackers

List of the trackers in the collection

Type

list

Parameters

trackers (*list[TrackerBase]* / *None*) – List of trackers that are to be handled.

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

info (*dict*) – Extra information from the simulation

Return type

None

classmethod from_data (*data, **kwargs*)

create tracker collection from given data

Parameters

data (*Sequence[TrackerBase | str] | TrackerBase | str | None*) – Data describing the tracker collection

Returns

An instance representing the tracker collection

Return type

TrackerCollection

handle (*state, t, atol=1e-08*)

handle all trackers

Parameters

- **state** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time
- **atol** (*float*) – An absolute tolerance that is used to determine whether a tracker should be called now or whether the simulation should be carried on more timesteps. This is basically used to predict the next time to decided which one is closer.

Returns

The next time the simulation needs to be interrupted to handle a tracker.

Return type

float

initialize (*field, info=None*)

initialize the tracker with information about the simulation

Parameters

- **field** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

time_next_action: *float*

The time of the next interrupt of the simulation

Type

float

tracker_action_times: `list[float]`

Times at which the trackers need to be handled next

Type

`list`

get_named_trackers()

returns all named trackers

Returns

a mapping of names to the actual tracker classes.

Return type

`dict`

4.7.2 `pde.trackers.interactive` module

Special module for defining an interactive tracker that uses napari to display fields

class InteractivePlotTracker (*interrupts='0:01', *, close=True, show_time=False, interval=None*)

Bases: `TrackerBase`

Tracker showing the state interactively in napari

Note: The interactive tracker uses the python `multiprocessing` module to run `napari` externally. The multiprocessing module has limitations on some platforms, which requires some care when writing your own programs. In particular, the main method needs to be safe-guarded so that the main module can be imported again after spawning a new process. An established pattern that works is to introduce a function *main* in your code, which you call using the following pattern

```
def main():
    # here goes your main code

if __name__ == "__main__":
    main()
```

The last two lines ensure that the *main* function is only called when the module is run initially and not again when it is re-imported.

Parameters

- **interrupts** (`InterruptData`) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.
- **close** (`bool`) – Flag indicating whether the napari window is closed automatically at the end of the simulation. If *False*, the tracker blocks when *finalize* is called until the user closes napari manually.
- **show_time** (`bool`) – Whether to indicate the time

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

info (*dict*) – Extra information from the simulation

Return type

None

handle (*state*, *t*)

handle data supplied to this tracker

Parameters

- **state** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

initialize (*state*, *info=None*)

initialize the tracker with information about the simulation

Parameters

- **state** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

name = 'interactive'

class NapariViewer (*state*, *t_initial=None*)

Bases: *object*

allows viewing and updating data in a separate napari process

Parameters

- **state** (*pde.fields.base.FieldBase*) – The initial state to be shown
- **t_initial** (*float*) – The initial time. If *None*, no time will be shown.

close (*force=True*)

closes the napari process

Parameters

force (*bool*) – Whether to force closing of the napari program. If this is *False*, this method blocks until the user closes napari manually.

update (*state*, *t*)

update the state in the napari viewer

Parameters

- **state** (*pde.fields.base.FieldBase*) – The new state
- **t** (*float*) – Current time

napari_process (*data_channel*, *initial_data*, *t_initial=None*, *viewer_args=None*)

multiprocessing.Process running `napari`

Parameters

- **data_channel** (*multiprocessing.Queue*) – queue instance to receive data to view
- **initial_data** (*dict*) – Initial data to be shown by napari. The layers are named according to the keys in the dictionary. The associated value needs to be a tuple, where the first item is a string indicating the type of the layer and the second carries the associated data
- **t_initial** (*float*) – Initial time
- **viewer_args** (*dict*) – Additional arguments passed to the napari viewer

4.7.3 pde.trackers.interrupts module

Module defining classes for time interrupts for trackers

The provided interrupt classes are:

<i>ConstantInterrupts</i>	class representing equidistantly spaced time interrupts
<i>FixedInterrupts</i>	class representing a list of interrupt times
<i>LogarithmicInterrupts</i>	class representing logarithmically spaced time interrupts
<i>RealtimeInterrupts</i>	class representing time interrupts spaced equidistantly in real time

class ConstantInterrupts (*dt=1*, *t_start=None*)

Bases: *InterruptsBase*

class representing equidistantly spaced time interrupts

Parameters

- **dt** (*float*) – The duration between subsequent interrupts. This is measured in simulation time units.
- **t_start** (*float*, *optional*) – The time after which the tracker becomes active. If omitted, the tracker starts recording right away. This argument can be used for an initial equilibration period during which no data is recorded.

copy ()

return a copy of this instance

initialize (*t*)

initialize the interrupt class

Parameters

- **t** (*float*) – The starting time of the simulation

Returns

The first time the simulation needs to be interrupted

Return type

float

next (*t*)

computes the next time point

Parameters

t (*float*) – The current time point of the simulation. The returned next time point lies later than this time, so interrupts might be skipped.

Returns

The next time point

Return type

float

class FixedInterrupts (*interrupts*)

Bases: *InterruptsBase*

class representing a list of interrupt times

Parameters

interrupts (*np.ndarray* | *Sequence[float]*) –

copy ()

return a copy of this instance

initialize (*t*)

initialize the interrupt class

Parameters

t (*float*) – The starting time of the simulation

Returns

The first time the simulation needs to be interrupted

Return type

float

next (*t*)

computes the next time point

Parameters

t (*float*) – The current time point of the simulation. The returned next time point lies later than this time, so interrupts might be skipped.

Returns

The next time point

Return type

float

class InterruptsBase

Bases: *object*

base class for implementing interrupts

abstract copy ()

return a copy of this instance

Parameters

self (*TInterrupt*) –

Return type

TInterrupt

dt: `float`

current time difference between interrupts

Type

`float`

abstract initialize (*t*)

initialize the interrupt class

Parameters

t (`float`) – The starting time of the simulation

Returns

The first time the simulation needs to be interrupted

Return type

`float`

abstract next (*t*)

computes the next time point

Parameters

t (`float`) – The current time point of the simulation. The returned next time point lies later than this time, so interrupts might be skipped.

Returns

The next time point

Return type

`float`

class LogarithmicInterrupts (*dt_initial=1, factor=1, t_start=None*)

Bases: `ConstantInterrupts`

class representing logarithmically spaced time interrupts

Parameters

- **dt_initial** (`float`) – The initial duration between subsequent interrupts. This is measured in simulation time units.
- **factor** (`float`) – The factor by which the time between interrupts is increased every time. Values larger than one lead to time interrupts that are increasingly further apart.
- **t_start** (`float`, *optional*) – The time after which the tracker becomes active. If omitted, the tracker starts recording right away. This argument can be used for an initial equilibration period during which no data is recorded.

next (*t*)

computes the next time point

Parameters

t (`float`) – The current time point of the simulation. The returned next time point lies later than this time, so interrupts might be skipped.

Returns

The next time point

Return type

`float`

class `RealtimeInterrupts` (*duration*, *dt_initial*=0.01)

Bases: `ConstantInterrupts`

class representing time interrupts spaced equidistantly in real time

This spacing is only achieved approximately and depends on the initial value set by *dt_initial* and the actual variation in computation speed.

Parameters

- **duration** (*float* or *str*) – The duration (in real seconds) that the interrupts should be spaced apart. The duration can also be given as a string, which is then parsed using the function `parse_duration()`.
- **dt_initial** (*float*) – The initial duration between subsequent interrupts. This is measured in simulation time units.

initialize (*t*)

initialize the interrupt class

Parameters

t (*float*) – The starting time of the simulation

Returns

The first time the simulation needs to be interrupted

Return type

float

next (*t*)

computes the next time point

Parameters

t (*float*) – The current time point of the simulation. The returned next time point lies later than this time, so interrupts might be skipped.

Returns

The next time point

Return type

float

parse_interrupt (*data*)

create interrupt class from various data formats

Parameters

data (str or number or `InterruptsBase`) – Data determining the interrupt class. If this is a `InterruptsBase`, it is simply returned, numbers imply `ConstantInterrupts`, a string is parsed as a time for `RealtimeInterrupts`, and lists are interpreted as `FixedInterrupts`.

Returns

An instance that represents the interrupt

Return type

`InterruptsBase`

4.7.4 `pde.trackers.trackers` module

Module defining classes for tracking results from simulations.

The trackers defined in this module are:

<code>CallbackTracker</code>	Tracker calling a function periodically
<code>ProgressTracker</code>	Tracker showing the progress of the simulation
<code>PrintTracker</code>	Tracker printing data to a stream (default: stdout)
<code>PlotTracker</code>	Tracker plotting data on screen, to files, or writes a movie
<code>LivePlotTracker</code>	PlotTracker with defaults for live plotting
<code>DataTracker</code>	Tracker storing custom data obtained by calling a function
<code>SteadyStateTracker</code>	Tracker aborting the simulation once steady state is reached
<code>RuntimeTracker</code>	Tracker interrupting the simulation once a duration has passed
<code>ConsistencyTracker</code>	Tracker interrupting the simulation when the state is not finite
<code>MaterialConservationTracker</code>	Tracking interrupting the simulation when material conservation is broken

class `CallbackTracker` (*func*, *interrupts=1*, *, *interval=None*)

Bases: `TrackerBase`

Tracker calling a function periodically

Example

The callback tracker can be used to check for conditions during the simulation:

```
def check_simulation(state, time):
    if state.integral < 0:
        raise StopIteration

tracker = CallbackTracker(check_simulation, interval="0:10")
```

Adding `tracker` to the simulation will perform a check every 10 real time seconds. If the integral of the entire state falls below zero, the simulation will be aborted.

Parameters

- **func** (*Callable*) – The function to call periodically. The function signature should be (*state*) or (*state*, *time*), where *state* contains the current state as an instance of `FieldBase` and *time* is a float value indicating the current time. Note that only a view of the state is supplied, implying that a copy needs to be made if the data should be stored. The function can thus adjust the state by modifying it in-place and it can even interrupt the simulation by raising the special exception `StopIteration`.
- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in `interrupts`.

handle (*field*, *t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

class ConsistencyTracker (*interrupts=None*, *, *interval=None*)

Bases: *TrackerBase*

Tracker interrupting the simulation when the state is not finite

Parameters

interrupts (*InterruptData* | *None*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*. The default value *None* checks for consistency approximately every (real) second.

handle (*field*, *t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

name = 'consistency'

class DataTracker (*func*, *interrupts=1*, *, *filename=None*, *interval=None*)

Bases: *CallbackTracker*

Tracker storing custom data obtained by calling a function

Example

The data tracker can be used to gather statistics during the run

```
def get_statistics(state, time):  
    return {"mean": state.data.mean(), "variance": state.data.var()}  
  
data_tracker = DataTracker(get_statistics, interval=10)
```

Adding `data_tracker` to the simulation will gather the statistics every 10 time units. After the simulation, the final result will be accessible via the `data` attribute or conveniently as a pandas from the `dataframe` attribute.

times

The time points at which the data is stored

Type

list

data

The actually stored data, which is a list of the objects returned by the callback function.

Type

list

Parameters

- **func** (*Callable*) – The function to call periodically. The function signature should be (*state*) or (*state, time*), where *state* contains the current state as an instance of `FieldBase` and *time* is a float value indicating the current time. Note that only a view of the state is supplied, implying that a copy needs to be made if the data should be stored. Typical return values of the function are either a single number, a numpy array, a list of number, or a dictionary to return multiple numbers with assigned labels.
- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.
- **filename** (*str*) – A path to a file to which the data is written at the end of the tracking. The data format will be determined by the extension of the filename. ‘.pickle’ indicates a python pickle file storing a tuple (*self.times, self.data*), whereas any other data format requires pandas.

property dataframe: pandas.DataFrame

the data in a dataframe

If *func* returns a dictionary, the keys are used as column names. Otherwise, the returned data is enumerated starting with ‘0’. In any case the time point at which the data was recorded is stored in the column ‘time’.

Type

pandas.DataFrame

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

info (*dict*) – Extra information from the simulation

Return type

None

handle (*field, t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

to_file (*filename, **kwargs*)

store data in a file

The extension of the filename determines what format is being used. For instance, ‘.pickle’ indicates a python pickle file storing a tuple (*self.times*, *self.data*), whereas any other data format requires *pandas*. Supported formats include ‘csv’, ‘json’.

Parameters

- **filename** (*str*) – Path where the data is stored
- ****kwargs** – Additional parameters may be supported for some formats

class LivePlotTracker (*interrupts='0:03', *, show=True, max_fps=2, interval=None, **kwargs*)

Bases: *PlotTracker*

PlotTracker with defaults for live plotting

The only difference to *PlotTracker* are the changed default values, where output is by default shown on screen and the *interval* is set something more suitable for interactive plotting. In particular, this tracker can be enabled by simply listing ‘plot’ as a tracker.

Parameters

- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.
- **title** (*str*) – Text to show in the title. The current time point will be appended to this text, so include a space for optimal results.
- **output_file** (*str*, *optional*) – Specifies a single image file, which is updated periodically, so that the progress can be monitored (e.g. on a compute cluster)
- **output_folder** (*str*, *optional*) – Specifies a folder to which all images are written. The files will have names with increasing numbers.
- **movie_file** (*str*, *optional*) – Specifies a filename to which a movie of all the frames is written after the simulation.
- **show** (*bool*, *optional*) – Determines whether the plot is shown while the simulation is running. If *False*, the files are created in the background. This option can slow down a simulation severely.
- **max_fps** (*float*) – Determines the maximal rate (frames per second) at which the plots are updated. Some plots are skipped if the tracker receives data at a higher rate. A larger value (e.g., *math.inf*) can be used to ensure every frame is drawn, which might penalizes the overall performance.
- **plot_args** (*dict*) – Extra arguments supplied to the plot call. For example, this can be used to specify axes ranges when a single panel is shown. For instance, the value `{‘ax_style’: {‘ylim’: (0, 1)}}` enforces the y-axis to lie between 0 and 1.

name = ‘plot’

class MaterialConservationTracker (*interrupts=1, atol=0.0001, rtol=0.0001, *, interval=None*)

Bases: *TrackerBase*

Tracking interrupting the simulation when material conservation is broken

Parameters

- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular

interruption. A string is interpreted as a duration in real time assuming the format 'hh:mm:ss'. A list of numbers is taken as explicit simulation time points. More fine-grained control is possible by passing an instance of classes defined in *interrupts*.

- **atol** (*float*) – Absolute tolerance for amount deviations
- **rtol** (*float*) – Relative tolerance for amount deviations

handle (*field*, *t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

initialize (*field*, *info=None*)

Parameters

- **field** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

name = 'material_conservation'

```
class PlotTracker (interrupts=1, *, title='Time: {time:g}', output_file=None, movie=None, show=None,
                  tight_layout=False, max_fps=inf, plot_args=None, interval=None)
```

Bases: *TrackerBase*

Tracker plotting data on screen, to files, or writes a movie

This tracker can be used to create movies from simulations or to simply update a single image file on the fly (i.e. to monitor simulations running on a cluster). The default values of this tracker are chosen with regular output to a file in mind.

Example

To create a movie while running the simulation, you can use

```
movie_tracker = PlotTracker(interval=10, movie="my_movie.mp4")
eq.solve(..., tracker=movie_tracker)
```

This will create the file *my_movie.mp4* during the simulation. Note that you can display the frames interactively by setting *show=True*.

Parameters

- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format 'hh:mm:ss'.

A list of numbers is taken as explicit simulation time points. More fine-grained control is possible by passing an instance of classes defined in *interrupts*.

- **title** (*str* or *callable*) – Title text of the figure. If this is a string, it is shown with a potential placeholder named *time* being replaced by the current simulation time. Conversely, if *title* is a function, it is called with the current state and the time as arguments. This function is expected to return a string.
- **output_file** (*str*, *optional*) – Specifies a single image file, which is updated periodically, so that the progress can be monitored (e.g. on a compute cluster)
- **movie** (*str* or *Movie*) – Create a movie. If a filename is given, all frames are written to this file in the format deduced from the extension after the simulation ran. If a *Movie* is supplied, frames are appended to the instance.
- **show** (*bool*, *optional*) – Determines whether the plot is shown while the simulation is running. If set to *None*, the images are only shown if neither *output_file* nor *movie* is set, otherwise they are kept hidden. Note that showing the plot can slow down a simulation severely.
- **tight_layout** (*bool*) – Determines whether `tight_layout()` is used.
- **max_fps** (*float*) – Determines the maximal rate (frames per second) at which the plots are updated in real time during the simulation. Some plots are skipped if the tracker receives data at a higher rate. A larger value (e.g., *math.inf*) can be used to ensure every frame is drawn, which might penalizes the overall performance.
- **plot_args** (*dict*) – Extra arguments supplied to the plot call. For example, this can be used to specify axes ranges when a single panel is shown. For instance, the value `{'ax_style': {'ylim': (0, 1)}}` enforces the y-axis to lie between 0 and 1.

Note: If an instance of *Movie* is given as the *movie* argument, it can happen that the movie is not written to the file when the simulation ends. This is because, the movie could still be extended by appending frames. To write the movie to a file call its *save()* method. Beside adding frames before and after the simulation, an explicit movie object can also be used to adjust the output. For instance, the following example code creates a movie with a framerate of 15, a resolution of 200 dpi, and a bitrate of 6000 kilobits per second:

```
movie = Movie("movie.mp4", framerate=15, dpi=200, bitrate=6000)
eq.solve(..., tracker=PlotTracker(1, movie=movie))
movie.save()
```

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

info (*dict*) – Extra information from the simulation

Return type

None

handle (*state*, *t*)

handle data supplied to this tracker

Parameters

- **state** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

initialize (*state*, *info=None*)

initialize the tracker with information about the simulation

Parameters

- **state** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

```
class PrintTracker (interrupts=1, stream=<_io.TextIOWrapper name='<stdout>' mode='w' encoding='utf-8'>,
                    *, interval=None)
```

Bases: *TrackerBase*

Tracker printing data to a stream (default: stdout)

Parameters

- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format 'hh:mm:ss'. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.
- **stream** (*IO[str]*) – The stream used for printing

handle (*field*, *t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

name = 'print'

```
class ProgressTracker (interrupts=None, *, fancy=True, ndigits=5, leave=True, interval=None)
```

Bases: *TrackerBase*

Tracker showing the progress of the simulation

Parameters

- **interrupts** (*InterruptData | None*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format 'hh:mm:ss'. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*. The default value *None* updates the progress bar approximately every (real) second.
- **fancy** (*bool*) – Flag determining whether a fancy progress bar should be used in jupyter notebooks (if *ipywidgets* is installed)

- **ndigits** (*int*) – The number of digits after the decimal point that are shown maximally.
- **leave** (*bool*) – Whether to leave the progress bar after the simulation has finished (default: True)

finalize (*info=None*)

finalize the tracker, supplying additional information

Parameters

- **info** (*dict*) – Extra information from the simulation

Return type

None

handle (*field, t*)

handle data supplied to this tracker

Parameters

- **field** (*FieldBase*) – The current state of the simulation
- **t** (*float*) – The associated time

Return type

None

initialize (*field, info=None*)

initialize the tracker with information about the simulation

Parameters

- **field** (*FieldBase*) – An example of the data that will be analyzed by the tracker
- **info** (*dict*) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type

float

name = 'progress'

class RuntimeTracker (*max_runtime, interrupts=1, *, interval=None*)

Bases: *TrackerBase*

Tracker interrupting the simulation once a duration has passed

Parameters

- **max_runtime** (*float or str*) – The maximal runtime of the simulation. If the runtime is exceeded, the simulation is interrupted. Values can be either given as a number (interpreted as seconds) or as a string, which is then parsed using the function *parse_duration()*.
- **interrupts** (*InterruptData*) – Determines when the tracker interrupts the simulation. A single numbers determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format 'hh:mm:ss'. A list of numbers is taken as explicit simulation time points. More fine- grained control is possible by passing an instance of classes defined in *interrupts*.

handle (*field, t*)

handle data supplied to this tracker

Parameters

- **field** (`FieldBase`) – The current state of the simulation
- **t** (`float`) – The associated time

Return type

None

initialize (*field*, *info*=None)**Parameters**

- **field** (`FieldBase`) – An example of the data that will be analyzed by the tracker
- **info** (`dict`) – Extra information from the simulation

Returns

The first time the tracker needs to handle data

Return type`float`

class SteadyStateTracker (*interrupts*=None, *atol*=1e-08, *rtol*=1e-05, *, *progress*=False, *evolution_rate*=None, *interval*=None)

Bases: `TrackerBase`

Tracker aborting the simulation once steady state is reached

Steady state is obtained when the state does not change anymore, i.e., when the evolution rate is close to zero. If the argument *evolution_rate* is specified, it is used to calculate the evolution rate directly. If it is omitted, the evolution rate is estimated by comparing the current state *cur* to the state *prev* at the previous time step. In both cases, convergence is assumed when the absolute value of the evolution rate falls below `atol + rtol * cur` for all points. Here, *atol* and *rtol* denote absolute and relative tolerances, respectively.

Parameters

- **interrupts** (`InterruptData` | `None`) – Determines when the tracker interrupts the simulation. A single number determines an interval (measured in the simulation time unit) of regular interruption. A string is interpreted as a duration in real time assuming the format ‘hh:mm:ss’. A list of numbers is taken as explicit simulation time points. More fine-grained control is possible by passing an instance of classes defined in `interrupts`. The default value `None` checks for the steady state approximately every (real) second.
- **atol** (`float`) – Absolute tolerance that must be reached to abort the simulation
- **rtol** (`float`) – Relative tolerance that must be reached to abort the simulation
- **progress** (`bool`) – Flag indicating whether the progress towards convergence is shown graphically during the simulation
- **evolution_rate** (`callable`) – Function to evaluate the current evolution rate. If omitted, the evolution rate is estimated from the change in the state variable, which can be less accurate. A suitable form of the function is returned by `eq.make_pde_rhs(state)` when *eq* is the PDE class.

handle (*field*, *t*)

handle data supplied to this tracker

Parameters

- **field** (`FieldBase`) – The current state of the simulation
- **t** (`float`) – The associated time

Return type

None

`name = 'steady_state'``progress_bar_format = 'Convergence: {percentage:3.0f}%|{bar}|
[{elapsed}<{remaining}]'`determines the format of the progress bar shown when *progress = True*

4.8 pde.visualization package

Functions and classes for visualizing simulations.

<code>movies</code>	Functions for creating movies of simulation results
<code>plotting</code>	Functions and classes for plotting simulation data

4.8.1 pde.visualization.movies module

Functions for creating movies of simulation results

<code>Movie</code>	Class for creating movies from matplotlib figures using ffmpeg
<code>movie_scalar</code>	produce a movie for a simulation of a scalar field
<code>movie_multiple</code>	produce a movie for a simulation with n components
<code>movie</code>	produce a movie by simply plotting each frame

class `Movie` (*filename*, *framerate=30*, *dpi=None*, ***kwargs*)

Bases: `object`

Class for creating movies from matplotlib figures using ffmpeg

Note: Internally, this class uses `matplotlib.animation.FFMpegWriter`. Note that the *ffmpeg* program needs to be installed in a system path, so that *matplotlib* can find it.

Warning: The movie is only fully written after the `save()` method has been called. To aid with this, it is best practice to use a contextmanager:

```
with Movie("output.mp4") as movie:  
    movie.add_figure()
```

Parameters

- **filename** (*str*) – The filename where the movie is stored. The suffix of this path also determines the default movie codec.
- **framerate** (*float*) – The number of frames per second, which determines how fast the movie will appear to run.
- **dpi** (*float*) – The resolution of the resulting movie

- ****kwargs** – Additional parameters are used to initialize `matplotlib.animation.FFMpegWriter`. Here, we can for instance set the bit rate of the resulting video using the *bitrate* parameter.

add_figure (*fig=None*)

adds the figure *fig* as a frame to the current movie

Parameters

fig (*Figure*) – The plot figure that is added to the movie

classmethod is_available ()

check whether the movie infrastructure is available

Returns

True if movies can be created

Return type

`bool`

save ()

convert the recorded images to a movie using ffmpeg

movie (*storage, filename, *, progress=True, show_time=True, plot_args=None, movie_args=None*)

produce a movie by simply plotting each frame

Parameters

- **storage** (*StorageBase*) – The storage instance that contains all the data for the movie
- **filename** (*str*) – The filename to which the movie is written. The extension determines the format used.
- **progress** (*bool*) – Flag determining whether the progress of making the movie is shown.
- **show_time** (*bool*) – Whether to show the simulation time in the movie
- **plot_args** (*dict*) – Additional arguments for the function plotting the state
- **movie_args** (*dict*) – Additional arguments for *Movie*. For example, this can be used to set the resolution (*dpi*), the framerate (*framerate*), and the bitrate (*bitrate*).

Return type

None

movie_multiple (*storage, filename, quantities=None, scale='automatic', progress=True*)

produce a movie for a simulation with n components

Parameters

- **storage** (*StorageBase*) – The storage instance that contains all the data for the movie
- **filename** (*str*) – The filename to which the movie is written. The extension determines the format used.
- **quantities** – A 2d list of quantities that are shown in a rectangular arrangement. If *quantities* is a simple list, the panels will be rendered as a single row. Each panel is defined by a dictionary, where the mandatory item 'source' defines what is being shown. Here, an integer specifies the component that is extracted from the field while a function is evaluate with the full state as an input and the result is shown. Additional items in the dictionary can be 'title' (setting the title of the panel), 'scale' (defining the color range shown; these are typically two numbers defining the lower and upper bound, but if only one is given the range [0, scale] is assumed), and 'cmap' (defining the colormap being used).

- **scale** (*str*, *float*, *tuple of float*) – Flag determining how the range of the color scale is determined. In the simplest case a tuple of numbers marks the lower and upper end of the scalar values that will be shown. If only a single number is supplied, the range starts at zero and ends at the given number. Additionally, the special value ‘automatic’ determines the range from the range of scalar values.
- **progress** (*bool*) – Flag determining whether the progress of making the movie is shown.

Return type

None

movie_scalar (*storage*, *filename*, *scale*='automatic', *extras*=None, *progress*=True, *tight*=False, *show*=True)

produce a movie for a simulation of a scalar field

Parameters

- **storage** (*StorageBase*) – The storage instance that contains all the data for the movie
- **filename** (*str*) – The filename to which the movie is written. The extension determines the format used.
- **scale** (*str*, *float*, *tuple of float*) – Flag determining how the range of the color scale is determined. In the simplest case a tuple of numbers marks the lower and upper end of the scalar values that will be shown. If only a single number is supplied, the range starts at zero and ends at the given number. Additionally, the special value ‘automatic’ determines the range from the range of scalar values.
- **extras** (*dict*, *optional*) – Additional functions that are evaluated and shown for each time step. The key of the dictionary is used as a panel title.
- **progress** (*bool*) – Flag determining whether the progress of making the movie is shown.
- **tight** (*bool*) – Whether to call `matplotlib.pyplot.tight_layout()`. This affects the layout of all plot elements.
- **show** (*bool*) – Flag determining whether images are shown during making the movie

Return type

None

4.8.2 `pde.visualization.plotting` module

Functions and classes for plotting simulation data

<code>ScalarFieldPlot</code>	class managing compound plots of scalar fields
<code>plot_magnitudes</code>	plot spatially averaged quantities as a function of time
<code>plot_kymograph</code>	plots a single kymograph from stored data
<code>plot_kymographs</code>	plots kymographs for all fields stored in <i>storage</i>
<code>plot_interactive</code>	plots stored data interactively using the napari viewer

class **ScalarFieldPlot** (*fields*, *quantities*=None, *scale*='automatic', *fig*=None, *title*=None, *tight*=False, *show*=True)Bases: `object`

class managing compound plots of scalar fields

Parameters

- **fields** (*FieldBase*) – Collection of fields

- **quantities** – A 2d list of quantities that are shown in a rectangular arrangement. If *quantities* is a simple list, the panels will be rendered as a single row. Each panel is defined by a dictionary, where the mandatory item ‘source’ defines what is being shown. Here, an integer specifies the component that is extracted from the field while a function is evaluate with the full state as an input and the result is shown. Additional items in the dictionary can be ‘title’ (setting the title of the panel), ‘scale’ (defining the color range shown; these are typically two numbers defining the lower and upper bound, but if only one is given the range [0, scale] is assumed), and ‘cmap’ (defining the colormap being used).
- **scale** (*str*, *float*, *tuple of float*) – Flag determining how the range of the color scale is determined. In the simplest case a tuple of numbers marks the lower and upper end of the scalar values that will be shown. If only a single number is supplied, the range starts at zero and ends at the given number. Additionally, the special value ‘automatic’ determines the range from the range of scalar values.
- **(fig)** – *class:matplotlib.figure.Figure*: Figure to be used for plotting. If ‘None’, a new figure is created.
- **title** (*str*) – Title of the plot.
- **tight** (*bool*) – Whether to call `matplotlib.pyplot.tight_layout()`. This affects the layout of all plot elements.
- **show** (*bool*) – Flag determining whether to show a plot. If *False*, the plot is kept in the background, which can be useful if it only needs to be written to a file.

classmethod from_storage (*storage*, *quantities=None*, *scale='automatic'*, *tight=False*, *show=True*)
create ScalarFieldPlot from storage

Parameters

- **storage** (*StorageBase*) – Instance of the storage class that contains the data
- **quantities** – A 2d list of quantities that are shown in a rectangular arrangement. If *quantities* is a simple list, the panels will be rendered as a single row. Each panel is defined by a dictionary, where the mandatory item ‘source’ defines what is being shown. Here, an integer specifies the component that is extracted from the field while a function is evaluate with the full state as an input and the result is shown. Additional items in the dictionary can be ‘title’ (setting the title of the panel), ‘scale’ (defining the color range shown; these are typically two numbers defining the lower and upper bound, but if only one is given the range [0, scale] is assumed), and ‘cmap’ (defining the colormap being used).
- **scale** (*str*, *float*, *tuple of float*) – Flag determining how the range of the color scale is determined. In the simplest case a tuple of numbers marks the lower and upper end of the scalar values that will be shown. If only a single number is supplied, the range starts at zero and ends at the given number. Additionally, the special value ‘automatic’ determines the range from the range of scalar values.
- **tight** (*bool*) – Whether to call `matplotlib.pyplot.tight_layout()`. This affects the layout of all plot elements.
- **show** (*bool*) – Flag determining whether to show a plot. If *False*, the plot is kept in the background.

Returns

ScalarFieldPlot

Return type

ScalarFieldPlot

make_movie (*storage, filename, progress=True*)

make a movie from the data stored in storage

Parameters

- **storage** (*StorageBase*) – The storage instance that contains all the data for the movie
- **filename** (*str*) – The filename to which the movie is written. The extension determines the format used.
- **progress** (*bool*) – Flag determining whether the progress of making the movie is shown.

Return type

None

savefig (*path, **kwargs*)

save plot to file

Parameters

- **path** (*str*) – The path to the file where the image is written. The file extension determines the image format
- ****kwargs** – Additional arguments are forwarded to `matplotlib.figure.Figure.savefig()`.

update (*fields, title=None*)

update the plot with the given fields

Parameters

- **fields** (*FieldBase*) – The field or field collection of which the defined quantities are shown.
- **title** (*str, optional*) – The title of this view. If *None*, the current title is not changed.

Return type

None

extract_field (*fields, source=None, check_rank=None*)

Extracts a single field from a possible collection.

Parameters

- **fields** (*FieldBase*) – The field from which data is extracted
- **source** (*int or callable, optional*) – Determines how a field is extracted from *fields*. If *None*, *fields* is passed as is, assuming it is already a scalar field. This works for the simple, standard case where only a single *ScalarField* is treated. Alternatively, *source* can be an integer, indicating which field is extracted from an instance of *FieldCollection*. Lastly, *source* can be a function that takes *fields* as an argument and returns the desired field.
- **check_rank** (*int, optional*) – Can be given to check whether the extracted field has the correct rank (0 = *ScalarField*, 1 = *VectorField*, ...).

Returns

The extracted field

Return type

DataFieldBase

plot_interactive (*storage, time_scaling='exact', viewer_args=None, **kwargs*)

plots stored data interactively using the *napari* viewer

Parameters

- **storage** (`StorageBase`) – The storage instance that contains all the data
- **time_scaling** (`str`) – Defines how the time axis is scaled. Possible options are “exact” (the actual time points are used), or “scaled” (the axis is scaled so that it has similar dimension to the spatial axes). Note that the spatial axes will never be scaled.
- **viewer_args** (`dict`) – Arguments passed to `napari.viewer.Viewer` to affect the viewer.
- ****kwargs** – Extra arguments passed to the plotting function

plot_kymograph (*storage*, *field_index=None*, *scalar='auto'*, *extract='auto'*, *colorbar=True*, *transpose=False*, **args*, *title=None*, *filename=None*, *action='auto'*, *ax_style=None*, *fig_style=None*, *ax=None*, ***kwargs*)

plots a single kymograph from stored data

The kymograph shows line data stacked along time. Consequently, the resulting image shows space along the horizontal axis and time along the vertical axis.

Parameters

- **storage** (`StorageBase`) – The storage instance that contains all the data
- **field_index** (`int`) – An index to choose a single field out of many in a collection stored in *storage*. This option should not be used if only a single field is stored in a collection.
- **scalar** (`str`) – The method for extracting scalars as described in `DataFieldBase.to_scalar()`.
- **extract** (`str`) – The method used for extracting the line data. See the docstring of the grid method `get_line_data` to find supported values.
- **colorbar** (`bool`) – Whether to show a colorbar or not
- **transpose** (`bool`) – Determines whether the transpose of the data should be plotted
- **title** (`str`) – Title of the plot. If omitted, the title might be chosen automatically.
- **filename** (`str`, *optional*) – If given, the plot is written to the specified file.
- **action** (`str`) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **ax_style** (`dict`) – Dictionary with properties that will be changed on the axis after the plot has been drawn by calling `matplotlib.pyplot.setp()`. A special item in this dictionary is *use_offset*, which is a flag that can be used to control whether offsets are shown along the axes of the plot.
- **fig_style** (`dict`) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.
- **ax** (`matplotlib.axes.Axes`) – Figure axes to be used for plotting. The special value “create” creates a new figure, while “reuse” attempts to reuse an existing figure, which is the default.
- ****kwargs** – Additional keyword arguments are passed to `matplotlib.pyplot.imshow()`.

Returns

The reference to the plot

Return type

PlotReference

plot_kymographs (*storage*, *scalar*='auto', *extract*='auto', *colorbar*=True, *transpose*=False, *resize_fig*=True, *args, *title*=None, *constrained_layout*=True, *filename*=None, *action*='auto', *fig_style*=None, *fig*=None, **kwargs)

plots kymographs for all fields stored in *storage*

The kymograph shows line data stacked along time. Consequently, the resulting image shows space along the horizontal axis and time along the vertical axis.

Parameters

- **storage** (*StorageBase*) – The storage instance that contains all the data
- **scalar** (*str*) – The method for extracting scalars as described in *DataFieldBase.to_scalar()*.
- **extract** (*str*) – The method used for extracting the line data. See the docstring of the grid method *get_line_data* to find supported values.
- **colorbar** (*bool*) – Whether to show a colorbar or not
- **transpose** (*bool*) – Determines whether the transpose of the data should be plotted
- **resize_fig** (*bool*) – Whether to resize the figure to adjust to the number of panels
- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically. This is shown above all panels.
- **constrained_layout** (*bool*) – Whether to use *constrained_layout* in *matplotlib.pyplot.figure()* call to create a figure. This affects the layout of all plot elements. Generally, spacing might be better with this flag enabled, but it can also lead to problems when plotting multiple plots successively, e.g., when creating a movie.
- **filename** (*str*, *optional*) – If given, the figure is written to the specified file.
- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, *matplotlib.pyplot.show()* will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling *matplotlib.pyplot.setp()*. For instance, using *fig_style={'dpi': 200}* increases the resolution of the figure.
- **fig** (*matplotlib.figure.Figure*) – Figure that is used for plotting. If omitted, a new figure is created.
- ****kwargs** – Additional keyword arguments are passed to the calls to *matplotlib.pyplot.imshow()*.

Returns

The references to all plots

Return type

list of *PlotReference*

plot_magnitudes (*storage*, *quantities=None*, **args*, *title=None*, *filename=None*, *action='auto'*, *ax_style=None*, *fig_style=None*, *ax=None*, ***kwargs*)

plot spatially averaged quantities as a function of time

For scalar fields, the default is to plot the average value while the averaged norm is plotted for vector fields.

Parameters

- **storage** (*StorageBase*) – Instance of *StorageBase* that contains the simulation data that will be plotted
- **quantities** – A 2d list of quantities that are shown in a rectangular arrangement. If *quantities* is a simple list, the panels will be rendered as a single row. Each panel is defined by a dictionary, where the mandatory item ‘source’ defines what is being shown. Here, an integer specifies the component that is extracted from the field while a function is evaluate with the full state as an input and the result is shown. Additional items in the dictionary can be ‘title’ (setting the title of the panel), ‘scale’ (defining the color range shown; these are typically two numbers defining the lower and upper bound, but if only one is given the range [0, scale] is assumed), and ‘cmap’ (defining the colormap being used).
- **title** (*str*) – Title of the plot. If omitted, the title might be chosen automatically.
- **filename** (*str*, *optional*) – If given, the plot is written to the specified file.
- **action** (*str*) – Decides what to do with the final figure. If the argument is set to *show*, `matplotlib.pyplot.show()` will be called to show the plot. If the value is *none*, the figure will be created, but not necessarily shown. The value *close* closes the figure, after saving it to a file when *filename* is given. The default value *auto* implies that the plot is shown if it is not a nested plot call.
- **ax_style** (*dict*) – Dictionary with properties that will be changed on the axis after the plot has been drawn by calling `matplotlib.pyplot.setp()`. A special item in this dictionary is *use_offset*, which is flag that can be used to control whether offset are shown along the axes of the plot.
- **fig_style** (*dict*) – Dictionary with properties that will be changed on the figure after the plot has been drawn by calling `matplotlib.pyplot.setp()`. For instance, using `fig_style={'dpi': 200}` increases the resolution of the figure.
- **ax** (`matplotlib.axes.Axes`) – Figure axes to be used for plotting. The special value “create” creates a new figure, while “reuse” attempts to reuse an existing figure, which is the default.
- ****kwargs** – All remaining parameters are forwarded to the *ax.plot* method

Returns

The reference to the plot

Return type

PlotReference

Indices and tables

- [genindex](#)
- [modindex](#)
- [search](#)

PYTHON MODULE INDEX

f

- pde.fields, 59
- pde.fields.base, 60
- pde.fields.collection, 74
- pde.fields.scalar, 80
- pde.fields.tensorial, 85
- pde.fields.vectorial, 89

g

- pde.grids, 94
- pde.grids.base, 144
- pde.grids.boundaries, 95
- pde.grids.boundaries.axes, 97
- pde.grids.boundaries.axis, 99
- pde.grids.boundaries.local, 102
- pde.grids.cartesian, 157
- pde.grids.coordinates, 127
- pde.grids.coordinates.base, 127
- pde.grids.coordinates.bipolar, 130
- pde.grids.coordinates.bispherical, 130
- pde.grids.coordinates.cartesian, 131
- pde.grids.coordinates.cylindrical, 131
- pde.grids.coordinates.polar, 132
- pde.grids.coordinates.spherical, 132
- pde.grids.cylindrical, 161
- pde.grids.operators, 133
- pde.grids.operators.cartesian, 133
- pde.grids.operators.common, 135
- pde.grids.operators.cylindrical_sym, 136
- pde.grids.operators.polar_sym, 139
- pde.grids.operators.spherical_sym, 141
- pde.grids.spherical, 165

p

- pde, 59
- pde.pdes, 170
- pde.pdes.allen_cahn, 170
- pde.pdes.base, 171
- pde.pdes.cahn_hilliard, 175
- pde.pdes.diffusion, 176
- pde.pdes.kpz_interface, 177
- pde.pdes.kuramoto_sivashinsky, 178

- pde.pdes.laplace, 180
- pde.pdes.pde, 181
- pde.pdes.swift_hohenberg, 183
- pde.pdes.wave, 184

s

- pde.solvers, 185
- pde.solvers.adams_bashforth, 188
- pde.solvers.base, 188
- pde.solvers.controller, 190
- pde.solvers.crank_nicolson, 192
- pde.solvers.explicit, 192
- pde.solvers.explicit_mpi, 193
- pde.solvers.implicit, 194
- pde.solvers.scipy, 195
- pde.storage, 195
- pde.storage.base, 196
- pde.storage.file, 201
- pde.storage.memory, 202
- pde.storage.movie, 204

t

- pde.tools, 207
- pde.tools.cache, 207
- pde.tools.config, 213
- pde.tools.cuboid, 214
- pde.tools.docstrings, 217
- pde.tools.expressions, 217
- pde.tools.ffmpeg, 223
- pde.tools.math, 225
- pde.tools.misc, 226
- pde.tools.mpi, 229
- pde.tools.numba, 231
- pde.tools.output, 233
- pde.tools.parameters, 234
- pde.tools.parse_duration, 237
- pde.tools.plotting, 237
- pde.tools.spectral, 242
- pde.tools.typing, 243
- pde.trackers, 243
- pde.trackers.base, 244
- pde.trackers.interactive, 247

`pde.trackers.interrupts`, [249](#)
`pde.trackers.trackers`, [253](#)

V

`pde.visualization`, [262](#)
`pde.visualization.movies`, [262](#)
`pde.visualization.plotting`, [264](#)

A

AdamsBashforthSolver (class in *pde.solvers*), 185
 AdamsBashforthSolver (class in *pde.solvers.adams_bashforth*), 188
 AdaptiveSolverBase (class in *pde.solvers.base*), 188
 add_figure() (Movie method), 263
 add_scaled_colorbar() (in module *pde.tools.plotting*), 239
 AdjacentEvaluator (class in *pde.tools.typing*), 243
 AllenCahnPDE (class in *pde.pdes.allen_cahn*), 170
 append() (FieldCollection method), 75
 append() (StorageBase method), 196
 apply() (FieldBase method), 69
 apply() (StorageBase method), 196
 apply_operator() (DataFieldBase method), 60
 asanyarray_flags() (in module *pde.tools.cuboid*), 216
 assert_field_compatible() (FieldBase method), 70
 assert_field_compatible() (FieldCollection method), 75
 assert_grid_compatible() (GridBase method), 144
 attributes (FieldBase property), 70
 attributes (FieldCollection property), 75
 attributes_serialized (FieldBase property), 70
 attributes_serialized (FieldCollection property), 75
 average (DataFieldBase property), 60
 averages (FieldCollection property), 75
 ax (PlotReference attribute), 238
 axes (BipolarCoordinates attribute), 130
 axes (BisphericalCoordinates attribute), 130
 axes (CoordinatesBase attribute), 127
 axes (CylindricalCoordinates attribute), 131
 axes (GridBase attribute), 145
 axes (PolarCoordinates attribute), 132
 axes (SphericalCoordinates attribute), 132
 axes_bounds (GridBase property), 145
 axes_coords (GridBase property), 145
 axes_symmetric (GridBase attribute), 145
 axis (BoundaryAxisBase property), 99

axis_coord (BCBase property), 103

B

BasicOutput (class in *pde.tools.output*), 233
 BasicPlottingContext (class in *pde.tools.plotting*), 238
 basis_rotation() (CoordinatesBase method), 127
 BCBase (class in *pde.grids.boundaries.local*), 103
 BCDataError, 107
 BipolarCoordinates (class in *pde.grids.coordinates.bipolar*), 130
 BisphericalCoordinates (class in *pde.grids.coordinates.bispherical*), 130
 bits_per_channel (FFmpegFormat attribute), 223
 boundaries (Boundaries property), 97
 Boundaries (class in *pde.grids.boundaries.axes*), 97
 boundary_names (CartesianGrid attribute), 157
 boundary_names (CylindricalSymGrid attribute), 162
 boundary_names (GridBase attribute), 145
 boundary_names (SphericalSymGridBase attribute), 167
 BoundaryAxisBase (class in *pde.grids.boundaries.axis*), 99
 BoundaryPair (class in *pde.grids.boundaries.axis*), 101
 BoundaryPeriodic (class in *pde.grids.boundaries.axis*), 101
 bounds (Cuboid property), 214
 bounds (SmoothData1D property), 225
 buffer() (Cuboid method), 214
 bytes_per_channel (FFmpegFormat property), 223

C

c (CylindricalSymGrid attribute), 162
 c (GridBase attribute), 145
 c (PolarSymGrid attribute), 166
 c (SphericalSymGrid attribute), 166
 cache_rhs (PDEBase attribute), 172
 cached_method (class in *pde.tools.cache*), 208
 cached_property (class in *pde.tools.cache*), 209
 CahnHilliardPDE (class in *pde.pdes.cahn_hilliard*), 175
 CallbackTracker (class in *pde.trackers.trackers*), 253

- CartesianCoordinates (class in *pde.grids.coordinates.cartesian*), 131
- CartesianGrid (class in *pde.grids.cartesian*), 157
- cell_coords (GridBase attribute), 145
- cell_volume() (CoordinatesBase method), 127
- cell_volume_data (CartesianGrid property), 157
- cell_volume_data (CylindricalSymGrid attribute), 162
- cell_volume_data (GridBase attribute), 145
- cell_volume_data (SphericalSymGridBase attribute), 167
- cell_volumes (GridBase attribute), 145
- CellVolume (class in *pde.tools.typing*), 243
- centroid (Cuboid property), 215
- channels (FFmpegFormat attribute), 223
- check_implementation (PDEBase attribute), 172
- check_length() (DictFiniteCapacity method), 207
- check_package_version() (in module *pde.tools.config*), 213
- check_rhs_consistency() (PDEBase method), 172
- check_value_rank() (BCBase method), 104
- check_value_rank() (Boundaries method), 97
- check_value_rank() (BoundaryPair method), 101
- check_value_rank() (BoundaryPeriodic method), 101
- class_type (OnlineStatistics attribute), 225
- classmethod() (hybridmethod method), 228
- classproperty (class in *pde.tools.misc*), 226
- clear() (FileStorage method), 201
- clear() (MemoryStorage method), 202
- clear() (MovieStorage method), 205
- clear() (StorageBase method), 196
- close() (FileStorage method), 201
- close() (JupyterPlottingContext method), 238
- close() (MovieStorage method), 205
- close() (NapariViewer method), 248
- close() (PlottingContextBase method), 239
- codec (FFmpegFormat attribute), 224
- compatible_with() (GridBase method), 145
- complex (ExpressionBase property), 218
- complex_valued (PDEBase attribute), 172
- Config (class in *pde.tools.config*), 213
- conjugate() (FieldBase method), 70
- ConsistencyTracker (class in *pde.trackers.trackers*), 254
- constant (ExpressionBase property), 218
- ConstantInterrupts (class in *pde.trackers.interrupts*), 249
- ConstBC1stOrderBase (class in *pde.grids.boundaries.local*), 107
- ConstBC2ndOrderBase (class in *pde.grids.boundaries.local*), 109
- ConstBCBase (class in *pde.grids.boundaries.local*), 111
- contains_point() (Cuboid method), 215
- contains_point() (GridBase method), 146
- Controller (class in *pde.solvers*), 185
- Controller (class in *pde.solvers.controller*), 190
- ConvergenceError, 189
- convert() (Parameter method), 235
- coordinate_arrays (GridBase attribute), 146
- coordinate_constraints (CylindricalSymGrid attribute), 162
- coordinate_constraints (GridBase attribute), 146
- coordinate_constraints (PolarSymGrid attribute), 166
- coordinate_constraints (SphericalSymGrid attribute), 166
- coordinate_limits (BipolarCoordinates attribute), 130
- coordinate_limits (BisphericalCoordinates attribute), 130
- coordinate_limits (CoordinatesBase attribute), 128
- coordinate_limits (CylindricalCoordinates attribute), 131
- coordinate_limits (PolarCoordinates attribute), 132
- coordinate_limits (SphericalCoordinates attribute), 132
- CoordinatesBase (class in *pde.grids.coordinates.base*), 127
- copy() (BCBase method), 104
- copy() (Boundaries method), 98
- copy() (BoundaryAxisBase method), 99
- copy() (BoundaryPeriodic method), 102
- copy() (ConstantInterrupts method), 249
- copy() (ConstBCBase method), 111
- copy() (Cuboid method), 215
- copy() (DataFieldBase method), 61
- copy() (ExpressionBC method), 115
- copy() (FieldBase method), 70
- copy() (FieldCollection method), 75
- copy() (FixedInterrupts method), 250
- copy() (GridBase method), 146
- copy() (InterruptsBase method), 250
- copy() (MixedBC method), 120
- copy() (ScalarExpression method), 220
- copy() (StorageBase method), 196
- copy() (UserBC method), 125
- corners (Cuboid property), 215
- count (OnlineStatistics attribute), 225
- Counter (class in *pde.tools.numba*), 231
- CrankNicolsonSolver (class in *pde.solvers*), 186
- CrankNicolsonSolver (class in *pde.solvers.crank_nicolson*), 192
- cuboid (CartesianGrid attribute), 157
- Cuboid (class in *pde.tools.cuboid*), 214
- CurvatureBC (class in *pde.grids.boundaries.local*), 112

- CylindricalCoordinates (class in *pde.grids.coordinates.cylindrical*), 131
- CylindricalSymGrid (class in *pde.grids.cylindrical*), 161
- ## D
- data (*DataTracker* attribute), 254
- data (*FieldBase* property), 71
- data (*FileStorage* property), 202
- data (*MovieStorage* property), 205
- data (*StorageBase* attribute), 197
- data_from_frame() (*FFmpegFormat* method), 224
- data_shape (*DataFieldBase* property), 61
- data_shape (*StorageBase* property), 197
- data_to_frame() (*FFmpegFormat* method), 224
- DataFieldBase (class in *pde.fields.base*), 60
- dataframe (*DataTracker* property), 255
- DataTracker (class in *pde.trackers.trackers*), 254
- decorator_arguments() (in module *pde.tools.misc*), 227
- default_capacity (*DictFiniteCapacity* attribute), 207
- deleter() (classproperty method), 227
- depends_on() (*ExpressionBase* method), 218
- DeprecatedParameter (class in *pde.tools.parameters*), 234
- derivative() (*SmoothData1D* method), 225
- derivatives (*ScalarExpression* attribute), 220
- derivatives (*TensorExpression* attribute), 221
- diagnostics (*Controller* attribute), 186, 191
- diagnostics (*PDEBase* attribute), 172
- diagonal (*Cuboid* property), 215
- DictFiniteCapacity (class in *pde.tools.cache*), 207
- difference_vector() (*CartesianGrid* method), 157
- difference_vector() (*CylindricalSymGrid* method), 162
- difference_vector() (*GridBase* method), 146
- difference_vector_real() (*GridBase* method), 146
- differentiate() (*ScalarExpression* method), 220
- differentiate() (*TensorExpression* method), 221
- DiffusionPDE (class in *pde.pdes.diffusion*), 176
- dim (*BipolarCoordinates* attribute), 130
- dim (*BisphericalCoordinates* attribute), 131
- dim (*CoordinatesBase* attribute), 128
- dim (*Cuboid* property), 215
- dim (*CylindricalCoordinates* attribute), 131
- dim (*GridBase* property), 147
- dim (*PolarCoordinates* attribute), 132
- dim (*SphericalCoordinates* attribute), 132
- DimensionError, 130
- DirichletBC (class in *pde.grids.boundaries.local*), 113
- disable_interactive() (in module *pde.tools.plotting*), 239
- discretization (*GridBase* property), 147
- discretize_interval() (in module *pde.grids.base*), 156
- display_progress() (in module *pde.tools.output*), 233
- distance() (*CoordinatesBase* method), 128
- distance() (*GridBase* method), 147
- distance_real() (*GridBase* method), 147
- divergence() (*Tensor2Field* method), 85
- divergence() (*VectorField* method), 89
- DomainError, 144
- dot() (*Tensor2Field* method), 86
- dot() (*VectorField* method), 90
- dt (*InterruptsBase* attribute), 250
- dt_default (*SolverBase* attribute), 189
- dt_max (*AdaptiveSolverBase* attribute), 189
- dt_min (*AdaptiveSolverBase* attribute), 189
- dtype (*FFmpegFormat* attribute), 224
- dtype (*FieldBase* property), 71
- dtype (*StorageBase* property), 197
- ## E
- element (*PlotReference* attribute), 238
- end_writing() (*FileStorage* method), 202
- end_writing() (*MovieStorage* method), 205
- end_writing() (*StorageBase* method), 197
- ensure_directory_exists() (in module *pde.tools.misc*), 227
- environment variable
PYTHONPATH, 5
- environment() (in module *pde.tools.config*), 213
- estimate_computation_speed() (in module *pde.tools.misc*), 227
- evaluate() (in module *pde.tools.expressions*), 221
- evolution_rate() (*AllenCahnPDE* method), 171
- evolution_rate() (*CahnHilliardPDE* method), 176
- evolution_rate() (*DiffusionPDE* method), 177
- evolution_rate() (*KPZInterfacePDE* method), 178
- evolution_rate() (*KuramotoSivashinskyPDE* method), 179
- evolution_rate() (*PDE* method), 182
- evolution_rate() (*PDEBase* method), 172
- evolution_rate() (*SwiftHohenbergPDE* method), 183
- evolution_rate() (*WavePDE* method), 184
- explicit_time_dependence (*AllenCahnPDE* attribute), 171
- explicit_time_dependence (*CahnHilliardPDE* attribute), 176
- explicit_time_dependence (*DiffusionPDE* attribute), 177
- explicit_time_dependence (*KPZInterfacePDE* attribute), 178
- explicit_time_dependence (*KuramotoSivashinskyPDE* attribute), 179

- explicit_time_dependence (*PDEBase* attribute), 173
- explicit_time_dependence (*SwiftHohenbergPDE* attribute), 183
- explicit_time_dependence (*WavePDE* attribute), 184
- ExplicitMPISolver (class in *pde.solvers.explicit_mpi*), 193
- ExplicitSolver (class in *pde.solvers*), 187
- ExplicitSolver (class in *pde.solvers.explicit*), 192
- expr_prod() (in module *pde.pdes.base*), 175
- expression (*AllenCahnPDE* property), 171
- expression (*CahnHilliardPDE* property), 176
- expression (*DiffusionPDE* property), 177
- expression (*ExpressionBase* property), 219
- expression (*KPZInterfacePDE* property), 178
- expression (*KuramotoSivashinskyPDE* property), 179
- expression (*SwiftHohenbergPDE* property), 183
- ExpressionBase (class in *pde.tools.expressions*), 218
- ExpressionBC (class in *pde.grids.boundaries.local*), 114
- ExpressionDerivativeBC (class in *pde.grids.boundaries.local*), 116
- ExpressionMixedBC (class in *pde.grids.boundaries.local*), 117
- expressions (*PDE* property), 182
- expressions (*WavePDE* property), 184
- ExpressionValueBC (class in *pde.grids.boundaries.local*), 118
- extract_field() (in module *pde.visualization.plotting*), 266
- extract_field() (*StorageBase* method), 197
- extract_time_range() (*StorageBase* method), 197
- ## F
- factory (*OperatorInfo* attribute), 156
- FFmpegFormat (class in *pde.tools.ffmpeg*), 223
- FieldBase (class in *pde.fields.base*), 69
- FieldCollection (class in *pde.fields.collection*), 74
- fields (*FieldCollection* property), 76
- fig (*PlottingContextBase* attribute), 239
- FileStorage (class in *pde.storage.file*), 201
- fill_in_docstring() (in module *pde.tools.docstrings*), 217
- finalize() (*DataTracker* method), 255
- finalize() (*InteractivePlotTracker* method), 247
- finalize() (*PlotTracker* method), 258
- finalize() (*ProgressTracker* method), 260
- finalize() (*StorageTracker* method), 200
- finalize() (*TrackerBase* method), 244
- finalize() (*TrackerCollection* method), 245
- find_format() (in module *pde.tools.ffmpeg*), 224
- FinishedSimulation, 244
- FixedInterrupts (class in *pde.trackers.interrupts*), 250
- flat_idx() (in module *pde.tools.numba*), 231
- flip_sign (*BoundaryPeriodic* property), 102
- fluctuations (*DataFieldBase* property), 61
- formats (in module *pde.tools.ffmpeg*), 224
- from_bounds() (*CartesianGrid* class method), 158
- from_bounds() (*Cuboid* class method), 215
- from_bounds() (*CylindricalSymGrid* class method), 163
- from_bounds() (*GridBase* class method), 147
- from_bounds() (*SphericalSymGridBase* class method), 167
- from_centerpoint() (*Cuboid* class method), 215
- from_collection() (*MemoryStorage* class method), 203
- from_data() (*BCBase* class method), 104
- from_data() (*Boundaries* class method), 98
- from_data() (*BoundaryPair* class method), 101
- from_data() (*FieldCollection* class method), 76
- from_data() (*TrackerBase* class method), 245
- from_data() (*TrackerCollection* class method), 246
- from_dict() (*BCBase* class method), 104
- from_expression() (*ScalarField* class method), 80
- from_expression() (*Tensor2Field* class method), 86
- from_expression() (*VectorField* class method), 90
- from_fields() (*MemoryStorage* class method), 203
- from_file() (*FieldBase* class method), 71
- from_image() (*ScalarField* class method), 81
- from_name() (*SolverBase* class method), 190
- from_points() (*Cuboid* class method), 215
- from_scalar_expressions() (*FieldCollection* class method), 76
- from_scalars() (*VectorField* class method), 91
- from_state() (*CartesianGrid* class method), 158
- from_state() (*CylindricalSymGrid* class method), 163
- from_state() (*DataFieldBase* class method), 61
- from_state() (*FieldBase* class method), 71
- from_state() (*FieldCollection* class method), 77
- from_state() (*GridBase* class method), 147
- from_state() (*SphericalSymGridBase* class method), 167
- from_state() (*UnitGrid* class method), 161
- from_storage() (*ScalarFieldPlot* class method), 265
- from_str() (*BCBase* class method), 105
- ## G
- get_all_parameters() (in module *pde.tools.parameters*), 236
- get_axis_index() (*GridBase* method), 148
- get_boundary_axis() (in module *pde.grids.boundaries.axis*), 102
- get_boundary_conditions() (*GridBase* method), 148

`get_boundary_field()` (*ScalarField method*), 81
`get_boundary_values()` (*DataFieldBase method*), 61
`get_cartesian_grid()` (*CylindricalSymGrid method*), 163
`get_cartesian_grid()` (*SphericalSymGridBase method*), 167
`get_class_by_rank()` (*DataFieldBase class method*), 62
`get_common_dtype()` (*in module pde.tools.misc*), 227
`get_common_numba_dtype()` (*in module pde.tools.numba*), 231
`get_compiled()` (*ExpressionBase method*), 219
`get_compiled_array()` (*TensorExpression method*), 221
`get_help()` (*BCBase class method*), 105
`get_help()` (*Boundaries class method*), 98
`get_help()` (*BoundaryAxisBase class method*), 99
`get_image_data()` (*CartesianGrid method*), 158
`get_image_data()` (*CylindricalSymGrid method*), 163
`get_image_data()` (*DataFieldBase method*), 62
`get_image_data()` (*FieldBase method*), 72
`get_image_data()` (*FieldCollection method*), 77
`get_image_data()` (*GridBase method*), 148
`get_image_data()` (*SphericalSymGridBase method*), 168
`get_initial_condition()` (*WavePDE method*), 185
`get_line_data()` (*CartesianGrid method*), 158
`get_line_data()` (*CylindricalSymGrid method*), 164
`get_line_data()` (*DataFieldBase method*), 62
`get_line_data()` (*FieldBase method*), 72
`get_line_data()` (*FieldCollection method*), 77
`get_line_data()` (*GridBase method*), 149
`get_line_data()` (*SphericalSymGridBase method*), 168
`get_mathematical_representation()` (*BCBase method*), 105
`get_mathematical_representation()` (*Boundaries method*), 98
`get_mathematical_representation()` (*BoundaryAxisBase method*), 99
`get_mathematical_representation()` (*CurvatureBC method*), 112
`get_mathematical_representation()` (*DirichletBC method*), 113
`get_mathematical_representation()` (*ExpressionBC method*), 115
`get_mathematical_representation()` (*MixedBC method*), 120
`get_mathematical_representation()` (*NeumannBC method*), 121
`get_mathematical_representation()` (*UserBC method*), 125
`get_memory_storage()` (*in module pde.storage.memory*), 203
`get_named_trackers()` (*in module pde.trackers.base*), 247
`get_package_versions()` (*in module pde.tools.config*), 213
`get_parameter_default()` (*Parameterized method*), 235
`get_parameters()` (*Parameterized class method*), 235
`get_plotting_context()` (*in module pde.tools.plotting*), 240
`get_progress_bar_class()` (*in module pde.tools.output*), 234
`get_random_point()` (*CartesianGrid method*), 159
`get_random_point()` (*CylindricalSymGrid method*), 164
`get_random_point()` (*GridBase method*), 149
`get_random_point()` (*SphericalSymGridBase method*), 168
`get_sparse_matrix_data()` (*BCBase method*), 105
`get_sparse_matrix_data()` (*BoundaryAxisBase method*), 100
`get_sparse_matrix_data()` (*ConstBC1stOrderBase method*), 108
`get_sparse_matrix_data()` (*ConstBC2ndOrderBase method*), 109
`get_sparse_matrix_data()` (*ExpressionBC method*), 115
`get_text_block()` (*in module pde.tools.docstrings*), 217
`get_vector_data()` (*CartesianGrid method*), 159
`get_vector_data()` (*DataFieldBase method*), 63
`get_vector_data()` (*GridBase method*), 149
`get_vector_data()` (*VectorField method*), 91
`get_virtual_point()` (*BCBase method*), 105
`get_virtual_point()` (*ConstBC1stOrderBase method*), 108
`get_virtual_point()` (*ConstBC2ndOrderBase method*), 110
`get_virtual_point()` (*ExpressionBC method*), 115
`get_virtual_point_data()` (*ConstBC1stOrderBase method*), 108
`get_virtual_point_data()` (*ConstBC2ndOrderBase method*), 110
`get_virtual_point_data()` (*CurvatureBC method*), 113
`get_virtual_point_data()` (*DirichletBC method*), 114
`get_virtual_point_data()` (*MixedBC method*), 120
`get_virtual_point_data()` (*NeumannBC method*), 121

getter() (*classproperty method*), 227
 GhostCellSetter (*class in pde.tools.typing*), 243
 gradient() (*ScalarField method*), 82
 gradient() (*VectorField method*), 91
 gradient_squared() (*ScalarField method*), 82
 grid (*Boundaries attribute*), 98
 grid (*BoundaryAxisBase property*), 100
 grid (*FieldBase property*), 72
 grid (*StorageBase property*), 198
 grid (*StorageView property*), 201
 GridBase (*class in pde.grids.base*), 144

H

handle() (*CallbackTracker method*), 253
 handle() (*ConsistencyTracker method*), 254
 handle() (*DataTracker method*), 255
 handle() (*InteractivePlotTracker method*), 248
 handle() (*MaterialConservationTracker method*), 257
 handle() (*PlotTracker method*), 258
 handle() (*PrintTracker method*), 259
 handle() (*ProgressTracker method*), 260
 handle() (*RuntimeTracker method*), 260
 handle() (*SteadyStateTracker method*), 261
 handle() (*StorageTracker method*), 200
 handle() (*TrackerBase method*), 245
 handle() (*TrackerCollection method*), 246
 has_collection (*StorageBase property*), 198
 has_collection (*StorageView attribute*), 201
 has_hole (*CylindricalSymGrid property*), 164
 has_hole (*SphericalSymGridBase property*), 169
 hash_mutable() (*in module pde.tools.cache*), 211
 hash_readable() (*in module pde.tools.cache*), 211
 hdf_write_attributes() (*in module pde.tools.misc*), 227
 HideParameter (*class in pde.tools.parameters*), 235
 high (*BoundaryAxisBase attribute*), 100
 homogeneous (*BCBase attribute*), 105
 hybridmethod (*class in pde.tools.misc*), 228

I

imag (*FieldBase property*), 72
 ImplicitSolver (*class in pde.solvers*), 187
 ImplicitSolver (*class in pde.solvers.implicit*), 194
 import_class() (*in module pde.tools.misc*), 228
 in_ipython() (*in module pde.tools.plotting*), 240
 in_jupyter_notebook() (*in module pde.tools.output*), 234
 increment() (*Counter method*), 231
 info (*AdamsBashforthSolver attribute*), 188
 info (*Controller attribute*), 191
 info (*CrankNicolsonSolver attribute*), 192
 info (*ExplicitSolver attribute*), 192
 info (*ImplicitSolver attribute*), 194
 info (*ScipySolver attribute*), 195

initialize() (*ConstantInterrupts method*), 249
 initialize() (*FixedInterrupts method*), 250
 initialize() (*InteractivePlotTracker method*), 248
 initialize() (*InterruptsBase method*), 251
 initialize() (*MaterialConservationTracker method*), 257
 initialize() (*PlotTracker method*), 259
 initialize() (*ProgressTracker method*), 260
 initialize() (*RealtimeInterrupts method*), 252
 initialize() (*RuntimeTracker method*), 261
 initialize() (*StorageTracker method*), 200
 initialize() (*TrackerBase method*), 245
 initialize() (*TrackerCollection method*), 246
 initialized (*in module pde.tools.mpi*), 229
 insert() (*DataFieldBase method*), 63
 instancemethod() (*hybridmethod method*), 228
 integral (*DataFieldBase property*), 63
 integral (*ScalarField property*), 83
 integral (*Tensor2Field property*), 87
 integral (*VectorField property*), 92
 integrals (*FieldCollection property*), 77
 integrate() (*GridBase method*), 149
 InteractivePlotTracker (*class in pde.trackers.interactive*), 247
 interface_width (*AllenCahnPDE attribute*), 171
 interpolate() (*DataFieldBase method*), 63
 interpolate_to_grid() (*DataFieldBase method*), 64
 interpolate_to_grid() (*FieldCollection method*), 77
 interpolate_to_grid() (*ScalarField method*), 83
 interpolate_to_grid() (*VectorField method*), 92
 InterruptsBase (*class in pde.trackers.interrupts*), 250
 is_available() (*Movie class method*), 263
 is_complex (*FieldBase property*), 72
 is_main (*in module pde.tools.mpi*), 230
 is_sde (*PDEBase property*), 173
 is_zero (*ScalarExpression property*), 220
 items() (*MovieStorage method*), 205
 items() (*StorageBase method*), 198
 items() (*StorageView method*), 201
 iter_mirror_points() (*CartesianGrid method*), 159
 iter_mirror_points() (*CylindricalSymGrid method*), 164
 iter_mirror_points() (*GridBase method*), 150

J

jit() (*in module pde.tools.numba*), 232
 JupyterOutput (*class in pde.tools.output*), 233
 JupyterPlottingContext (*class in pde.tools.plotting*), 238

K

KPZInterfacePDE (class in *pde.pdes.kpz_interface*), 177

KuramotoSivashinskyPDE (class in *pde.pdes.kuramoto_sivashinsky*), 178

L

label (*FieldBase* property), 72

labels (*FieldCollection* property), 78

laplace() (*ScalarField* method), 83

laplace() (*VectorField* method), 93

length (*CylindricalSymGrid* property), 165

link_value() (*ConstBCBase* method), 111

LivePlotTracker (class in *pde.trackers.trackers*), 256

LogarithmicInterrupts (class in *pde.trackers.interrupts*), 251

low (*BoundaryAxisBase* attribute), 100

M

magnitude (*DataFieldBase* property), 64

magnitudes (*FieldCollection* property), 78

major_axis (*SphericalCoordinates* attribute), 132

make_adjacent_evaluator() (*BCBase* method), 105

make_adjacent_evaluator() (*ConstBC1stOrderBase* method), 108

make_adjacent_evaluator() (*ConstBC2ndOrderBase* method), 110

make_adjacent_evaluator() (*ExpressionBC* method), 115

make_array_constructor() (in module *pde.tools.numba*), 232

make_cell_volume_compiled() (*GridBase* method), 150

make_colored_noise() (in module *pde.tools.spectral*), 242

make_derivative() (in module *pde.grids.operators.common*), 135

make_derivative2() (in module *pde.grids.operators.common*), 135

make_divergence() (in module *pde.grids.operators.cartesian*), 133

make_divergence() (in module *pde.grids.operators.cylindrical_sym*), 136

make_divergence() (in module *pde.grids.operators.polar_sym*), 139

make_divergence() (in module *pde.grids.operators.spherical_sym*), 141

make_dot_operator() (*DataFieldBase* method), 64

make_general_poisson_solver() (in module *pde.grids.operators.common*), 135

make_ghost_cell_sender() (*BCBase* method), 106

make_ghost_cell_sender() (*BCBase* method), 106

make_ghost_cell_sender() (*Boundaries* method), 98

make_ghost_cell_sender() (*BoundaryAxisBase* method), 100

make_ghost_cell_sender() (*UserBC* method), 125

make_gradient() (in module *pde.grids.operators.cartesian*), 133

make_gradient() (in module *pde.grids.operators.cylindrical_sym*), 137

make_gradient() (in module *pde.grids.operators.polar_sym*), 139

make_gradient() (in module *pde.grids.operators.spherical_sym*), 142

make_gradient_squared() (in module *pde.grids.operators.cylindrical_sym*), 137

make_gradient_squared() (in module *pde.grids.operators.polar_sym*), 139

make_gradient_squared() (in module *pde.grids.operators.spherical_sym*), 142

make_inserter_compiled() (*GridBase* method), 150

make_integrator() (*GridBase* method), 150

make_interpolator() (*DataFieldBase* method), 65

make_laplace() (in module *pde.grids.operators.cartesian*), 134

make_laplace() (in module *pde.grids.operators.cylindrical_sym*), 137

make_laplace() (in module *pde.grids.operators.polar_sym*), 140

make_laplace() (in module *pde.grids.operators.spherical_sym*), 142

make_laplace_from_matrix() (in module *pde.grids.operators.common*), 136

make_modify_after_step() (*PDEBase* method), 173

make_movie() (*ScalarFieldPlot* method), 265

make_normalize_point_compiled() (*GridBase* method), 151

make_operator() (*GridBase* method), 151

make_operator_no_bc() (*GridBase* method), 152

make_outer_prod_operator() (*VectorField* method), 93

make_pde_rhs() (*PDEBase* method), 173

make_poisson_solver() (in module *pde.grids.operators.cartesian*), 134

make_poisson_solver() (in module *pde.grids.operators.cylindrical_sym*), 138

make_poisson_solver() (in module *pde.grids.operators.polar_sym*), 140

make_poisson_solver() (in module *pde.grids.operators.spherical_sym*), 143

`make_sde_rhs()` (*PDEBase method*), 173
`make_serializer()` (*in module `pde.tools.cache`*), 212
`make_stepper()` (*AdaptiveSolverBase method*), 189
`make_stepper()` (*ExplicitMPISolver method*), 194
`make_stepper()` (*ScipySolver method*), 187, 195
`make_stepper()` (*SolverBase method*), 190
`make_tensor_divergence()` (*in module `pde.grids.operators.cartesian`*), 134
`make_tensor_divergence()` (*in module `pde.grids.operators.cylindrical_sym`*), 138
`make_tensor_divergence()` (*in module `pde.grids.operators.polar_sym`*), 140
`make_tensor_divergence()` (*in module `pde.grids.operators.spherical_sym`*), 143
`make_tensor_double_divergence()` (*in module `pde.grids.operators.spherical_sym`*), 143
`make_unserializer()` (*in module `pde.tools.cache`*), 212
`make_vector_gradient()` (*in module `pde.grids.operators.cartesian`*), 134
`make_vector_gradient()` (*in module `pde.grids.operators.cylindrical_sym`*), 138
`make_vector_gradient()` (*in module `pde.grids.operators.polar_sym`*), 141
`make_vector_gradient()` (*in module `pde.grids.operators.spherical_sym`*), 144
`make_vector_laplace()` (*in module `pde.grids.operators.cartesian`*), 135
`make_vector_laplace()` (*in module `pde.grids.operators.cylindrical_sym`*), 138
`make_virtual_point_evaluator()` (*BCBase method*), 106
`make_virtual_point_evaluator()` (*Con-
stBC1stOrderBase method*), 109
`make_virtual_point_evaluator()` (*Con-
stBC2ndOrderBase method*), 110
`make_virtual_point_evaluator()` (*Expres-
sionBC method*), 115
`make_virtual_point_evaluator()` (*UserBC
method*), 126
`mapping_jacobian()` (*CoordinatesBase method*), 128
`MaterialConservationTracker` (*class in `pde.trackers.trackers`*), 256
`max_value` (*FFmpegFormat property*), 224
`mean` (*OnlineStatistics attribute*), 225
`MemoryStorage` (*class in `pde.storage.memory`*), 202
`metric()` (*CoordinatesBase method*), 128
`MixedBC` (*class in `pde.grids.boundaries.local`*), 119
`module`
 pde.fields, 59
 pde.fields.base, 60
 pde.fields.collection, 74
 pde.fields.scalar, 80
 pde.fields.tensorial, 85
 pde.fields.vectorial, 89
 pde.grids, 94
 pde.grids.base, 144
 pde.grids.boundaries, 95
 pde.grids.boundaries.axes, 97
 pde.grids.boundaries.axis, 99
 pde.grids.boundaries.local, 102
 pde.grids.cartesian, 157
 pde.grids.coordinates, 127
 pde.grids.coordinates.base, 127
 pde.grids.coordinates.bipolar, 130
 pde.grids.coordinates.bispherical, 130
 pde.grids.coordinates.cartesian, 131
 pde.grids.coordinates.cylindrical, 131
 pde.grids.coordinates.polar, 132
 pde.grids.coordinates.spherical, 132
 pde.grids.cylindrical, 161
 pde.grids.operators, 133
 pde.grids.operators.cartesian, 133
 pde.grids.operators.common, 135
 pde.grids.operators.cylindrical_sym, 136
 pde.grids.operators.polar_sym, 139
 pde.grids.operators.spherical_sym, 141
 pde.grids.spherical, 165
 pde.pdes, 170
 pde.pdes.allen_cahn, 170
 pde.pdes.base, 171
 pde.pdes.cahn_hilliard, 175
 pde.pdes.diffusion, 176
 pde.pdes.kpz_interface, 177
 pde.pdes.kuramoto_sivashinsky, 178
 pde.pdes.laplace, 180
 pde.pdes.pde, 181
 pde.pdes.swift_hohenberg, 183
 pde.pdes.wave, 184
 pde.solvers, 185
 pde.solvers.adams_bashforth, 188
 pde.solvers.base, 188
 pde.solvers.controller, 190
 pde.solvers.crank_nicolson, 192
 pde.solvers.explicit, 192
 pde.solvers.explicit_mpi, 193
 pde.solvers.implicit, 194
 pde.solvers.scipy, 195
 pde.storage, 195
 pde.storage.base, 196
 pde.storage.file, 201
 pde.storage.memory, 202

pde.storage.movie, 204
 pde.tools, 207
 pde.tools.cache, 207
 pde.tools.config, 213
 pde.tools.cuboid, 214
 pde.tools.docstrings, 217
 pde.tools.expressions, 217
 pde.tools.ffmpeg, 223
 pde.tools.math, 225
 pde.tools.misc, 226
 pde.tools.mpi, 229
 pde.tools.numba, 231
 pde.tools.output, 233
 pde.tools.parameters, 234
 pde.tools.parse_duration, 237
 pde.tools.plotting, 237
 pde.tools.spectral, 242
 pde.tools.typing, 243
 pde.trackers, 243
 pde.trackers.base, 244
 pde.trackers.interactive, 247
 pde.trackers.interrupts, 249
 pde.trackers.trackers, 253
 pde.visualization, 262
 pde.visualization.movies, 262
 pde.visualization.plotting, 264
 module_available() (in module pde.tools.misc), 228
 Movie (class in pde.visualization.movies), 262
 movie() (in module pde.visualization.movies), 263
 movie_multiple() (in module pde.visualization.movies), 263
 movie_scalar() (in module pde.visualization.movies), 264
 MovieStorage (class in pde.storage.movie), 204
 mpi_allreduce() (in module pde.tools.mpi), 230
 mpi_recv() (in module pde.tools.mpi), 230
 mpi_send() (in module pde.tools.mpi), 230
 mutable (Cuboid property), 216

N

name (AdamsBashforthSolver attribute), 185, 188
 name (ConsistencyTracker attribute), 254
 name (CrankNicolsonSolver attribute), 187, 192
 name (ExplicitMPSolver attribute), 194
 name (ExplicitSolver attribute), 187, 192
 name (ImplicitSolver attribute), 187, 194
 name (InteractivePlotTracker attribute), 248
 name (LivePlotTracker attribute), 256
 name (MaterialConservationTracker attribute), 257
 name (OperatorInfo attribute), 156
 name (PrintTracker attribute), 259
 name (ProgressTracker attribute), 260
 name (ScipySolver attribute), 188, 195
 name (SteadyStateTracker attribute), 262

names (BCBase attribute), 106
 names (CurvatureBC attribute), 113
 names (DirichletBC attribute), 114
 names (ExpressionBC attribute), 116
 names (ExpressionDerivativeBC attribute), 117
 names (ExpressionMixedBC attribute), 118
 names (ExpressionValueBC attribute), 119
 names (MixedBC attribute), 120
 names (NeumannBC attribute), 121
 names (NormalCurvatureBC attribute), 122
 names (NormalDirichletBC attribute), 123
 names (NormalMixedBC attribute), 124
 names (NormalNeumannBC attribute), 124
 names (UserBC attribute), 126
 napari_add_layers() (in module pde.tools.plotting), 240
 napari_process() (in module pde.trackers.interactive), 248
 napari_viewer() (in module pde.tools.plotting), 240
 NapariViewer (class in pde.trackers.interactive), 248
 nested_plotting_check (class in pde.tools.plotting), 240
 NeumannBC (class in pde.grids.boundaries.local), 121
 next() (ConstantInterrupts method), 249
 next() (FixedInterrupts method), 250
 next() (InterruptsBase method), 251
 next() (LogarithmicInterrupts method), 251
 next() (RealtimeInterrupts method), 252
 noise_realization() (PDEBase method), 174
 normal (BCBase attribute), 106
 normal (NormalCurvatureBC attribute), 122
 normal (NormalDirichletBC attribute), 123
 normal (NormalMixedBC attribute), 124
 normal (NormalNeumannBC attribute), 125
 NormalCurvatureBC (class in pde.grids.boundaries.local), 121
 NormalDirichletBC (class in pde.grids.boundaries.local), 122
 normalize_point() (GridBase method), 152
 NormalMixedBC (class in pde.grids.boundaries.local), 123
 NormalNeumannBC (class in pde.grids.boundaries.local), 124
 num_axes (GridBase attribute), 152
 num_cells (GridBase property), 152
 numba_dict() (in module pde.tools.numba), 232
 numba_environment() (in module pde.tools.numba), 232
 numba_type (GridBase property), 152
 number() (in module pde.tools.misc), 228
 number_array() (in module pde.tools.misc), 228

O

objects_equal() (in module pde.tools.cache), 212

`ol_flat_idx()` (in module *pde.tools.numba*), 232
`ol_mpi_allreduce()` (in module *pde.tools.mpi*), 230
`ol_mpi_recv()` (in module *pde.tools.mpi*), 230
`ol_mpi_send()` (in module *pde.tools.mpi*), 231
`OnlineStatistics` (class in *pde.tools.math*), 225
`OperatorFactory` (class in *pde.tools.typing*), 243
`OperatorInfo` (class in *pde.grids.base*), 155
`operators` (*GridBase* attribute), 153
`OperatorType` (class in *pde.tools.typing*), 243
`outer_product()` (*VectorField* method), 93
`OutputBase` (class in *pde.tools.output*), 233

P

`packages_from_requirements()` (in module *pde.tools.config*), 214
`parallel_run` (in module *pde.tools.mpi*), 231
`Parameter` (class in *pde.tools.parameters*), 235
`Parameterized` (class in *pde.tools.parameters*), 235
`parameters` (*PlotReference* attribute), 238
`parameters_default` (*Parameterized* attribute), 236
`parse_duration()` (in module *pde.tools.parse_duration*), 237
`parse_interrupt()` (in module *pde.trackers.interrupts*), 252
`parse_number()` (in module *pde.tools.expressions*), 222
`parse_version_str()` (in module *pde.tools.config*), 214
`pde`
 module, 59
`PDE` (class in *pde.pdes.pde*), 181
`pde.fields`
 module, 59
`pde.fields.base`
 module, 60
`pde.fields.collection`
 module, 74
`pde.fields.scalar`
 module, 80
`pde.fields.tensorial`
 module, 85
`pde.fields.vectorial`
 module, 89
`pde.grids`
 module, 94
`pde.grids.base`
 module, 144
`pde.grids.boundaries`
 module, 95
`pde.grids.boundaries.axes`
 module, 97
`pde.grids.boundaries.axis`
 module, 99
`pde.grids.boundaries.local`

 module, 102
`pde.grids.cartesian`
 module, 157
`pde.grids.coordinates`
 module, 127
`pde.grids.coordinates.base`
 module, 127
`pde.grids.coordinates.bipolar`
 module, 130
`pde.grids.coordinates.bispherical`
 module, 130
`pde.grids.coordinates.cartesian`
 module, 131
`pde.grids.coordinates.cylindrical`
 module, 131
`pde.grids.coordinates.polar`
 module, 132
`pde.grids.coordinates.spherical`
 module, 132
`pde.grids.cylindrical`
 module, 161
`pde.grids.operators`
 module, 133
`pde.grids.operators.cartesian`
 module, 133
`pde.grids.operators.common`
 module, 135
`pde.grids.operators.cylindrical_sym`
 module, 136
`pde.grids.operators.polar_sym`
 module, 139
`pde.grids.operators.spherical_sym`
 module, 141
`pde.grids.spherical`
 module, 165
`pde.pdes`
 module, 170
`pde.pdes.allen_cahn`
 module, 170
`pde.pdes.base`
 module, 171
`pde.pdes.cahn_hilliard`
 module, 175
`pde.pdes.diffusion`
 module, 176
`pde.pdes.kpz_interface`
 module, 177
`pde.pdes.kuramoto_sivashinsky`
 module, 178
`pde.pdes.laplace`
 module, 180
`pde.pdes.pde`
 module, 181
`pde.pdes.swift_hohenberg`

module, 183
 pde.pdes.wave
 module, 184
 pde.solvers
 module, 185
 pde.solvers.adams_bashforth
 module, 188
 pde.solvers.base
 module, 188
 pde.solvers.controller
 module, 190
 pde.solvers.crank_nicolson
 module, 192
 pde.solvers.explicit
 module, 192
 pde.solvers.explicit_mpi
 module, 193
 pde.solvers.implicit
 module, 194
 pde.solvers.scipy
 module, 195
 pde.storage
 module, 195
 pde.storage.base
 module, 196
 pde.storage.file
 module, 201
 pde.storage.memory
 module, 202
 pde.storage.movie
 module, 204
 pde.tools
 module, 207
 pde.tools.cache
 module, 207
 pde.tools.config
 module, 213
 pde.tools.cuboid
 module, 214
 pde.tools.docstrings
 module, 217
 pde.tools.expressions
 module, 217
 pde.tools.ffmpeg
 module, 223
 pde.tools.math
 module, 225
 pde.tools.misc
 module, 226
 pde.tools.mpi
 module, 229
 pde.tools.numba
 module, 231
 pde.tools.output
 module, 233
 pde.tools.parameters
 module, 234
 pde.tools.parse_duration
 module, 237
 pde.tools.plotting
 module, 237
 pde.tools.spectral
 module, 242
 pde.tools.typing
 module, 243
 pde.trackers
 module, 243
 pde.trackers.base
 module, 244
 pde.trackers.interactive
 module, 247
 pde.trackers.interrupts
 module, 249
 pde.trackers.trackers
 module, 253
 pde.visualization
 module, 262
 pde.visualization.movies
 module, 262
 pde.visualization.plotting
 module, 264
 PDEBase (*class in pde.pdes.base*), 171
 periodic (*BCBase property*), 106
 periodic (*Boundaries property*), 99
 periodic (*BoundaryAxisBase property*), 100
 periodic (*GridBase property*), 153
 PeriodicityError, 156
 pix_fmt_data (*FFmpegFormat attribute*), 224
 pix_fmt_file (*FFmpegFormat attribute*), 224
 plot () (*CartesianGrid method*), 159
 plot () (*DataFieldBase method*), 65
 plot () (*FieldBase method*), 73
 plot () (*FieldCollection method*), 78
 plot () (*GridBase method*), 153
 plot () (*SphericalSymGridBase method*), 169
 plot_components () (*Tensor2Field method*), 87
 plot_interactive () (*FieldBase method*), 73
 plot_interactive () (in module *pde.visualization.plotting*), 266
 plot_kymograph () (in module *pde.visualization.plotting*), 267
 plot_kymographs () (in module *pde.visualization.plotting*), 268
 plot_magnitudes () (in module *pde.visualization.plotting*), 268
 plot_on_axes () (in module *pde.tools.plotting*), 241
 plot_on_figure () (in module *pde.tools.plotting*), 241
 PlotReference (*class in pde.tools.plotting*), 238

PlottingContextBase (class in *pde.tools.plotting*), 239
 PlotTracker (class in *pde.trackers.trackers*), 257
 point_from_cartesian() (GridBase method), 153
 point_to_cartesian() (GridBase method), 153
 PolarCoordinates (class in *pde.grids.coordinates.polar*), 132
 PolarSymGrid (class in *pde.grids.spherical*), 165
 pos_diff() (CoordinatesBase method), 128
 pos_from_cart() (CoordinatesBase method), 129
 pos_to_cart() (CoordinatesBase method), 129
 preserve_scalars() (in module *pde.tools.misc*), 229
 PrintTracker (class in *pde.trackers.trackers*), 259
 progress_bar_format (SteadyStateTracker attribute), 262
 ProgressTracker (class in *pde.trackers.trackers*), 259
 project() (ScalarField method), 84
 PYTHONPATH, 5

R

radius (CylindricalSymGrid property), 165
 radius (SphericalSymGridBase property), 169
 random_colored() (DataFieldBase class method), 66
 random_harmonic() (DataFieldBase class method), 67
 random_normal() (DataFieldBase class method), 67
 random_seed() (in module *pde.tools.numba*), 232
 random_uniform() (DataFieldBase class method), 68
 rank (BoundaryAxisBase property), 100
 rank (DataFieldBase attribute), 68
 rank (ExpressionBase property), 219
 rank (in module *pde.tools.mpi*), 231
 rank (ScalarField attribute), 84
 rank (Tensor2Field attribute), 88
 rank (TensorExpression property), 221
 rank (VectorField attribute), 94
 rank_in (OperatorInfo attribute), 156
 rank_out (OperatorInfo attribute), 156
 RankError, 74
 real (FieldBase property), 73
 RealtimeInterrupts (class in *pde.trackers.interrupts*), 251
 register_operator() (GridBase class method), 153
 registered_boundary_condition_classes() (in module *pde.grids.boundaries.local*), 126
 registered_boundary_condition_names() (in module *pde.grids.boundaries.local*), 126
 registered_operators() (in module *pde.grids.base*), 156
 registered_solvers (SolverBase attribute), 190
 registered_solvers() (in module *pde.solvers*), 188
 replace_in_docstring() (in module *pde.tools.docstrings*), 217
 run() (Controller method), 186, 191

RuntimeTracker (class in *pde.trackers.trackers*), 260

S

save() (Movie method), 263
 savefig() (ScalarFieldPlot method), 266
 scalar_random_uniform() (FieldCollection class method), 79
 ScalarExpression (class in *pde.tools.expressions*), 219
 ScalarField (class in *pde.fields.scalar*), 80
 ScalarFieldPlot (class in *pde.visualization.plotting*), 264
 scale_factors() (CoordinatesBase method), 129
 ScipySolver (class in *pde.solvers*), 187
 ScipySolver (class in *pde.solvers.scipy*), 195
 SerializedDict (class in *pde.tools.cache*), 208
 set_ghost_cells() (BCBase method), 106
 set_ghost_cells() (Boundaries method), 99
 set_ghost_cells() (BoundaryAxisBase method), 100
 set_ghost_cells() (ConstBC1stOrderBase method), 109
 set_ghost_cells() (ConstBC2ndOrderBase method), 110
 set_ghost_cells() (DataFieldBase method), 68
 set_ghost_cells() (ExpressionBC method), 116
 set_ghost_cells() (UserBC method), 126
 setter() (classproperty method), 227
 shape (ExpressionBase property), 219
 shape (GridBase property), 154
 shape (ScalarExpression attribute), 220
 shape (StorageBase property), 198
 shape (TensorExpression property), 221
 show() (BasicOutput method), 233
 show() (JupyterOutput method), 233
 show() (OutputBase method), 233
 show_parameters() (Parameterized method), 236
 sigma_auto_scale (SmoothData1D attribute), 226
 size (Cuboid property), 216
 size (in module *pde.tools.mpi*), 231
 skipUnlessModule() (in module *pde.tools.misc*), 229
 slice() (CartesianGrid method), 160
 slice() (CylindricalSymGrid method), 165
 slice() (GridBase method), 154
 slice() (ScalarField method), 84
 slice() (UnitGrid method), 161
 smooth() (DataFieldBase method), 69
 smooth() (FieldCollection method), 79
 SmoothData1D (class in *pde.tools.math*), 225
 solve() (PDEBase method), 174
 solve_laplace_equation() (in module *pde.pdes.laplace*), 180
 solve_poisson_equation() (in module *pde.pdes.laplace*), 180

- SolverBase (class in *pde.solvers.base*), 189
 SphericalCoordinates (class in *pde.grids.coordinates.spherical*), 132
 SphericalSymGrid (class in *pde.grids.spherical*), 166
 SphericalSymGridBase (class in *pde.grids.spherical*), 166
 sphinx_display_parameters() (in module *pde.tools.parameters*), 236
 split_mpi() (*FieldBase* method), 73
 start_writing() (*FileStorage* method), 202
 start_writing() (*MemoryStorage* method), 203
 start_writing() (*MovieStorage* method), 205
 start_writing() (*StorageBase* method), 198
 state (*CartesianGrid* property), 160
 state (*CylindricalSymGrid* property), 165
 state (*GridBase* property), 154
 state (*SphericalSymGridBase* property), 169
 state (*UnitGrid* property), 161
 state_serialized (*GridBase* property), 154
 SteadyStateTracker (class in *pde.trackers.trackers*), 261
 storage (*StorageTracker* attribute), 199
 StorageBase (class in *pde.storage.base*), 196
 StorageTracker (class in *pde.storage.base*), 199
 StorageView (class in *pde.storage.base*), 200
 supports_update (*JupyterPlottingContext* attribute), 238
 supports_update (*PlottingContextBase* attribute), 239
 surface_area (*Cuboid* property), 216
 SwiftHohenbergPDE (class in *pde.pdes.swift_hohenberg*), 183
 symmetrize() (*Tensor2Field* method), 88
- ## T
- t_range (*Controller* property), 186, 191
 Tensor2Field (class in *pde.fields.tensorial*), 85
 TensorExpression (class in *pde.tools.expressions*), 220
 time_next_action (*TrackerCollection* attribute), 246
 times (*DataTracker* attribute), 254
 times (*FileStorage* property), 202
 times (*MovieStorage* attribute), 206
 times (*StorageBase* attribute), 198
 times (*StorageView* property), 201
 to_cartesian() (*UnitGrid* method), 161
 to_dict() (*Config* method), 213
 to_file() (*DataTracker* method), 255
 to_file() (*FieldBase* method), 73
 to_scalar() (*DataFieldBase* method), 69
 to_scalar() (*ScalarField* method), 85
 to_scalar() (*Tensor2Field* method), 88
 to_scalar() (*VectorField* method), 94
 to_subgrid() (*BCBase* method), 107
 to_subgrid() (*ConstBCBase* method), 112
 to_subgrid() (*ExpressionBC* method), 116
 to_subgrid() (*MixedBC* method), 120
 to_subgrid() (*UserBC* method), 126
 trace() (*Tensor2Field* method), 88
 tracker() (*MovieStorage* method), 206
 tracker() (*StorageBase* method), 198
 tracker_action_times (*TrackerCollection* attribute), 246
 TrackerBase (class in *pde.trackers.base*), 244
 TrackerCollection (class in *pde.trackers.base*), 245
 trackers (*TrackerCollection* attribute), 245
 transform() (*GridBase* method), 154
 transpose() (*Tensor2Field* method), 89
 typical_discretization (*GridBase* property), 155
- ## U
- uniform_cell_volumes (*GridBase* attribute), 155
 uniform_discretization() (in module *pde.grids.operators.common*), 136
 UnitGrid (class in *pde.grids.cartesian*), 160
 unserialize_attributes() (*DataFieldBase* class method), 69
 unserialize_attributes() (*FieldBase* class method), 74
 unserialize_attributes() (*FieldCollection* class method), 80
 update() (*DictFiniteCapacity* method), 207
 update() (*NapariViewer* method), 248
 update() (*ScalarFieldPlot* method), 266
 UserBC (class in *pde.grids.boundaries.local*), 125
- ## V
- value (*ConstBCBase* property), 112
 value (*ScalarExpression* property), 220
 value (*TensorExpression* property), 221
 value_is_linked (*ConstBCBase* attribute), 112
 variables (*PDE* attribute), 181
 vec_to_cart() (*CoordinatesBase* method), 129
 VectorField (class in *pde.fields.vectorial*), 89
 vertices (*Cuboid* property), 216
 view_field() (*StorageBase* method), 199
 VirtualPointEvaluator (class in *pde.tools.typing*), 243
 volume (*CartesianGrid* property), 160
 volume (*Cuboid* property), 216
 volume (*CylindricalSymGrid* property), 165
 volume (*GridBase* property), 155
 volume (*SphericalSymGridBase* property), 169
 volume_factor() (*CoordinatesBase* method), 129
 volume_from_radius() (in module *pde.grids.spherical*), 169
- ## W
- WavePDE (class in *pde.pdes.wave*), 184

`write_mode` (*StorageBase attribute*), [199](#)
`writable` (*FieldBase property*), [74](#)