PyFR Documentation

Release 1.12.3

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PyFR 1.12.3 is an open-source flow solver that uses the high-order flux reconstruction method. For more information on the PyFR project visit our website, or to ask a question visit our forum.

Contents:

CHAPTER

ONE

INSTALLATION

1.1 Quick-start

PyFR 1.12.3 can be installed using pip and virtualenv, as shown in the quick-start guides below.

Alternatively, PyFR 1.12.3 can be installed from source, see *Compiling from source*.

1.1.1 macOS

We recommend using the package manager homebrew. Open the terminal and install the dependencies with the following commands:

```
brew install python3 open-mpi metis
pip3 install virtualenv
```

For visualisation of results, either install ParaView from the command line:

```
brew cask install paraview
```

or dowload the app from the ParaView website. Then create a virtual environment and activate it:

```
virtualenv --python=python3 ENV3
source ENV3/bin/activate
```

Finally install PyFR with pip in the virtual environment:

```
pip install pyfr
```

This concludes the installation. In order to run PyFR with the OpenMP backend (see *Running PyFR*), use the following settings in the *Configuration File (.ini)*:

```
[backend-openmp]
cc = gcc-8
```

Note the version of the compiler which must support the `openmp` flag. This has been tested on macOS 11.6 for ARM and Intel CPUs.

1.1.2 Ubuntu

Open the terminal and install the dependencies with the following commands:

```
sudo apt install python3 python3-pip libopenmpi-dev openmpi-bin
sudo apt install metis libmetis-dev
pip3 install virtualenv
```

For visualisation of results, either install ParaView from the command line:

```
sudo apt install paraview
```

or dowload the app from the ParaView website. Then create a virtual environment and activate it:

```
python3 -m virtualenv pyfr-venv
source pyfr-venv/bin/activate
```

Finally install PyFR with pip in the virtual environment:

```
pip install pyfr
```

This concludes the installation.

This has been tested on Ubuntu 20.04.

1.2 Compiling from source

PyFR can be obtained here. To install the software from source, use the provided `setup.py` installer or add the root PyFR directory to `PYTHONPATH` using:

```
user@computer ~/PyFR$ export PYTHONPATH=.:$PYTHONPATH
```

When installing from source, we strongly recommend using pip and virtualenv to manage the Python dependencies.

1.2.1 Dependencies

PyFR 1.12.3 has a hard dependency on Python 3.9+ and the following Python packages:

1. appdirs >= 1.4.0
2. gimmik >= 2.0
3. h5py >= 2.10
4. mako >= 1.0.0
5. mpi4py >= 3.0
6. numpy >= 1.20
7. pytools >= 2016.2.1

Note that due to a bug in NumPy, PyFR is not compatible with 32-bit Python distributions.

1.2.1.1 CUDA Backend

The CUDA backend targets NVIDIA GPUs with a compute capability of 3.0 or greater. The backend requires:

1. CUDA >= 8.0

1.2.1.2 HIP Backend

The HIP backend targets AMD GPUs which are supported by the ROCm stack. The backend requires:

1. ROCm >= 4.5.0
2. rocBLAS >= 2.41.0

1.2.1.3 OpenCL Backend

The OpenCL backend targets a range of accelerators including GPUs from AMD, Intel, and NVIDIA. The backend requires:

1. OpenCL
2. pyopencl >= 2015.2.4
3. CLBlast

1.2.1.4 OpenMP Backend

The OpenMP backend targets multi-core CPUs. The backend requires:

1. GCC >= 4.9 or another C compiler with OpenMP support
2. Optionally libxsmm >= commit 14b6cea61376653b2712e3eefa72b13c5e76e421 compiled as a shared library (STATIC=0) with BLAS=0 and CODE_BUF_MAXSIZE=262144

In order for PyFR to find libxsmm it must be located in a directory which is on the library search path. Alternatively, the path can be specified explicitly by exporting the environment variable `PYFR_XSMM_LIBRARY_PATH=/path/to/libxsmm.so`.

1.2.1.5 Parallel

To partition meshes for running in parallel it is also necessary to have one of the following partitioners installed:

1. METIS >= 5.0
2. SCOTCH >= 6.0

In order for PyFR to find these libraries they must be located in a directory which is on the library search path. Alternatively, the paths can be specified explicitly by exporting the environment variables `PYFR_METIS_LIBRARY_PATH=/path/to/libmetis.so` and/or `PYFR_SCOTCH_LIBRARY_PATH=/path/to/libscotch.so`.

CHAPTER

TWO

USER GUIDE

For information on how to install PyFR see *Installation*.

2.1 Running PyFR

PyFR 1.12.3 uses three distinct file formats:

1. `.ini` — configuration file
2. `.pyfrm` — mesh file
3. `.pyfrs` — solution file

The following commands are available from the `pyfr` program:

1. `pyfr import` — convert a Gmsh .msh file into a PyFR .pyfrm file.

   Example:

   ```
   pyfr import mesh.msh mesh.pyfrm
   ```

2. `pyfr partition` — partition an existing mesh and associated solution files.

   Example:

   ```
   pyfr partition 2 mesh.pyfrm solution.pyfrs .
   ```

3. `pyfr run` — start a new PyFR simulation. Example:

   ```
   pyfr run mesh.pyfrm configuration.ini
   ```

4. `pyfr restart` — restart a PyFR simulation from an existing solution file. Example:

   ```
   pyfr restart mesh.pyfrm solution.pyfrs
   ```

5. `pyfr export` — convert a PyFR `.pyfrs` file into an unstructured VTK `.vtu` or `.pvtu` file. If a `-k` flag is provided with an integer argument then `.pyfrs` elements are converted to high-order VTK cells which are exported, where the order of the VTK cells is equal to the value of the integer argument. Example:

   ```
   pyfr export -k 4 mesh.pyfrm solution.pyfrs solution.vtu
   ```

   If a `-d` flag is provided with an integer argument then `.pyfrs` elements are subdivided into linear VTK cells which are exported, where the number of sub-divisions is equal to the value of the integer argument. Example:

```
pyfr export -d 4 mesh.pyfrm solution.pyfrs solution.vtu
```

If no flags are provided then `.pyfrs` elements are converted to high-order VTK cells which are exported, where the order of the cells is equal to the order of the solution data in the `.pyfrs` file.

2.1.1 Running in Parallel

PyFR can be run in parallel. To do so prefix `pyfr` with `mpiexec -n <cores/devices>`. Note that the mesh must be pre-partitioned, and the number of cores or devices must be equal to the number of partitions.

2.2 Configuration File (.ini)

The .ini configuration file parameterises the simulation. It is written in the INI format. Parameters are grouped into sections. The roles of each section and their associated parameters are described below. Note that both `;` and `#` may be used as comment characters.

2.2.1 Backends

The backend sections detail how the solver will be configured for a range of different hardware platforms. If a hardware specific backend section is omitted, then PyFR will fall back to built-in default settings.

2.2.1.1 [backend]

Parameterises the backend with

1. `precision` — number precision:

   `single` | `double`

2. `rank-allocator` — MPI rank allocator:

   `linear` | `random`

Example:

```
[backend]
precision = double
rank-allocator = linear
```

2.2.1.2 [backend-cuda]

Parameterises the CUDA backend with

1. `device-id` — method for selecting which device(s) to run on:

   int | `round-robin` | `local-rank`

2. `mpi-type` — type of MPI library that is being used:

   `standard` | `cuda-aware`

3. `cflags` — additional NVIDIA realtime compiler (`nvrtc`) flags:

   string

Example:

```
[backend-cuda]
device-id = round-robin
mpi-type = standard
```

2.2.1.3 [backend-hip]

Parameterises the HIP backend with

1. `device-id` — method for selecting which device(s) to run on:

   int | `local-rank`

2. `mpi-type` — type of MPI library that is being used:

   `standard` | `hip-aware`

Example:

```
[backend-hip]
device-id = local-rank
mpi-type = standard
```

2.2.1.4 [backend-opencl]

Parameterises the OpenCL backend with

1. `platform-id` — for selecting platform id:

   int | *string*

2. `device-type` — for selecting what type of device(s) to run on:

   `all` | `cpu` | `gpu` | `accelerator`

3. `device-id` — for selecting which device(s) to run on:

   int | *string* | `local-rank`

4. `gimmik-max-nnz` — cutoff for GiMMiK in terms of the number of non-zero entires in a constant matrix:

   int

Example:

```
[backend-opencl]
platform-id = 0
device-type = gpu
device-id = local-rank
gimmik-max-nnz = 512
```

2.2.1.5 [backend-openmp]

Parameterises the OpenMP backend with

1. `cc` — C compiler:

   string

2. `cflags` — additional C compiler flags:

   string

3. `alignb` — alignment requirement in bytes; must be a power of two and at least 32:

   int

4. `gimmik-max-nnz` — cutoff for GiMMiK in terms of the number of non-zero entires in a constant matrix:

   int

Example:

```
[backend-openmp]
cc = gcc
```

2.2.2 Systems

These sections of the input file setup and control the physical system being solved, as well as charateristics of the spatial and temporal schemes to be used.

2.2.2.1 [constants]

Sets constants used in the simulation

1. `gamma` — ratio of specific heats for `euler` | `navier-stokes`:

   float

2. `mu` — dynamic viscosity for `navier-stokes`:

   float

3. `nu` — kinematic viscosity for `ac-navier-stokes`:

   float

4. `Pr` — Prandtl number for `navier-stokes`:

   float

5. `cpTref` — product of specific heat at constant pressure and reference temperature for `navier-stokes` with Sutherland's Law:

   float

6. `cpTs` — product of specific heat at constant pressure and Sutherland temperature for `navier-stokes` with Sutherland's Law:

   float

7. `ac-zeta` — artificial compressibility factor for `ac-euler` | `ac-navier-stokes`

   float

Other constant may be set by the user which can then be used throughout the `.ini` file.

Example:

```
[constants]
; PyFR Constants
gamma = 1.4
mu = 0.001
Pr = 0.72

; User Defined Constants
V_in = 1.0
P_out = 20.0
```

2.2.2.2 [solver]

Parameterises the solver with

1. `system` — governing system:

   `euler` | `navier-stokes` | `ac-euler` | `ac-navier-stokes`

   where

   `navier-stokes` requires

   - `viscosity-correction` — viscosity correction:

     `none` | `sutherland`

   - `shock-capturing` — shock capturing scheme:

     `none` | `artificial-viscosity`

2. `order` — order of polynomial solution basis:

   int

3. `anti-alias` — type of anti-aliasing:

   `flux` | `surf-flux` | `flux, surf-flux`

Example:

```
[solver]
system = navier-stokes
order = 3
anti-alias = flux
viscosity-correction = none
shock-capturing = artificial-viscosity
```

2.2.2.3 [solver-time-integrator]

Parameterises the time-integration scheme used by the solver with

1. `formulation` — formulation:

   `std` | `dual`

   where

   `std` requires

   - `scheme` — time-integration scheme

     `euler` | `rk34` | `rk4` | `rk45` | `tvd-rk3`

   - `tstart` — initial time

     float

   - `tend` — final time

     float

   - `dt` — time-step

     float

   - `controller` — time-step controller

     `none` | `pi`

     where

     `pi` only works with `rk34` and `rk45` and requires

     - `atol` — absolute error tolerance

       float

     - `rtol` — relative error tolerance

       float

     - `errest-norm` — norm to use for estimating the error

       `uniform` | `l2`

     - `safety-fact` — safety factor for step size adjustment (suitable range 0.80-0.95)

       float

     - `min-fact` — minimum factor by which the time-step can change between iterations (suitable range 0.1-0.5)

       float

     - `max-fact` — maximum factor by which the time-step can change between iterations (suitable range 2.0-6.0)

       float

     - `dt-max` — maximum permissible time-step

       float

   `dual` requires

   - `scheme` — time-integration scheme

`backward-euler` | `bdf2` | `bdf3`

- `pseudo-scheme` — pseudo time-integration scheme

  `euler` | `rk34` | `rk4` | `rk45` | `tvd-rk3` | `vermeire`

- `tstart` — initial time

  float

- `tend` — final time

  float

- `dt` — time-step

  float

- `pseudo-dt` — pseudo time-step

  float

- `controller` — pseudo time-step controller

  `none`

- `pseudo-niters-max` — minimum number of iterations

  int

- `pseudo-niters-min` — maximum number of iterations

  int

- `pseudo-resid-tol` — pseudo residual tolerance

  float

- `pseudo-resid-norm` — pseudo residual norm

  `uniform` | `l2`

- `pseudo-controller` — pseudo time-step controller

  `none` | `local-pi`

  where

  `local-pi` only works with `rk34` and `rk45` and requires

  - `atol` — absolute error tolerance

    float

  - `safety-fact` — safety factor for pseudo time-step size adjustment (suitable range 0.80-0.95)

    float

  - `min-fact` — minimum factor by which the local pseudo time-step can change between iterations (suitable range 0.98-0.998)

    float

  - `max-fact` — maximum factor by which the local pseudo time-step can change between iterations (suitable range 1.001-1.01)

    float

- `pseudo-dt-max-mult` — maximum permissible local pseudo time-step given as a multiplier of `pseudo-dt` (suitable range 2.0-5.0)

  float

Example:

```
[solver-time-integrator]
formulation = std
scheme = rk45
controller = pi
tstart = 0.0
tend = 10.0
dt = 0.001
atol = 0.00001
rtol = 0.00001
errest-norm = l2
safety-fact = 0.9
min-fact = 0.3
max-fact = 2.5
```

2.2.2.4 [solver-dual-time-integrator-multip]

Parameterises multi-p for dual time-stepping with

1. `pseudo-dt-fact` — factor by which the pseudo time-step size changes between multi-p levels:

   float

2. `cycle` — nature of a single multi-p cycle:

   `[(order,nsteps), (order,nsteps), ... (order,nsteps)]`

   where `order` in the first and last bracketed pair must be the overall polynomial order used for the simulation, and `order` can only change by one between subsequent bracketed pairs

Example:

```
[solver-dual-time-integrator-multip]
pseudo-dt-fact = 2.3
cycle = [(3, 1), (2, 1), (1, 1), (0, 2), (1, 1), (2, 1), (3, 3)]
```

2.2.2.5 [solver-interfaces]

Parameterises the interfaces with

1. `riemann-solver` — type of Riemann solver:

   `rusanov` | `hll` | `hllc` | `roe` | `roem`

   where

   `hll` | `hllc` | `roe` | `roem` do not work with `ac-euler` | `ac-navier-stokes`

2. `ldg-beta` — beta parameter used for LDG:

   float

3. `ldg-tau` — tau parameter used for LDG:

float

Example:

```
[solver-interfaces]
riemann-solver = rusanov
ldg-beta = 0.5
ldg-tau = 0.1
```

2.2.2.6 [solver-source-terms]

Parameterises solution, space (x, y, [z]), and time (t) dependent source terms with

1. `rho` — density source term for `euler` | `navier-stokes`:

   string

2. `rhou` — x-momentum source term for `euler` | `navier-stokes` :

   string

3. `rhov` — y-momentum source term for `euler` | `navier-stokes` :

   string

4. `rhow` — z-momentum source term for `euler` | `navier-stokes` :

   string

5. `E` — energy source term for `euler` | `navier-stokes` :

   string

6. `p` — pressure source term for `ac-euler` | `ac-navier-stokes`:

   string

7. `u` — x-velocity source term for `ac-euler` | `ac-navier-stokes`:

   string

8. `v` — y-velocity source term for `ac-euler` | `ac-navier-stokes`:

   string

9. `w` — w-velocity source term for `ac-euler` | `ac-navier-stokes`:

   string

Example:

```
[solver-source-terms]
rho = t
rhou = x*y*sin(y)
rhov = z*rho
rhow = 1.0
E = 1.0/(1.0+x)
```

2.2.2.7 [solver-artificial-viscosity]

Parameterises artificial viscosity for shock capturing with

1. `max-artvisc` — maximum artificial viscosity:

   float

2. `s0` — sensor cut-off:

   float

3. `kappa` — sensor range:

   float

Example:

```
[solver-artificial-viscosity]
max-artvisc = 0.01
s0 = 0.01
kappa = 5.0
```

2.2.2.8 [soln-filter]

Parameterises an exponential solution filter with

1. `nsteps` — apply filter every `nsteps`:

   int

2. `alpha` — strength of filter:

   float

3. `order` — order of filter:

   int

4. `cutoff` — cutoff frequency below which no filtering is applied:

   int

Example:

```
[soln-filter]
nsteps = 10
alpha = 36.0
order = 16
cutoff = 1
```

2.2.3 Boundary and Initial Conditions

These sections allow users to set the boundary and initial conditions of calculations.

2.2.3.1 [soln-bcs-*name*]

Parameterises constant, or if available space (x, y, [z]) and time (t) dependent, boundary condition labelled *name* in the .pyfrm file with

1. `type` — type of boundary condition:

   `ac-char-riem-inv | ac-in-fv | ac-out-fp | char-riem-inv | no-slp-adia-wall | no-slp-isot-wall | no-slp-wall | slp-adia-wall | slp-wall | sub-in-frv | sub-in-ftpttang | sub-out-fp | sup-in-fa | sup-out-fn`

   where

   `ac-char-riem-inv` only works with `ac-euler | ac-navier-stokes` and requires

   - `ac-zeta` — artificial compressibility factor for boundary (increasing `ac-zeta` makes the boundary less reflective allowing larger deviation from the target state)

     float

   - `niters` — number of Newton iterations

     int

   - `p` — pressure

     float | *string*

   - `u` — x-velocity

     float | *string*

   - `v` — y-velocity

     float | *string*

   - `w` — z-velocity

     float | *string*

   `ac-in-fv` only works with `ac-euler | ac-navier-stokes` and requires

   - `u` — x-velocity

     float | *string*

   - `v` — y-velocity

     float | *string*

   - `w` — z-velocity

     float | *string*

   `ac-out-fp` only works with `ac-euler | ac-navier-stokes` and requires

   - `p` — pressure

     float | *string*

   `char-riem-inv` only works with `euler | navier-stokes` and requires

   - `rho` — density

float | *string*

- `u` — x-velocity

  float | *string*

- `v` — y-velocity

  float | *string*

- `w` — z-velocity

  float | *string*

- `p` — static pressure

  float | *string*

`no-slp-adia-wall` only works with `navier-stokes`

`no-slp-isot-wall` only works with `navier-stokes` and requires

- `u` — x-velocity of wall

  float

- `v` — y-velocity of wall

  float

- `w` — z-velocity of wall

  float

- `cpTw` — product of specific heat capacity at constant pressure and temperature of wall

  float

`no-slp-wall` only works with `ac-navier-stokes` and requires

- `u` — x-velocity of wall

  float

- `v` — y-velocity of wall

  float

- `w` — z-velocity of wall

  float

`slp-adia-wall` only works with `euler` | `navier-stokes`

`slp-wall` only works with `ac-euler` | `ac-navier-stokes`

`sub-in-frv` only works with `navier-stokes` and requires

- `rho` — density

  float | *string*

- `u` — x-velocity

  float | *string*

- `v` — y-velocity

  float | *string*

- `w` — z-velocity

float | *string*

`sub-in-ftpttang` only works with `navier-stokes` and requires

- `pt` — total pressure

  float

- `cpTt` — product of specific heat capacity at constant pressure and total temperature

  float

- `theta` — azimuth angle (in degrees) of inflow measured in the x-y plane relative to the positive x-axis

  float

- `phi` — inclination angle (in degrees) of inflow measured relative to the positive z-axis

  float

`sub-out-fp` only works with `navier-stokes` and requires

- `p` — static pressure

  float | *string*

`sup-in-fa` only works with `euler` | `navier-stokes` and requires

- `rho` — density

  float | *string*

- `u` — x-velocity

  float | *string*

- `v` — y-velocity

  float | *string*

- `w` — z-velocity

  float | *string*

- `p` — static pressure

  float | *string*

`sup-out-fn` only works with `euler` | `navier-stokes`

Example:

```
[soln-bcs-bcwallupper]
type = no-slp-isot-wall
cpTw = 10.0
u = 1.0
```

Simple periodic boundary conditions are supported; however, their behaviour is not controlled through the `.ini` file, instead it is handled at the mesh generation stage. Two faces may be taged with `periodic_x_l` and `periodic_x_r`, where `x` is a unique identifier for the pair of boundaries. Currently, only periodicity in a single cardinal direction is supported, for example, the planes `(x,y,0)`` and `(x,y,10)`.

2.2.3.2 [soln-ics]

Parameterises space (x, y, [z]) dependent initial conditions with

1. `rho` — initial density distribution for `euler` | `navier-stokes`:

   string

2. `u` — initial x-velocity distribution for `euler` | `navier-stokes` | `ac-euler` | `ac-navier-stokes`:

   string

3. `v` — initial y-velocity distribution for `euler` | `navier-stokes` | `ac-euler` | `ac-navier-stokes`:

   string

4. `w` — initial z-velocity distribution for `euler` | `navier-stokes` | `ac-euler` | `ac-navier-stokes`:

   string

5. `p` — initial static pressure distribution for `euler` | `navier-stokes` | `ac-euler` | `ac-navier-stokes`:

   string

Example:

```
[soln-ics]
rho = 1.0
u = x*y*sin(y)
v = z
w = 1.0
p = 1.0/(1.0+x)
```

2.2.4 Nodal Point Sets

Solution point sets must be specified for each element type that is used and flux point sets must be specified for each interface type that is used. If anti-aliasing is enabled then quadrature point sets for each element and interface type that is used must also be specified. For example, a 3D mesh comprised only of prisms requires a solution point set for prism elements and flux point set for quadrilateral and triangular interfaces.

2.2.4.1 [solver-interfaces-line{-mg-p*order*}]

Parameterises the line interfaces, or if -mg-p*order* is suffixed the line interfaces at multi-p level *order*, with

1. `flux-pts` — location of the flux points on a line interface:

   `gauss-legendre` | `gauss-legendre-lobatto`

2. `quad-deg` — degree of quadrature rule for anti-aliasing on a line interface:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing on a line interface:

   `gauss-legendre` | `gauss-legendre-lobatto`

Example:

```
[solver-interfaces-line]
flux-pts = gauss-legendre
quad-deg = 10
quad-pts = gauss-legendre
```

2.2.4.2 [solver-interfaces-tri{-mg-p*order*}]

Parameterises the triangular interfaces, or if -mg-p*order* is suffixed the triangular interfaces at multi-p level *order*, with

1. `flux-pts` — location of the flux points on a triangular interface:

   `williams-shunn`

2. `quad-deg` — degree of quadrature rule for anti-aliasing on a triangular interface:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing on a triangular interface:

   `williams-shunn` | `witherden-vincent`

Example:

```
[solver-interfaces-tri]
flux-pts = williams-shunn
quad-deg = 10
quad-pts = williams-shunn
```

2.2.4.3 [solver-interfaces-quad{-mg-p*order*}]

Parameterises the quadrilateral interfaces, or if -mg-p*order* is suffixed the quadrilateral interfaces at multi-p level *order*, with

1. `flux-pts` — location of the flux points on a quadrilateral interface:

   `gauss-legendre` | `gauss-legendre-lobatto`

2. `quad-deg` — degree of quadrature rule for anti-aliasing on a quadrilateral interface:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing on a quadrilateral interface:

   `gauss-legendre` | `gauss-legendre-lobatto` | `witherden-vincent`

Example:

```
[solver-interfaces-quad]
flux-pts = gauss-legendre
quad-deg = 10
quad-pts = gauss-legendre
```

2.2.4.4 [solver-elements-tri{-mg-p*order*}]

Parameterises the triangular elements, or if -mg-p*order* is suffixed the triangular elements at multi-p level *order*, with

1. `soln-pts` — location of the solution points in a triangular element:

   `williams-shunn`

2. `quad-deg` — degree of quadrature rule for anti-aliasing in a triangular element:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing in a triangular element:

   `williams-shunn` | `witherden-vincent`

Example:

```
[solver-elements-tri]
soln-pts = williams-shunn
quad-deg = 10
quad-pts = williams-shunn
```

2.2.4.5 [solver-elements-quad{-mg-p*order*}]

Parameterises the quadrilateral elements, or if -mg-p*order* is suffixed the quadrilateral elements at multi-p level *order*, with

1. `soln-pts` — location of the solution points in a quadrilateral element:

   `gauss-legendre` | `gauss-legendre-lobatto`

2. `quad-deg` — degree of quadrature rule for anti-aliasing in a quadrilateral element:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing in a quadrilateral element:

   `gauss-legendre` | `gauss-legendre-lobatto` | `witherden-vincent`

Example:

```
[solver-elements-quad]
soln-pts = gauss-legendre
quad-deg = 10
quad-pts = gauss-legendre
```

2.2.4.6 [solver-elements-hex{-mg-p*order*}]

Parameterises the hexahedral elements, or if -mg-p*order* is suffixed the hexahedral elements at multi-p level *order*, with

1. `soln-pts` — location of the solution points in a hexahedral element:

   `gauss-legendre` | `gauss-legendre-lobatto`

2. `quad-deg` — degree of quadrature rule for anti-aliasing in a hexahedral element:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing in a hexahedral element:

   `gauss-legendre` | `gauss-legendre-lobatto` | `witherden-vincent`

Example:

```
[solver-elements-hex]
soln-pts = gauss-legendre
quad-deg = 10
quad-pts = gauss-legendre
```

2.2.4.7 [solver-elements-tet{-mg-p*order*}]

Parameterises the tetrahedral elements, or if -mg-p*order* is suffixed the tetrahedral elements at multi-p level *order*, with

1. `soln-pts` — location of the solution points in a tetrahedral element:

   `shunn-ham`

2. `quad-deg` — degree of quadrature rule for anti-aliasing in a tetrahedral element:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing in a tetrahedral element:

   `shunn-ham|witherden-vincent`

Example:

```
[solver-elements-tet]
soln-pts = shunn-ham
quad-deg = 10
quad-pts = shunn-ham
```

2.2.4.8 [solver-elements-pri{-mg-p*order*}]

Parameterises the prismatic elements, or if -mg-p*order* is suffixed the prismatic elements at multi-p level *order*, with

1. `soln-pts` — location of the solution points in a prismatic element:

   `williams-shunn~gauss-legendre|williams-shunn~gauss-legendre-lobatto`

2. `quad-deg` — degree of quadrature rule for anti-aliasing in a prismatic element:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing in a prismatic element:

   `williams-shunn~gauss-legendre | williams-shunn~gauss-legendre-lobatto | witherden-vincent`

Example:

```
[solver-elements-pri]
soln-pts = williams-shunn~gauss-legendre
quad-deg = 10
quad-pts = williams-shunn~gauss-legendre
```

2.2.4.9 [solver-elements-pyr{-mg-p*order*}]

Parameterises the pyramidal elements, or if -mg-p*order* is suffixed the pyramidal elements at multi-p level *order*, with

1. `soln-pts` — location of the solution points in a pyramidal element:

   `gauss-legendre` | `gauss-legendre-lobatto`

2. `quad-deg` — degree of quadrature rule for anti-aliasing in a pyramidal element:

   int

3. `quad-pts` — name of quadrature rule for anti-aliasing in a pyramidal element:

   `witherden-vincent`

Example:

```
[solver-elements-pyr]
soln-pts = gauss-legendre
quad-deg = 10
quad-pts = witherden-vincent
```

2.2.5 Plugins

Plugins allow for powerful additional functionality to be swapped in and out. It is possible to load multiple instances of the same plugin by appending a tag, for example:

```
[soln-plugin-writer]
...

[soln-plugin-writer-2]
...

[soln-plugin-writer-three]
...
```

2.2.5.1 [soln-plugin-writer]

Periodically write the solution to disk in the pyfrs format. Parameterised with

1. `dt-out` — write to disk every `dt-out` time units:

   float

2. `basedir` — relative path to directory where outputs will be written:

   string

3. `basename` — pattern of output names:

   string

4. `post-action` — command to execute after writing the file:

   string

5. `post-action-mode` — how the post-action command should be executed:

   `blocking` | `non-blocking`

4. `region` — region to be written, specified as either the entire domain using `*`, a cuboidal sub-region via diametrically opposite vertices, or a sub-region of elements that have faces on a specific domain boundary via the name of the domain boundary

   `*|[(x, y, [z]), (x, y, [z])]|`*string*

Example:

```
[soln-plugin-writer]
dt-out = 0.01
basedir = .
basename = files-{t:.2f}
post-action = echo "Wrote file {soln} at time {t} for mesh {mesh}."
post-action-mode = blocking
region = [(-5, -5, -5), (5, 5, 5)]
```

2.2.5.2 [soln-plugin-fluidforce-*name*]

Periodically integrates the pressure and viscous stress on the boundary labelled `name` and writes out the resulting force and moment (if requested) vectors to a CSV file. Parameterised with

1. `nsteps` — integrate every `nsteps`:

   int

2. `file` — output file path; should the file already exist it will be appended to:

   string

3. `header` — if to output a header row or not:

   boolean

4. `morigin` — origin used to compute moments (optional):

   `(x, y, [z])`

Example:

```
[soln-plugin-fluidforce-wing]
nsteps = 10
file = wing-forces.csv
header = true
morigin = (0.0, 0.0, 0.5)
```

2.2.5.3 [soln-plugin-nancheck]

Periodically checks the solution for NaN values. Parameterised with

1. `nsteps` — check every `nsteps`:

   int

Example:

```
[soln-plugin-nancheck]
nsteps = 10
```

2.2.5.4 [soln-plugin-residual]

Periodically calculates the residual and writes it out to a CSV file. Parameterised with

1. `nsteps` — calculate every `nsteps`:

   int

2. `file` — output file path; should the file already exist it will be appended to:

   string

3. `header` — if to output a header row or not:

   boolean

Example:

```
[soln-plugin-residual]
nsteps = 10
file = residual.csv
header = true
```

2.2.5.5 [soln-plugin-dtstats]

Write time-step statistics out to a CSV file. Parameterised with

1. `flushsteps` — flush to disk every `flushsteps`:

   int

2. `file` — output file path; should the file already exist it will be appended to:

   string

3. `header` — if to output a header row or not:

   boolean

Example:

```
[soln-plugin-dtstats]
flushsteps = 100
file = dtstats.csv
header = true
```

2.2.5.6 [soln-plugin-pseudostats]

Write pseudo-step convergence history out to a CSV file. Parameterised with

1. `flushsteps` — flush to disk every `flushsteps`:

   int

2. `file` — output file path; should the file already exist it will be appended to:

   string

3. `header` — if to output a header row or not:

   boolean

Example:

```
[soln-plugin-pseudostats]
flushsteps = 100
file = pseudostats.csv
header = true
```

2.2.5.7 [soln-plugin-sampler]

Periodically samples specific points in the volume and writes them out to a CSV file. The plugin actually samples the solution point closest to each sample point, hence a slight discrepancy in the output sampling locations is to be expected. A nearest-neighbour search is used to locate the closest solution point to the sample point. The location process automatically takes advantage of scipy.spatial.cKDTree where available. Parameterised with

1. `nsteps` — sample every `nsteps`:

   int

2. `samp-pts` — list of points to sample:

   `[(x, y), (x, y), ...]|[(x, y, z), (x, y, z), ...]`

3. `format` — output variable format:

   `primitive|conservative`

4. `file` — output file path; should the file already exist it will be appended to:

   string

5. `header` — if to output a header row or not:

   boolean

Example:

```
[soln-plugin-sampler]
nsteps = 10
samp-pts = [(1.0, 0.7, 0.0), (1.0, 0.8, 0.0)]
format = primitive
file = point-data.csv
header = true
```

2.2.5.8 [soln-plugin-tavg]

Time average quantities. Parameterised with

1. `nsteps` — accumulate the average every `nsteps` time steps:

   int

2. `dt-out` — write to disk every `dt-out` time units:

   float

3. `tstart` — time at which to start accumulating average data:

   float

4. `mode` — output file accumulation mode:

`continuous` | `windowed`

Windowed outputs averages over each `dt- out` period. Whereas, continuous outputs averages over all `dt-out` periods thus far completed within a given invocation of PyFR. The default is `windowed`.

5. `basedir` — relative path to directory where outputs will be written:

   string

6. `basename` — pattern of output names:

   string

7. `precision` — output file number precision:

   `single` | `double`

8. `region` — region to be averaged, specified as either the entire domain using `*`, a cuboidal sub-region via diametrically opposite vertices, or a sub-region of elements that have faces on a specific domain boundary via the name of the domain boundary

   `*` | `[(x, y, [z]), (x, y, [z])]` | *string*

9. `avg-`*name* — expression to time average, written as a function of the primitive variables and gradients thereof; multiple expressions, each with their own *name*, may be specified:

   string

10. `fun-avg-`*name* — expression to compute at file output time, written as a function of any ordinary average terms; multiple expressions, each with their own *name*, may be specified:

    string

    As `fun-avg` terms are evaluated at write time, these are only indirectly effected by the averaging mode.

Example:

```
[soln-plugin-tavg]
nsteps = 10
dt-out = 2.0
mode = windowed
basedir = .
basename = files-{t:06.2f}

avg-u = u
avg-v = v
avg-uu = u*u
avg-vv = v*v
avg-uv = u*v

fun-avg-upup = uu - u*u
fun-avg-vpvp = vv - v*v
fun-avg-upvp = uv - u*v
fun-avg-urms = sqrt(uu - u*u + vv - v*v)
```

2.2.5.9 [soln-plugin-integrate]

Integrate quantities over the compuational domain. Parameterised with:

1. `nsteps` — calculate the integral every `nsteps` time steps:

   int

2. `file` — output file path; should the file already exist it will be appended to:

   string

3. `header` — if to output a header row or not:

   boolean

4. `quad-deg` — degree of quadrature rule (optional):

5. `quad-pts-{etype}` — name of quadrature rule (optional):

6. `int-`*name* — expression to integrate, written as a function of the primitive variables and gradients thereof, the physical coordinates [x, y, [z]] and/or the physical time [t]; multiple expressions, each with their own *name*, may be specified:

   string

Example:

```
[soln-plugin-integrate]
nsteps = 50
file = integral.csv
header = true
quad-deg = 9
vor1 = (grad_w_y - grad_v_z)
vor2 = (grad_u_z - grad_w_x)
vor3 = (grad_v_x - grad_u_y)

int-E = rho*(u*u + v*v + w*w)
int-enst = rho*(%(vor1)s*%(vor1)s + %(vor2)s*%(vor2)s + %(vor3)s*%(vor3)s)
```

2.2.6 Additional Information

The *INI* file format is very versatile. A feature that can be useful in defining initial conditions is the substitution feature and this is demonstrated in the *[soln-plugin-integrate]* example.

To prevent situations where you have solutions files for unknown configurations, the contents of the `.ini` file are added as an attribute to `.pyfrs` files. These files use the HDF5 format and can be straightforwardly probed with tools such as h5dump.

In several places within the `.ini` file expressions may be used. As well as the constant `pi`, expressions containing the following functions are supported:

1. `+, -, *, /` — basic arithmetic
2. `sin, cos, tan` — basic trigonometric functions (radians)
3. `asin, acos, atan, atan2` — inverse trigonometric functions
4. `exp, log` — exponential and the natural logarithm
5. `tanh` — hyperbolic tangent

6. `pow` — power, note `**` is not supported
7. `sqrt` — square root
8. `abs` — absolute value

9. `min, max` — two variable minimum and maximum functions, arguments can be arrays

CHAPTER

THREE

DEVELOPER GUIDE

3.1 A Brief Overview of the PyFR Framework

3.1.1 Where to Start

The symbolic link `pyfr.scripts.pyfr` points to the script `pyfr.scripts.main`, which is where it all starts! Specifically, the function `process_run` calls the function `_process_common`, which in turn calls the function `get_solver`, returning an Integrator – a composite of a *Controller* and a *Stepper*. The Integrator has a method named `run`, which is then called to run the simulation.

3.1.2 Controller

A *Controller* acts to advance the simulation in time. Specifically, a *Controller* has a method named `advance_to` which advances a *System* to a specified time. There are three types of physical-time *Controller* available in PyFR 1.12.3:

StdNoneController **Click to show**

class pyfr.integrators.std.controllers.**StdNoneController**(**args*, ***kwargs*)

_accept_step(*dt*, *idxcurr*, *err=None*)

_add(**args*, *subdims=None*)

_check_abort()

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

_reject_step(*dt*, *idxold*, *err=None*)

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

controller_name = 'none'

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

StdPIController **Click to show**

class pyfr.integrators.std.controllers.StdPIController(**args*, ***kwargs*)

_accept_step(*dt*, *idxcurr*, *err=None*)

_add(**args*, *subdims=None*)

_check_abort()

_errest(*rcurr*, *rprev*, *rerr*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

_reject_step(*dt*, *idxold*, *err=None*)

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

controller_name = 'pi'

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

DualNoneController **Click to show**

class pyfr.integrators.dual.phys.controllers.DualNoneController(**args*, ***kwargs*)

_accept_step(*idxcurr*)

_check_abort()

_get_plugins(*initsoln*)

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

controller_name = 'none'

formulation = 'dual'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

property pseudostepinfo

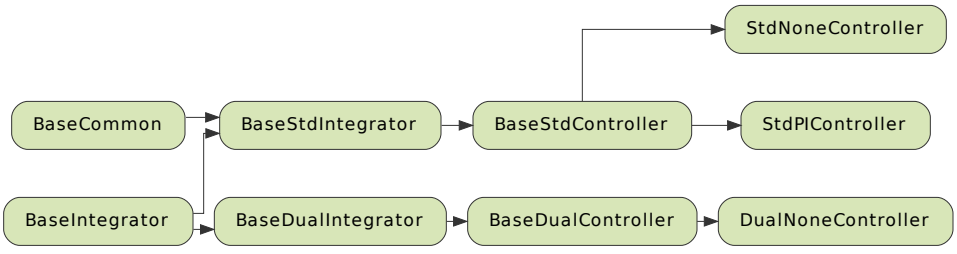
run()

property soln

step(*t*, *dt*)

property system

Types of physical-time *Controller* are related via the following inheritance diagram:



There are two types of pseudo-time *Controller* available in PyFR 1.12.3:

DualNonePseudoController **Click to show**

class pyfr.integrators.dual.pseudo.pseudocontrollers.**DualNonePseudoController**(**args*, ***kwargs*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

property _pseudo_stepper_regidx

_resid(*rcurr*, *rold*, *dt_fac*)

property _source_regidx

property _stepper_regidx

_update_pseudostepinfo(*niters*, *resid*)

aux_nregs = 0

convmon(*i*, *minniters*, *dt_fac=1*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

pseudo_advance(*tcurr*)

pseudo_controller_name = 'none'

pseudo_controller_needs_lerrest = False

DualPIPseudoController **Click to show**

class pyfr.integrators.dual.pseudo.pseudocontrollers.**DualPIPseudoController**(**args*, ***kwargs*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

property _pseudo_stepper_regidx

_resid(*rcurr*, *rold*, *dt_fac*)

property _source_regidx

property _stepper_regidx

_update_pseudostepinfo(*niters*, *resid*)

aux_nregs = 0

convmon(*i*, *minniters*, *dt_fac=1*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

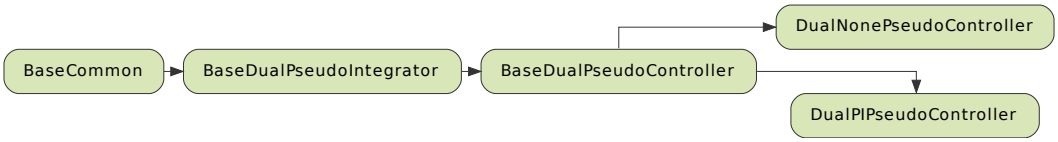
localerrest(*errbank*)

pseudo_advance(*tcurr*)

pseudo_controller_name = 'local-pi'

pseudo_controller_needs_lerrest = True

Types of pseudo-time *Controller* are related via the following inheritance diagram:



3.1.3 Stepper

A *Stepper* acts to advance the simulation by a single time-step. Specifically, a *Stepper* has a method named `step` which advances a *System* by a single time-step. There are eight types of *Stepper* available in PyFR 1.12.3:

StdEulerStepper **Click to show**

class pyfr.integrators.std.steppers.**StdEulerStepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*)

_add(**args*, *subdims=None*)

_check_abort()

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

property _stepper_nfevals

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

stepper_has_errest = False

stepper_name = 'euler'

stepper_nregs = 2

stepper_order = 1

StdRK4Stepper **Click to show**

class pyfr.integrators.std.steppers.**StdRK4Stepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*)

_add(**args*, *subdims=None*)

_check_abort()

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

property _stepper_nfevals

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

stepper_has_errest = False

stepper_name = 'rk4'

stepper_nregs = 3

stepper_order = 4

StdRK34Stepper **Click to show**

class pyfr.integrators.std.steppers.**StdRK34Stepper**(**args*, ***kwargs*)

_add(**args*, *subdims=None*)

_check_abort()

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

_get_rkvdh2_kerns(*stage*, *r1*, *r2*, *rold=None*, *rerr=None*)

property _stepper_nfevals

a = [0.32416573882874605, 0.5570978645055429, -0.08605491431272755]

advance_to(*t*)

b = [0.10407986927510238, 0.6019391368822611, 2.9750900268840206, -2.681109033041384]

bhat = [0.3406814840808433, 0.09091523008632837, 2.866496742725443, -2.298093456892615]

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

property stepper_has_errest

stepper_name = 'rk34'

property stepper_nregs

stepper_order = 3

StdRK45Stepper **Click to show**

class pyfr.integrators.std.steppers.**StdRK45Stepper**(**args*, ***kwargs*)

_add(**args*, *subdims=None*)

_check_abort()

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

_get_rkvdh2_kerns(*stage*, *r1*, *r2*, *rold=None*, *rerr=None*)

property _stepper_nfevals

a = [0.22502245872571303, 0.5440433129514047, 0.14456824349399464, 0.7866643421983568]

advance_to(*t*)

b = [0.05122930664033915, 0.3809548257264019, -0.3733525963923833, 0.5925012850263623, 0.34866717899927996]

bhat = [0.13721732210321927, 0.19188076232938728, -0.2292067211595315, 0.6242946765438954, 0.27581396018302956]

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

property stepper_has_errest

stepper_name = 'rk45'

property stepper_nregs

stepper_order = 4

StdTVDRK3Stepper **Click to show**

class pyfr.integrators.std.steppers.StdTVDRK3Stepper(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*)

_add(**args*, *subdims=None*)

_check_abort()

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_plugins(*initsoln*)

_get_reduction_kerns(**rs*, ***kwargs*)

property _stepper_nfevals

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

property controller_needs_errest

formulation = 'std'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

run()

property soln

step(*t*, *dt*)

stepper_has_errest = False

stepper_name = 'tvd-rk3'

stepper_nregs = 3

stepper_order = 3

DualBDF2Stepper **Click to show**

class pyfr.integrators.dual.phys.steppers.**DualBDF2Stepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*)

_check_abort()

_get_plugins(*initsoln*)

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

formulation = 'dual'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

property pseudostepinfo

run()

property soln

step(*t*, *dt*)

stepper_coeffs = [-1.5, 2.0, -0.5]

stepper_name = 'bdf2'

stepper_order = 2

property system

DualBDF3Stepper **Click to show**

class pyfr.integrators.dual.phys.steppers.**DualBDF3Stepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*)

_check_abort()

_get_plugins(*initsoln*)

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

formulation = 'dual'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

property pseudostepinfo

run()

property soln

step(*t*, *dt*)

stepper_coeffs = [-1.8333333333333333, 3.0, -1.5, 0.3333333333333333]

stepper_name = 'bdf3'

stepper_order = 3

property system

DualBackwardEulerStepper **Click to show**

class pyfr.integrators.dual.phys.steppers.**DualBackwardEulerStepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*)

_check_abort()

_get_plugins(*initsoln*)

advance_to(*t*)

call_plugin_dt(*dt*)

property cfgmeta

collect_stats(*stats*)

formulation = 'dual'

static get_plugin_data_prefix(*name*, *suffix*)

property grad_soln

property nsteps

property pseudostepinfo

run()

property soln

step(*t*, *dt*)

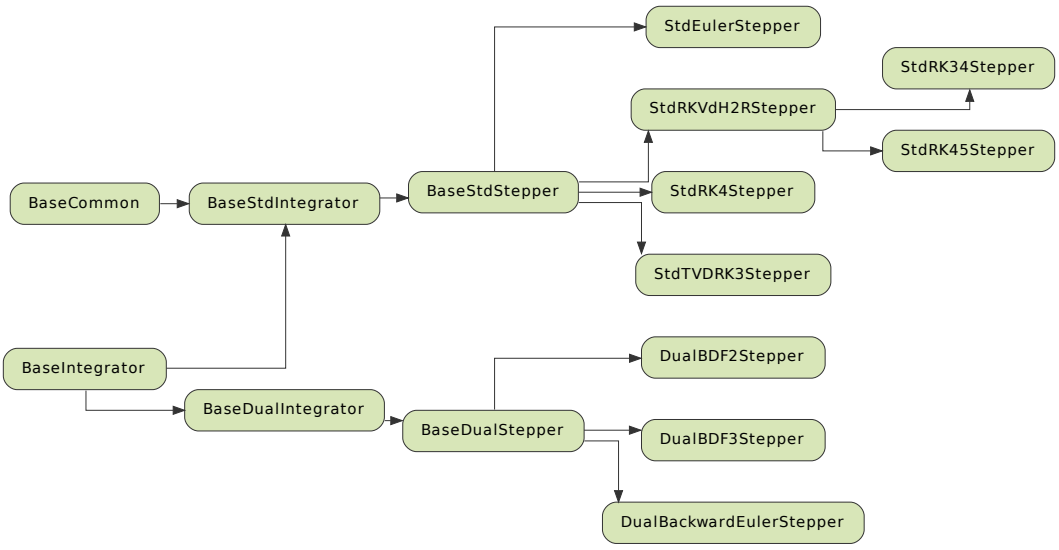
stepper_coeffs = [-1.0, 1.0]

stepper_name = 'backward-euler'

stepper_order = 1

property system

Types of *Stepper* are related via the following inheritance diagram:



3.1.4 PseudoStepper

A *PseudoStepper* acts to advance the simulation by a single pseudo-time-step. They are used to converge implicit *Stepper* time-steps via a dual time-stepping formulation. There are six types of *PseudoStepper* available in PyFR 1.12.3:

DualDenseRKPseudoStepper **Click to show**

class pyfr.integrators.dual.pseudo.pseudosteppers.**DualDenseRKPseudoStepper**(**args*, ***kwargs*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

property _pseudo_stepper_regidx

_rhs_with_dts(*t*, *uin*, *fout*)

property _source_regidx

property _stepper_regidx

aux_nregs = 0

collect_stats(*stats*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

property ntotiters

property pseudo_stepper_nfevals

step(*t*)

DualRK4PseudoStepper **Click to show**

class pyfr.integrators.dual.pseudo.pseudosteppers.**DualRK4PseudoStepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*, *stepper_coeffs*, *dt*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

property _pseudo_stepper_regidx

_rhs_with_dts(*t*, *uin*, *fout*)

property _source_regidx

property _stepper_regidx

aux_nregs = 0

collect_stats(*stats*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

property ntotiters

pseudo_stepper_has_lerrest = False

pseudo_stepper_name = 'rk4'

property pseudo_stepper_nfevals

pseudo_stepper_nregs = 3

pseudo_stepper_order = 4

step(*t*)

DualTVDRK3PseudoStepper **Click to show**

class pyfr.integrators.dual.pseudo.pseudosteppers.**DualTVDRK3PseudoStepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*, *stepper_coeffs*, *dt*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

property _pseudo_stepper_regidx

_rhs_with_dts(*t*, *uin*, *fout*)

property _source_regidx

property _stepper_regidx

aux_nregs = 0

collect_stats(*stats*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

property ntotiters

pseudo_stepper_has_lerrest = False

pseudo_stepper_name = 'tvd-rk3'

property pseudo_stepper_nfevals

pseudo_stepper_nregs = 3

pseudo_stepper_order = 3

step(*t*)

DualEulerPseudoStepper **Click to show**

class pyfr.integrators.dual.pseudo.pseudosteppers.**DualEulerPseudoStepper**(*backend*, *systemcls*, *rallocs*, *mesh*, *initsoln*, *cfg*, *stepper_coeffs*, *dt*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

property _pseudo_stepper_regidx

_rhs_with_dts(*t*, *uin*, *fout*)

property _source_regidx

property _stepper_regidx

aux_nregs = 0

collect_stats(*stats*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

property ntotiters

pseudo_stepper_has_lerrest = False

pseudo_stepper_name = 'euler'

property pseudo_stepper_nfevals

pseudo_stepper_nregs = 2

pseudo_stepper_order = 1

step(*t*)

DualRK34PseudoStepper **Click to show**

class pyfr.integrators.dual.pseudo.pseudosteppers.**DualRK34PseudoStepper**(**args*, ***kwargs*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

_get_rkvdh2pseudo_kerns(*stage*, *r1*, *r2*, *rold*, *rerr=None*)

property _pseudo_stepper_regidx

_rhs_with_dts(*t*, *uin*, *fout*)

property _source_regidx

property _stepper_regidx

a = [0.32416573882874605, 0.5570978645055429, -0.08605491431272755]

aux_nregs = 0

b = [0.10407986927510238, 0.6019391368822611, 2.9750900268840206, -2.681109033041384]

bhat = [0.3406814840808433, 0.09091523008632837, 2.866496742725443, -2.298093456892615]

collect_stats(*stats*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

property ntotiters

property pseudo_stepper_has_lerrest

pseudo_stepper_name = 'rk34'

property pseudo_stepper_nfevals

property pseudo_stepper_nregs

pseudo_stepper_order = 3

step(*t*)

DualRK45PseudoStepper **Click to show**

class pyfr.integrators.dual.pseudo.pseudosteppers.**DualRK45PseudoStepper**(**args*, ***kwargs*)

_accumulate_source()

_add(**args*, *subdims=None*)

_get_axnpby_kerns(**rs*, *subdims=None*)

_get_gndofs()

_get_reduction_kerns(**rs*, ***kwargs*)

_get_rkvdh2pseudo_kerns(*stage*, *r1*, *r2*, *rold*, *rerr=None*)

property _pseudo_stepper_regidx

_rhs_with_dts(*t*, *uin*, *fout*)

property _source_regidx

property _stepper_regidx

a = [0.22502245872571303, 0.5440433129514047, 0.14456824349399464, 0.7866643421983568]

aux_nregs = 0

b = [0.05122930664033915, 0.3809548257264019, -0.3733525963923833, 0.5925012850263623, 0.34866717899927996]

bhat = [0.13721732210321927, 0.19188076232938728, -0.2292067211595315, 0.6242946765438954, 0.27581396018302956]

collect_stats(*stats*)

finalise_pseudo_advance(*currsoln*)

formulation = 'dual'

property ntotiters

property pseudo_stepper_has_lerrest

pseudo_stepper_name = 'rk45'

property pseudo_stepper_nfevals

property pseudo_stepper_nregs

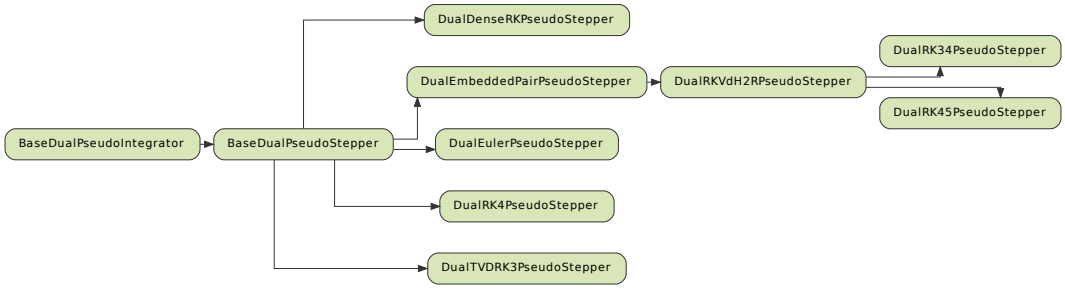
pseudo_stepper_order = 4

step(*t*)

Note that DualDenseRKPseudoStepper includes families of *PseudoStepper* whose coefficients are read from .txt files named thus:

{scheme name}-s{stage count}-p{temporal order}-sp{optimal spatial polynomial order}.txt

Types of *PseudoStepper* are related via the following inheritance diagram:



3.1.5 System

A *System* holds information/data for the system, including *Elements*, *Interfaces*, and the *Backend* with which the simulation is to run. A *System* has a method named `rhs`, which obtains the divergence of the flux (the 'right-hand-side') at each solution point. The method `rhs` invokes various kernels which have been pre-generated and loaded into queues. A *System* also has a method named `_gen_kernels` which acts to generate all the kernels required by a particular *System*. A kernel is an instance of a 'one-off' class with a method named `run` that implements the required kernel functionality. Individual kernels are produced by a kernel provider. PyFR 1.12.3 has various types of kernel provider. A *Pointwise Kernel Provider* produces point-wise kernels such as Riemann solvers and flux functions etc. These point-wise kernels are specified using an in-built platform-independent templating language derived from Mako, henceforth referred to as *PyFR-Mako*. There are four types of *System* available in PyFR 1.12.3:

ACEulerSystem **Click to show**

class pyfr.solvers.aceuler.system.**ACEulerSystem**(*backend*, *rallocs*, *mesh*, *initsoln*, *nregs*, *cfg*)

_gen_kernels(*eles*, *iint*, *mpiint*, *bcint*)

_gen_queues()

_load_bc_inters(*rallocs*, *mesh*, *elemap*)

_load_eles(*rallocs*, *mesh*, *initsoln*, *nregs*, *nonce*)

_load_int_inters(*rallocs*, *mesh*, *elemap*)

_load_mpi_inters(*rallocs*, *mesh*, *elemap*)

_nonce_seq = count(0)

_nqueues = 2

bbcinterscls
alias of pyfr.solvers.aceuler.inters.ACEulerBaseBCInters

compute_grads(*t*, *uinbank*)

ele_scal_upts(*idx*)

elementscls
alias of *pyfr.solvers.aceuler.elements.ACEulerElements*

filt(*uinoutbank*)

intinterscls
alias of *pyfr.solvers.aceuler.inters.ACEulerIntInters*

mpiinterscls
alias of *pyfr.solvers.aceuler.inters.ACEulerMPIInters*

name = 'ac-euler'

rhs(*t*, *uinbank*, *foutbank*)

ACNavierStokesSystem **Click to show**

class pyfr.solvers.acnavstokes.system.**ACNavierStokesSystem**(*backend*, *rallocs*, *mesh*, *initsoln*, *nregs*, *cfg*)

_gen_kernels(*eles*, *iint*, *mpiint*, *bcint*)

_gen_queues()

_load_bc_inters(*rallocs*, *mesh*, *elemap*)

_load_eles(*rallocs*, *mesh*, *initsoln*, *nregs*, *nonce*)

_load_int_inters(*rallocs*, *mesh*, *elemap*)

_load_mpi_inters(*rallocs*, *mesh*, *elemap*)

_nonce_seq = count(0)

_nqueues = 2

bbcinterscls
alias of pyfr.solvers.acnavstokes.inters.ACNavierStokesBaseBCInters

compute_grads(*t*, *uinbank*)

ele_scal_upts(*idx*)

elementscls
alias of *pyfr.solvers.acnavstokes.elements.ACNavierStokesElements*

filt(*uinoutbank*)

intinterscls
alias of *pyfr.solvers.acnavstokes.inters.ACNavierStokesIntInters*

mpiinterscls
alias of *pyfr.solvers.acnavstokes.inters.ACNavierStokesMPIInters*

name = 'ac-navier-stokes'

rhs(*t*, *uinbank*, *foutbank*)

EulerSystem **Click to show**

class pyfr.solvers.euler.system.**EulerSystem**(*backend*, *rallocs*, *mesh*, *initsoln*, *nregs*, *cfg*)

_gen_kernels(*eles*, *iint*, *mpiint*, *bcint*)

_gen_queues()

_load_bc_inters(*rallocs*, *mesh*, *elemap*)

_load_eles(*rallocs*, *mesh*, *initsoln*, *nregs*, *nonce*)

_load_int_inters(*rallocs*, *mesh*, *elemap*)

_load_mpi_inters(*rallocs*, *mesh*, *elemap*)

_nonce_seq = count(0)

_nqueues = 2

bbcinterscls
alias of pyfr.solvers.euler.inters.EulerBaseBCInters

compute_grads(*t*, *uinbank*)

ele_scal_upts(*idx*)

elementscls
alias of *pyfr.solvers.euler.elements.EulerElements*

filt(*uinoutbank*)

intinterscls
alias of *pyfr.solvers.euler.inters.EulerIntInters*

mpiinterscls
alias of *pyfr.solvers.euler.inters.EulerMPIInters*

name = 'euler'

rhs(*t*, *uinbank*, *foutbank*)

NavierStokesSystem **Click to show**

class pyfr.solvers.navstokes.system.**NavierStokesSystem**(*backend*, *rallocs*, *mesh*, *initsoln*, *nregs*, *cfg*)

_gen_kernels(*eles*, *iint*, *mpiint*, *bcint*)

_gen_queues()

_load_bc_inters(*rallocs*, *mesh*, *elemap*)

_load_eles(*rallocs*, *mesh*, *initsoln*, *nregs*, *nonce*)

_load_int_inters(*rallocs*, *mesh*, *elemap*)

_load_mpi_inters(*rallocs*, *mesh*, *elemap*)

_nonce_seq = count(0)

_nqueues = 2

bbcinterscls
alias of `pyfr.solvers.navstokes.inters.NavierStokesBaseBCInters`

compute_grads(*t*, *uinbank*)

ele_scal_upts(*idx*)

elementscls
alias of *pyfr.solvers.navstokes.elements.NavierStokesElements*

filt(*uinoutbank*)

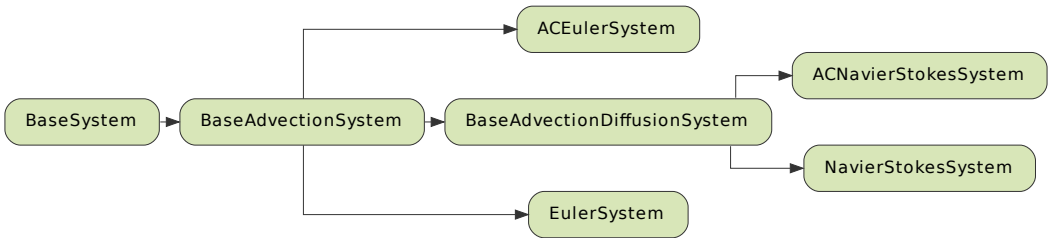
intinterscls
alias of *pyfr.solvers.navstokes.inters.NavierStokesIntInters*

mpiinterscls
alias of *pyfr.solvers.navstokes.inters.NavierStokesMPIInters*

name = 'navier-stokes'

rhs(*t*, *uinbank*, *foutbank*)

Types of *System* are related via the following inheritance diagram:



3.1.6 Elements

An *Elements* holds information/data for a group of elements. There are four types of *Elements* available in PyFR 1.12.3:

ACEulerElements **Click to show**

class pyfr.solvers.aceuler.elements.**ACEulerElements**(*basiscls*, *eles*, *cfg*)

_gen_pnorm_fpts()

_mag_pnorm_fpts = None

property _mesh_regions

_norm_pnorm_fpts = None

_ploc_in_src_exprs = None

property _scratch_bufs

_slice_mat(*mat*, *region*, *ra=None*, *rb=None*)

_smats_djacs_mpts = None

_soln_in_src_exprs = None

_src_exprs = None

_srtd_face_fpts = None

static con_to_pri(*convs*, *cfg*)

convarmap = {2: ['p', 'u', 'v'], 3: ['p', 'u', 'v', 'w']}

dualcoeffs = {2: ['u', 'v'], 3: ['u', 'v', 'w']}

formulations = ['dual']

get_mag_pnorms(*eidx*, *fidx*)

get_mag_pnorms_for_inter(*eidx*, *fidx*)

get_norm_pnorms(*eidx*, *fidx*)

get_norm_pnorms_for_inter(*eidx*, *fidx*)

get_ploc_for_inter(*eidx*, *fidx*)

get_scal_fpts_for_inter(*eidx*, *fidx*)

get_vect_fpts_for_inter(*eidx*, *fidx*)

opmat(*expr*)

ploc_at(*name*, *side=None*)

ploc_at_np(*name*)

plocfpts = None

static pri_to_con(*pris*, *cfg*)

privarmap = {2: ['p', 'u', 'v'], 3: ['p', 'u', 'v', 'w']}

qpts = None

rcpdjac_at(*name*, *side=None*)

rcpdjac_at_np(*name*)

set_backend(**args*, ***kwargs*)

set_ics_from_cfg()

set_ics_from_soln(*solnmat*, *solncfg*)

sliceat()

smat_at(*name*, *side=None*)

smat_at_np(*name*)

upts = None

visvarmap = {2: [('velocity', ['u', 'v']), ('pressure', ['p'])], 3: [('velocity', ['u', 'v', 'w']), ('pressure', ['p'])]}

ACNavierStokesElements **Click to show**

class pyfr.solvers.acnavstokes.elements.**ACNavierStokesElements**(*basiscls*, *eles*, *cfg*)

_gen_pnorm_fpts()

_mag_pnorm_fpts = None

property _mesh_regions

_norm_pnorm_fpts = None

_ploc_in_src_exprs = None

property _scratch_bufs

_slice_mat(*mat*, *region*, *ra=None*, *rb=None*)

_smats_djacs_mpts = None

_soln_in_src_exprs = None

_src_exprs = None

_srtd_face_fpts = None

static con_to_pri(*convs*, *cfg*)

convarmap = {2: ['p', 'u', 'v'], 3: ['p', 'u', 'v', 'w']}

dualcoeffs = {2: ['u', 'v'], 3: ['u', 'v', 'w']}

formulations = ['dual']

get_artvisc_fpts_for_inter(*eidx*, *fidx*)

get_mag_pnorms(*eidx*, *fidx*)

get_mag_pnorms_for_inter(*eidx*, *fidx*)

get_norm_pnorms(*eidx*, *fidx*)

get_norm_pnorms_for_inter(*eidx*, *fidx*)

get_ploc_for_inter(*eidx*, *fidx*)

get_scal_fpts_for_inter(*eidx*, *fidx*)

get_vect_fpts_for_inter(*eidx*, *fidx*)

static grad_con_to_pri(*cons*, *grad_cons*, *cfg*)

opmat(*expr*)

ploc_at(*name*, *side=None*)

ploc_at_np(*name*)

plocfpts = None

static pri_to_con(*pris*, *cfg*)

privarmap = {2: ['p', 'u', 'v'], 3: ['p', 'u', 'v', 'w']}

qpts = None

rcpdjac_at(*name*, *side=None*)

rcpdjac_at_np(*name*)

set_backend(**args*, ***kwargs*)

set_ics_from_cfg()

set_ics_from_soln(*solnmat*, *solncfg*)

sliceat()

smat_at(*name*, *side=None*)

smat_at_np(*name*)

upts = None

visvarmap = {2: [('velocity', ['u', 'v']), ('pressure', ['p'])], 3: [('velocity', ['u', 'v', 'w']), ('pressure', ['p'])]}

EulerElements **Click to show**

class pyfr.solvers.euler.elements.**EulerElements**(*basiscls*, *eles*, *cfg*)

_gen_pnorm_fpts()

_mag_pnorm_fpts = None

property _mesh_regions

_norm_pnorm_fpts = None

_ploc_in_src_exprs = None

property _scratch_bufs

_slice_mat(*mat*, *region*, *ra=None*, *rb=None*)

_smats_djacs_mpts = None

_soln_in_src_exprs = None

_src_exprs = None

_srtd_face_fpts = None

static con_to_pri(*cons*, *cfg*)

convarmap = {2: ['rho', 'rhou', 'rhov', 'E'], 3: ['rho', 'rhou', 'rhov', 'rhow', 'E']}

dualcoeffs = {2: ['rho', 'rhou', 'rhov', 'E'], 3: ['rho', 'rhou', 'rhov', 'rhow', 'E']}

formulations = ['std', 'dual']

get_mag_pnorms(*eidx*, *fidx*)

get_mag_pnorms_for_inter(*eidx*, *fidx*)

get_norm_pnorms(*eidx*, *fidx*)

get_norm_pnorms_for_inter(*eidx*, *fidx*)

get_ploc_for_inter(*eidx*, *fidx*)

get_scal_fpts_for_inter(*eidx*, *fidx*)

get_vect_fpts_for_inter(*eidx*, *fidx*)

opmat(*expr*)

ploc_at(*name*, *side=None*)

ploc_at_np(*name*)

plocfpts = None

static pri_to_con(*pris*, *cfg*)

privarmap = {2: ['rho', 'u', 'v', 'p'], 3: ['rho', 'u', 'v', 'w', 'p']}

qpts = None

rcpdjac_at(*name*, *side=None*)

rcpdjac_at_np(*name*)

set_backend(**args*, ***kwargs*)

set_ics_from_cfg()

set_ics_from_soln(*solnmat*, *solncfg*)

sliceat()

smat_at(*name*, *side=None*)

smat_at_np(*name*)

upts = None

visvarmap = {2: [('density', ['rho']), ('velocity', ['u', 'v']), ('pressure', ['p'])], 3: [('density', ['rho']), ('velocity', ['u', 'v', 'w']), ('pressure', ['p'])]}

NavierStokesElements **Click to show**

class pyfr.solvers.navstokes.elements.**NavierStokesElements**(*basiscls*, *eles*, *cfg*)

_gen_pnorm_fpts()

_mag_pnorm_fpts = None

property _mesh_regions

_norm_pnorm_fpts = None

_ploc_in_src_exprs = None

property _scratch_bufs

_slice_mat(*mat*, *region*, *ra=None*, *rb=None*)

_smats_djacs_mpts = None

_soln_in_src_exprs = None

_src_exprs = None

_srtd_face_fpts = None

static con_to_pri(*cons*, *cfg*)

convarmap = {2: ['rho', 'rhou', 'rhov', 'E'], 3: ['rho', 'rhou', 'rhov', 'rhow', 'E']}

dualcoeffs = {2: ['rho', 'rhou', 'rhov', 'E'], 3: ['rho', 'rhou', 'rhov', 'rhow', 'E']}

formulations = ['std', 'dual']

get_artvisc_fpts_for_inter(*eidx*, *fidx*)

get_mag_pnorms(*eidx*, *fidx*)

get_mag_pnorms_for_inter(*eidx*, *fidx*)

get_norm_pnorms(*eidx*, *fidx*)

get_norm_pnorms_for_inter(*eidx*, *fidx*)

get_ploc_for_inter(*eidx*, *fidx*)

get_scal_fpts_for_inter(*eidx*, *fidx*)

get_vect_fpts_for_inter(*eidx*, *fidx*)

static grad_con_to_pri(*cons*, *grad_cons*, *cfg*)

opmat(*expr*)

ploc_at(*name*, *side=None*)

ploc_at_np(*name*)

plocfpts = None

static pri_to_con(*pris*, *cfg*)

privarmap = {2: ['rho', 'u', 'v', 'p'], 3: ['rho', 'u', 'v', 'w', 'p']}

qpts = None

rcpdjac_at(*name*, *side=None*)

rcpdjac_at_np(*name*)

set_backend(**args*, ***kwargs*)

set_ics_from_cfg()

set_ics_from_soln(*solnmat*, *solncfg*)

shockvar = 'rho'

sliceat()

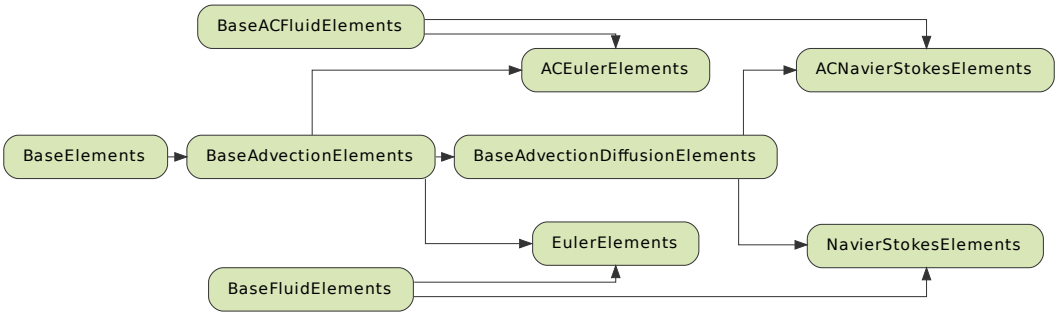
smat_at(*name*, *side=None*)

smat_at_np(*name*)

upts = None

```
visvarmap = {2:  [('density', ['rho']), ('velocity', ['u', 'v']), ('pressure',
['p'])], 3:  [('density', ['rho']), ('velocity', ['u', 'v', 'w']), ('pressure',
['p'])]}
```

Types of *Elements* are related via the following inheritance diagram:



3.1.7 Interfaces

An *Interfaces* holds information/data for a group of interfaces. There are eight types of (non-boundary) *Interfaces* available in PyFR 1.12.3:

ACEulerIntInters **Click to show**

class pyfr.solvers.aceuler.inters.**ACEulerIntInters**(**args*, ***kwargs*)

_const_mat(*inter*, *meth*)

_gen_perm(*lhs*, *rhs*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

ACEulerMPIInters **Click to show**

class pyfr.solvers.aceuler.inters.**ACEulerMPIInters**(**args*, ***kwargs*)

MPI_TAG = 2314

_const_mat(*inter*, *meth*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

ACNavierStokesIntInters **Click to show**

class pyfr.solvers.acnavstokes.inters.**ACNavierStokesIntInters**(*be*, *lhs*, *rhs*, *elemap*, *cfg*)

_const_mat(*inter*, *meth*)

_gen_perm(*lhs*, *rhs*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

ACNavierStokesMPIInters **Click to show**

class pyfr.solvers.acnavstokes.inters.**ACNavierStokesMPIInters**(*be*, *lhs*, *rhsrank*, *rallocs*, *elemap*, *cfg*)

MPI_TAG = 2314

_const_mat(*inter*, *meth*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

EulerIntInters **Click to show**

class pyfr.solvers.euler.inters.**EulerIntInters**(**args*, ***kwargs*)

_const_mat(*inter*, *meth*)

_gen_perm(*lhs*, *rhs*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

EulerMPIInters **Click to show**

class pyfr.solvers.euler.inters.**EulerMPIInters**(**args*, ***kwargs*)

MPI_TAG = 2314

_const_mat(*inter*, *meth*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

NavierStokesIntInters **Click to show**

class pyfr.solvers.navstokes.inters.**NavierStokesIntInters**(*be*, *lhs*, *rhs*, *elemap*, *cfg*)

_const_mat(*inter*, *meth*)

_gen_perm(*lhs*, *rhs*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

NavierStokesMPIInters **Click to show**

class pyfr.solvers.navstokes.inters.**NavierStokesMPIInters**(*be*, *lhs*, *rhsrank*, *rallocs*, *elemap*, *cfg*)

MPI_TAG = 2314

_const_mat(*inter*, *meth*)

_get_perm_for_view(*inter*, *meth*)

_scal_view(*inter*, *meth*)

_scal_xchg_view(*inter*, *meth*)

_set_external(*name*, *spec*, *value=None*)

_vect_view(*inter*, *meth*)

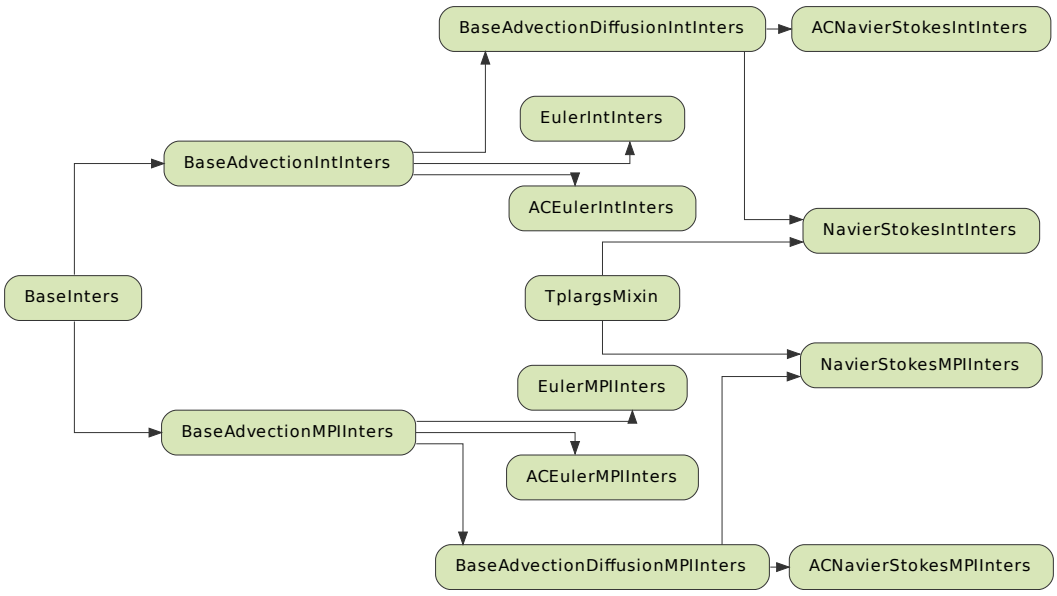
_vect_xchg_view(*inter*, *meth*)

_view(*inter*, *meth*, *vshape=()*)

_xchg_view(*inter*, *meth*, *vshape=()*)

prepare(*t*)

Types of (non-boundary) *Interfaces* are related via the following inheritance diagram:



3.1.8 Backend

A *Backend* holds information/data for a backend. There are four types of *Backend* available in PyFR 1.12.3:

CUDABackend **Click to show**

class pyfr.backends.cuda.base.**CUDABackend**(*cfg*)

_malloc_impl(*nbytes*)

alias(*obj*, *aobj*)

blocks = False

commit()

const_matrix(*initval*, *extent=None*, *tags={}*)

kernel(*name*, **args*, ***kwargs*)

lookup = None

malloc(*obj*, *extent*)

matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

matrix_bank(*mats*, *initbank=0*, *tags={}*)

matrix_slice(*mat*, *ra*, *rb*, *ca*, *cb*)

name = 'cuda'

queue()

runall(*sequence*)

view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

xchg_matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

xchg_matrix_for_view(*view*, *tags={}*)

xchg_view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

HIPBackend **Click to show**

class pyfr.backends.hip.base.**HIPBackend**(*cfg*)

_malloc_impl(*nbytes*)

alias(*obj*, *aobj*)

blocks = False

commit()

const_matrix(*initval*, *extent=None*, *tags={}*)

kernel(*name*, **args*, ***kwargs*)

lookup = None

malloc(*obj*, *extent*)

matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

matrix_bank(*mats*, *initbank=0*, *tags={}*)

matrix_slice(*mat*, *ra*, *rb*, *ca*, *cb*)

name = 'hip'

queue()

runall(*sequence*)

view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

xchg_matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

xchg_matrix_for_view(*view*, *tags={}*)

xchg_view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

OpenCLBackend **Click to show**

class pyfr.backends.opencl.base.**OpenCLBackend**(*cfg*)

_malloc_impl(*nbytes*)

alias(*obj*, *aobj*)

blocks = False

commit()

const_matrix(*initval*, *extent=None*, *tags={}*)

kernel(*name*, **args*, ***kwargs*)

lookup = None

malloc(*obj*, *extent*)

matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

matrix_bank(*mats*, *initbank=0*, *tags={}*)

matrix_slice(*mat*, *ra*, *rb*, *ca*, *cb*)

name = 'opencl'

queue()

runall(*sequence*)

view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

xchg_matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

xchg_matrix_for_view(*view*, *tags={}*)

xchg_view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

OpenMPBackend **Click to show**

class pyfr.backends.openmp.base.**OpenMPBackend**(*cfg*)

_malloc_impl(*nbytes*)

alias(*obj*, *aobj*)

blocks = True

commit()

const_matrix(*initval*, *extent=None*, *tags={}*)

kernel(*name*, **args*, ***kwargs*)

lookup = None

malloc(*obj*, *extent*)

matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

matrix_bank(*mats*, *initbank=0*, *tags={}*)

matrix_slice(*mat*, *ra*, *rb*, *ca*, *cb*)

name = 'openmp'

queue()

runall(*sequence*)

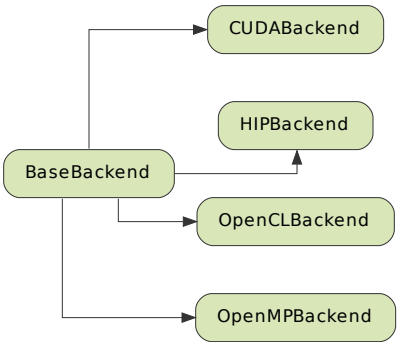
view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

xchg_matrix(*ioshape*, *initval=None*, *extent=None*, *aliases=None*, *tags={}*)

xchg_matrix_for_view(*view*, *tags={}*)

xchg_view(*matmap*, *rmap*, *cmap*, *rstridemap=None*, *vshape=()*, *tags={}*)

Types of *Backend* are related via the following inheritance diagram:



3.1.9 Pointwise Kernel Provider

A *Pointwise Kernel Provider* produces point-wise kernels. Specifically, a *Pointwise Kernel Provider* has a method named `register`, which adds a new method to an instance of a *Pointwise Kernel Provider*. This new method, when called, returns a kernel. A kernel is an instance of a 'one-off' class with a method named `run` that implements the required kernel functionality. The kernel functionality itself is specified using *PyFR-Mako*. Hence, a *Pointwise Kernel Provider* also has a method named `_render_kernel`, which renders *PyFR-Mako* into low-level platform-specific code. The `_render_kernel` method first sets the context for Mako (i.e. details about the *Backend* etc.) and then uses Mako to begin rendering the *PyFR-Mako* specification. When Mako encounters a `pyfr:kernel` an instance of a *Kernel Generator* is created, which is used to render the body of the `pyfr:kernel`. There are four types of *Pointwise Kernel Provider* available in PyFR 1.12.3:

CUDAPointwiseKernelProvider **Click to show**

class pyfr.backends.cuda.provider.**CUDAPointwiseKernelProvider**(*backend*)

_build_arglst(*dims*, *argn*, *argt*, *argdict*)

_build_kernel(*name*, *src*, *argtypes*)

_instantiate_kernel(*dims*, *fun*, *arglst*)

_render_kernel(*name*, *mod*, *extrns*, *tplargs*)

kernel_generator_cls
alias of *pyfr.backends.cuda.generator.CUDAKernelGenerator*

register(*mod*)

HIPPointwiseKernelProvider **Click to show**

class pyfr.backends.hip.provider.**HIPPointwiseKernelProvider**(**args*, ***kwargs*)

_build_arglst(*dims*, *argn*, *argt*, *argdict*)

_build_kernel(*name*, *src*, *argtypes*)

_instantiate_kernel(*dims*, *fun*, *arglst*)

_render_kernel(*name*, *mod*, *extrns*, *tplargs*)

kernel_generator_cls = None

register(*mod*)

OpenCLPointwiseKernelProvider **Click to show**

class pyfr.backends.opencl.provider.**OpenCLPointwiseKernelProvider**(*backend*)

_build_arglst(*dims*, *argn*, *argt*, *argdict*)

_build_kernel(*name*, *src*, *argtypes*)

_instantiate_kernel(*dims*, *fun*, *arglst*)

_render_kernel(*name*, *mod*, *extrns*, *tplargs*)

kernel_generator_cls
alias of *pyfr.backends.opencl.generator.OpenCLKernelGenerator*

register(*mod*)

OpenMPPointwiseKernelProvider **Click to show**

class pyfr.backends.openmp.provider.**OpenMPPointwiseKernelProvider**(*backend*)

_build_arglst(*dims*, *argn*, *argt*, *argdict*)

_build_kernel(*name*, *src*, *argtypes*, *restype=None*)

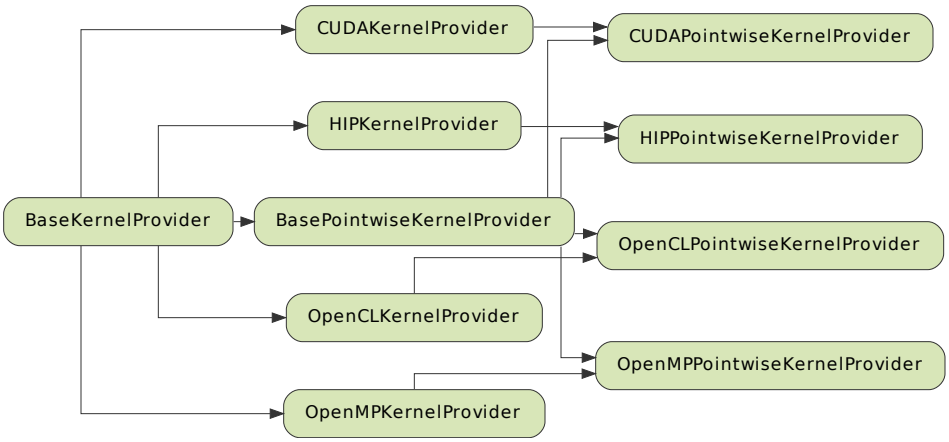
_instantiate_kernel(*dims*, *fun*, *arglst*)

_render_kernel(*name*, *mod*, *extrns*, *tplargs*)

kernel_generator_cls
alias of *pyfr.backends.openmp.generator.OpenMPKernelGenerator*

register(*mod*)

Types of *Pointwise Kernel Provider* are related via the following inheritance diagram:



3.1.10 Kernel Generator

A *Kernel Generator* renders the *PyFR-Mako* in a `pyfr:kernel` into low-level platform-specific code. Specifically, a *Kernel Generator* has a method named `render`, which applies *Backend* specific regex and adds *Backend* specific 'boiler plate' code to produce the low-level platform-specific source – which is compiled, linked, and loaded. There are four types of *Kernel Generator* available in PyFR 1.12.3:

CUDAKernelGenerator **Click to show**

class pyfr.backends.cuda.generator.**CUDAKernelGenerator**(**args*, ***kwargs*)

_deref_arg_array_1d(*arg*)

_deref_arg_array_2d(*arg*)

_deref_arg_view(*arg*)

_render_body(*body*)

_render_spec()

argspec()

ldim_size(*name*, **factor*)

needs_ldim(*arg*)

render()

HIPKernelGenerator **Click to show**

class pyfr.backends.hip.generator.**HIPKernelGenerator**(**args*, ***kwargs*)

_deref_arg_array_1d(*arg*)

_deref_arg_array_2d(*arg*)

_deref_arg_view(*arg*)

_render_body(*body*)

_render_spec()

argspec()

block1d = None

block2d = None

ldim_size(*name*, **factor*)

needs_ldim(*arg*)

render()

OpenCLKernelGenerator **Click to show**

class pyfr.backends.opencl.generator.**OpenCLKernelGenerator**(**args*, ***kwargs*)

_deref_arg_array_1d(*arg*)

_deref_arg_array_2d(*arg*)

_deref_arg_view(*arg*)

_render_body(*body*)

_render_spec()

argspec()

ldim_size(*name*, **factor*)

needs_ldim(*arg*)

render()

OpenMPKernelGenerator **Click to show**

class pyfr.backends.openmp.generator.**OpenMPKernelGenerator**(*name*, *ndim*, *args*, *body*, *fpdtype*)

_deref_arg_array_1d(*arg*)

_deref_arg_array_2d(*arg*)

_deref_arg_view(*arg*)

_render_body(*body*)

_render_spec()

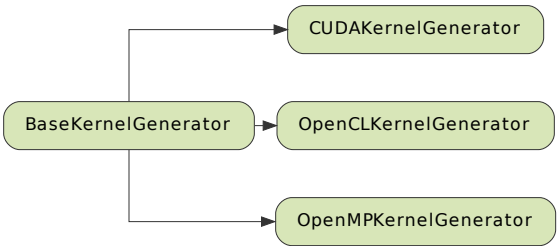
argspec()

ldim_size(*name*, **factor*)

needs_ldim(*arg*)

render()

Types of *Kernel Generator* are related via the following inheritance diagram:



3.2 PyFR-Mako

3.2.1 PyFR-Mako Kernels

PyFR-Mako kernels are specifications of point-wise functionality that can be invoked directly from within PyFR. They are opened with a header of the form:

```
<%pyfr:kernel name='kernel-name' ndim='data-dimensionality' [argument-name='argument-
↪intent argument-attribute argument-data-type' ...]>
```

where

1. `kernel-name` — name of kernel

   string

2. `data-dimensionality` — dimensionality of data

   int

3. `argument-name` — name of argument

   string

4. `argument-intent` — intent of argument

   `in` | `out` | `inout`

5. `argument-attribute` — attribute of argument

   `mpi` | `scalar` | `view`

6. `argument-data-type` — data type of argument

   string

and are closed with a footer of the form:

```
</%pyfr:kernel>
```

3.2.2 PyFR-Mako Macros

PyFR-Mako macros are specifications of point-wise functionality that cannot be invoked directly from within PyFR, but can be embedded into PyFR-Mako kernels. PyFR-Mako macros can be viewed as building blocks for PyFR-mako kernels. They are opened with a header of the form:

```
<%pyfr:macro name='macro-name' params='[parameter-name, ...]'>
```

where

1. `macro-name` — name of macro

   string

2. `parameter-name` — name of parameter

   string

and are closed with a footer of the form:

```
</%pyfr:macro>
```

PyFR-Mako macros are embedded within a kernel using an expression of the following form:

```
${pyfr.expand('macro-name', ['parameter-name', ...])};
```

where

1. `macro-name` — name of the macro

   string

2. `parameter-name` — name of parameter

   string

3.2.3 Syntax

3.2.3.1 Basic Functionality

Basic functionality can be expressed using a restricted subset of the C programming language. Specifically, use of the following is allowed:

1. `+,-,*,/` — basic arithmetic
2. `sin, cos, tan` — basic trigonometric functions
3. `exp` — exponential
4. `pow` — power
5. `fabs` — absolute value
6. `output = ( condition ? satisfied :  unsatisfied )` — ternary if
7. `min` — minimum
8. `max` — maximum

However, conditional if statements, as well as for/while loops, are not allowed.

3.2.3.2 Expression Substitution

Mako expression substitution can be used to facilitate PyFR-Mako kernel specification. A Python expression `expression` prescribed thus `${expression}` is substituted for the result when the PyFR-Mako kernel specification is interpreted at runtime.

Example:

```
E = s[${ndims - 1}]
```

3.2.3.3 Conditionals

Mako conditionals can be used to facilitate PyFR-Mako kernel specification. Conditionals are opened with `% if condition:` and closed with `% endif`. Note that such conditionals are evaluated when the PyFR-Mako kernel specification is interpreted at runtime, they are not embedded into the low-level kernel.

Example:

```
% if ndims == 2:
    fout[0][1] += t_xx;     fout[1][1] += t_xy;
    fout[0][2] += t_xy;     fout[1][2] += t_yy;
    fout[0][3] += u*t_xx + v*t_xy + ${-c['mu']*c['gamma']/c['Pr']}*T_x;
    fout[1][3] += u*t_xy + v*t_yy + ${-c['mu']*c['gamma']/c['Pr']}*T_y;
% endif
```

3.2.3.4 Loops

Mako loops can be used to facilitate PyFR-Mako kernel specification. Loops are opened with `% for condition:` and closed with `% endfor`. Note that such loops are unrolled when the PyFR-Mako kernel specification is interpreted at runtime, they are not embedded into the low-level kernel.

Example:

```
% for i in range(ndims):
    rhov[${i}] = s[${i + 1}];
    v[${i}] = invrho*rhov[${i}];
% endfor
```

CHAPTER

FOUR

PERFORMANCE TUNING

The following sections contain best practices for *tuning* the performance of PyFR. Note, however, that it is typically not worth pursuing the advice in this section until a simulation is working acceptably and generating the desired results.

4.1 OpenMP Backend

4.1.1 libxsmm

If libxsmm is not available then PyFR will make use of GiMMiK for all matrix-matrix multiplications. Although functional, the performance is typically sub-par compared with that of libxsmm. As such libxsmm is *highly* recommended.

4.1.2 AVX-512

When running on an AVX-512 capable CPU Clang and GCC will, by default, only make use of 256-bit vectors. Given that the kernels in PyFR benefit meaningfully from longer vectors it is desirable to override this behaviour. This can be accomplished through the `cflags` key as:

```
[backend-openmp]
cflags = -mprefer-vector-width=512
```

4.1.3 Cores vs. threads

PyFR does not typically derive any benefit from SMT. As such the number of OpenMP threads should be chosen to be equal to the number of physical cores.

4.1.4 MPI processes vs. OpenMP threads

When using the OpenMP backend it is recommended to employ *one MPI rank per NUMA zone*. For most systems each socket represents its own NUMA zone. Thus, on a two socket system it is suggested to run PyFR with two MPI ranks, with each process being bound to a single socket. The specifics of how to accomplish this depend on both the job scheduler and MPI distribution.

4.2 CUDA Backend

4.2.1 CUDA-aware MPI

PyFR is capable of taking advantage of CUDA-aware MPI. This enables CUDA device pointers to be directly to passed MPI routines. Under the right circumstances this can result in improved performance for simulations which are near the strong scaling limit. Assuming mpi4py has been built against an MPI distribution which is CUDA-aware this functionality can be enabled through the `mpi-type` key as:

```
[backend-cuda]
mpi-type = cuda-aware
```

Note that if UCX is used as a transport, as is the case for recent builds of OpenMPI, it may be necessary to set:

```
$ export UCX_MEMTYPE_CACHE=n
```

4.3 Partitioning

4.3.1 METIS vs SCOTCH

The partitioning module in PyFR includes support for both METIS and SCOTCH. Both usually result in high-quality decompositions. However, for long running simulations on complex geometries it may be worth partitioning a grid with both and observing which decomposition performs best.

4.3.2 Mixed grids

When running PyFR in parallel on mixed element grids it is necessary to take some additional care when partitioning the grid. A good domain decomposition is one where each partition contains the same amount of computational work. For grids with a single element type the amount of computational work is very well approximated by the number of elements assigned to a partition. Thus the goal is simply to ensure that all of the partitions have roughly the same number of elements. However, when considering mixed grids this relationship begins to break down since the computational cost of one element type can be appreciably more than that of another.

Thus in order to obtain a good decomposition it is necessary to assign a weight to each type of element in the domain. Element types which are more computationally intensive should be assigned a larger weight than those that are less intensive. Unfortunately, the relative cost of different element types depends on a variety of factors, including:

- The polynomial order.
- If anti-aliasing is enabled in the simulation, and if so, to what extent.
- The hardware which the simulation will be run on.

Weights can be specified when partitioning the mesh as `-e shape:weight`. For example, if on a particular system a quadrilateral is found to be 50% more expensive than a triangle this can be specified as:

```
pyfr partition -e quad:3 -e tri:2 ...
```

If precise profiling data is not available regarding the performance of each element type in a given configuration a helpful rule of thumb is to under-weight the dominant element type in the domain. For example, if a domain is 90% tetrahedra and 10% prisms then, absent any additional information about the relative performance of tetrahedra and prisms, a safe choice is to assume the prisms are appreciably *more* expensive than the tetrahedra.

4.4 Parallel I/O

PyFR incorporates support for parallel file I/O via HDF5 and will use it automatically where available. However, for this work several prerequisites must be satisfied:

- HDF5 must be explicitly compiled with support for parallel I/O.
- The mpi4py Python module *must* be compiled against the same MPI distribution as HDF5. A version mismatch here can result in subtle and difficult to diagnose errors.
- The h5py Python module *must* be built with support for parallel I/O.

After completing this process it is highly recommended to verify everything is working by trying the h5py parallel hdf5 example.

4.5 Start-up Time

The start-up time required by PyFR can be reduced by ensuring that Python is compiled from source with profile guided optimisations (PGO) which can be enabled by passing `--enable-optimizations` to the `configure` script.

It is also important that NumPy be configured to use an optimized BLAS/LAPACK distribution. Further details can be found in the NumPy building from source guide.

If the point sampler plugin is being employed with a large number of sample points it is further recommended to install SciPy.

CHAPTER

FIVE

EXAMPLES

PyFR includes several test cases to showcase the functionality of the solver. It is important to note, however, that these examples are all relatively small 2D simulations and, as such, are *not* suitable for scalability or performance studies.

5.1 Euler Equations

5.1.1 2D Euler Vortex

Proceed with the following steps to run a parallel 2D Euler vortex simulation on a structured mesh:

1. Create a working directory called `euler_vortex_2d/`
2. Copy the configuration file `PyFR/examples/euler_vortex_2d/euler_vortex_2d.ini` into `euler_vortex_2d/`
3. Copy the Gmsh file `PyFR/examples/euler_vortex_2d/euler_vortex_2d.msh` into `euler_vortex_2d/`
4. Run pyfr to convert the Gmsh mesh file into a PyFR mesh file called `euler_vortex_2d.pyfrm`:

```
pyfr import euler_vortex_2d.msh euler_vortex_2d.pyfrm
```

5. Run pyfr to partition the PyFR mesh file into two pieces:

```
pyfr partition 2 euler_vortex_2d.pyfrm .
```

6. Run pyfr to solve the Euler equations on the mesh, generating a series of PyFR solution files called `euler_vortex_2d*.pyfrs`:

```
mpiexec -n 2 pyfr run -b cuda -p euler_vortex_2d.pyfrm euler_vortex_2d.ini
```

7. Run pyfr on the solution file `euler_vortex_2d-100.0.pyfrs` converting it into an unstructured VTK file called `euler_vortex_2d-100.0.vtu`:

```
pyfr export euler_vortex_2d.pyfrm euler_vortex_2d-100.0.pyfrs euler_vortex_2d-100.0.
↪vtu
```

8. Visualise the unstructured VTK file in Paraview

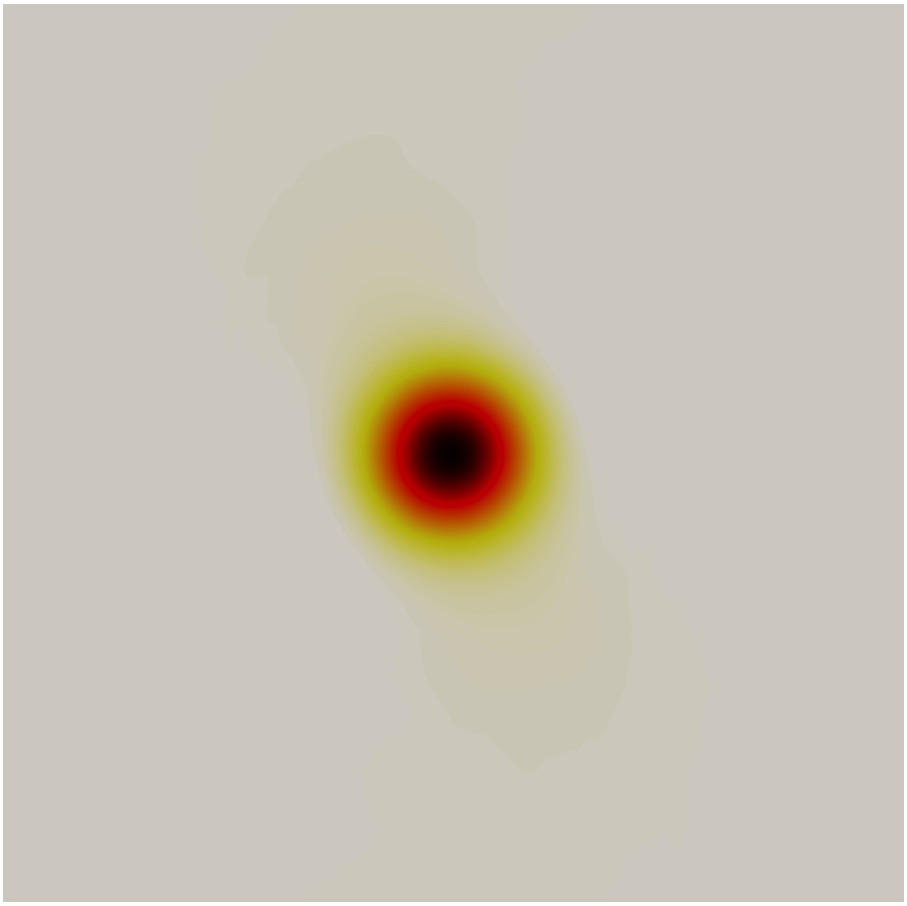


Fig. 1: Colour map of density distribution at 100 time units.

5.2 Compressible Navier–Stokes Equations

5.2.1 2D Couette Flow

Proceed with the following steps to run a serial 2D Couette flow simulation on a mixed unstructured mesh:

1. Create a working directory called `couette_flow_2d/`
2. Copy the configuration file `PyFR/examples/couette_flow_2d/couette_flow_2d.ini` into `couette_flow_2d/`
3. Copy the Gmsh mesh file `PyFR/examples/couette_flow_2d/couette_flow_2d.msh` into `couette_flow_2d/`
4. Run pyfr to covert the Gmsh mesh file into a PyFR mesh file called `couette_flow_2d.pyfrm`:

```
pyfr import couette_flow_2d.msh couette_flow_2d.pyfrm
```

5. Run pyfr to solve the Navier-Stokes equations on the mesh, generating a series of PyFR solution files called `couette_flow_2d-*.pyfrs`:

```
pyfr run -b cuda -p couette_flow_2d.pyfrm couette_flow_2d.ini
```

6. Run pyfr on the solution file `couette_flow_2d-040.pyfrs` converting it into an unstructured VTK file called `couette_flow_2d-040.vtu`:

```
pyfr export couette_flow_2d.pyfrm couette_flow_2d-040.pyfrs couette_flow_2d-040.vtu
```

7. Visualise the unstructured VTK file in Paraview

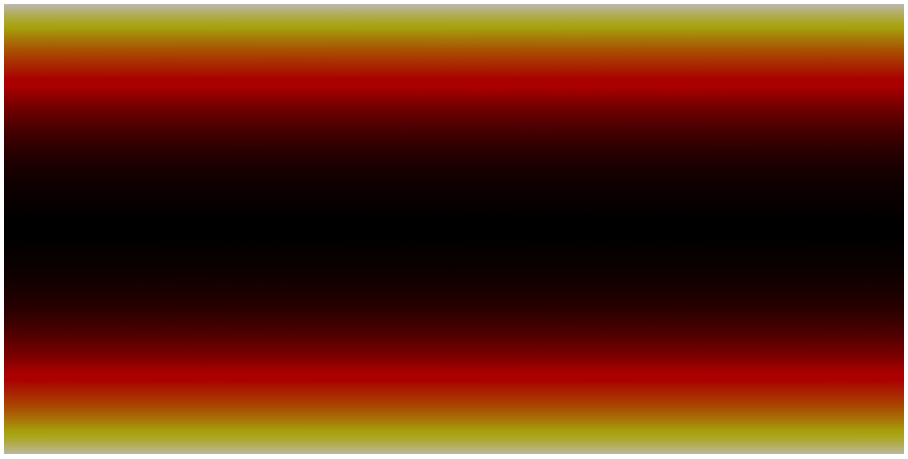


Fig. 2: Colour map of steady-state density distribution.

5.3 Incompressible Navier–Stokes Equations

5.3.1 2D Incompressible Cylinder Flow

Proceed with the following steps to run a serial 2D incompressible cylinder flow simulation on a mixed unstructured mesh:

1. Create a working directory called `inc_cylinder_2d/`
2. Copy the configuration file `PyFR/examples/inc_cylinder_2d/inc_cylinder_2d.ini` into `inc_cylinder_2d/`
3. Copy the compressed Gmsh mesh file `PyFR/examples/inc_cylinder_2d/inc_cylinder_2d.msh.gz` into `inc_cylinder_2d/`
4. Unzip the file and run pyfr to covert the Gmsh mesh file into a PyFR mesh file called `inc_cylinder_2d.pyfrm`:

```
zcat inc_cylinder_2d.msh.gz | pyfr import -tgmsh - inc_cylinder_2d.pyfrm
```

5. Run pyfr to solve the incompressible Navier-Stokes equations on the mesh, generating a series of PyFR solution files called `inc_cylinder_2d-*.pyfrs`:

```
pyfr run -b cuda -p inc_cylinder_2d.pyfrm inc_cylinder_2d.ini
```

6. Run pyfr on the solution file `inc_cylinder_2d-75.00.pyfrs` converting it into an unstructured VTK file called `inc_cylinder_2d-75.00.vtu`:

```
pyfr export inc_cylinder_2d.pyfrm inc_cylinder_2d-75.00.pyfrs inc_cylinder_2d-75.00.
↪vtu
```

7. Visualise the unstructured VTK file in Paraview

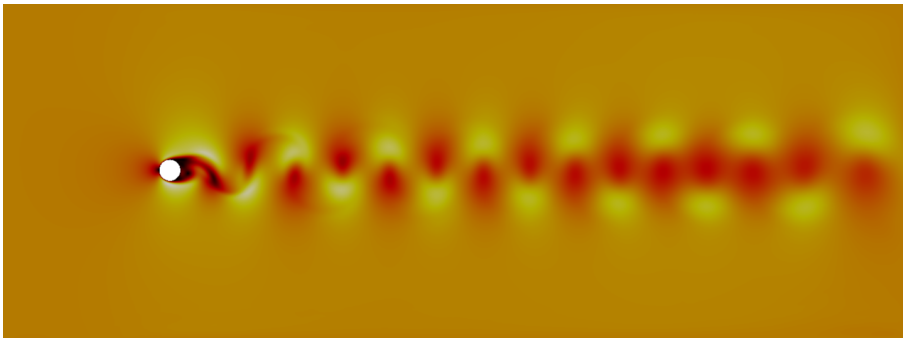


Fig. 3: Colour map of velocity magnitude distribution at 75 time units.

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