Struphy - solving plasma physics PDEs within the `Python` ecosystem

Struphy development team
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MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

```python
from struphy.pic.particles import Particles3D
from struphy.feec.psydac_derham import Derham
from mpi4py import MPI

Nel = [128, 128, 16]  # number of elements
p = [2, 2, 3] # spline degrees
spl_kind = [False, True, True] # periodic splines?
comm = MPI.COMM_WORLD
derham = Derham(Nel, p, spl_kind, comm=comm)
particles = Particles3D('ions', comm=comm)
particles.draw_markers()
```
✓ 4.6s

Outline

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Why Python? - Philospohy of Struphy development

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Why Python? - Philospohy of Struphy development

1. `Python` is the English of programming languages.
2. **Clarity, usability and flexibility first**.
3. Be <u>easily</u> accessible/usable by all scientists, for free.
4. Seamless integration with `Python` ecosystem:
   - `psydac` : MPI-distributed high-order spline library
   - `pyccel` : translate and compile in C or Fortran, use OpenMP
   - `mpi4py` : use MPI from Python
   - `numpy` : fast linear algebra
   - `desc-opt` : Stellarator equilibria
   - `pytest` : unit testing
   - and countless more ...
5. Provide an abstract framework for adding **new physics models, quickly**.

How Struphy works

1. Through the command line: `$ struphy run LinearMHD --mpi 8 -o DIR`
2. Through the Struphy API:


```
1  from struphy.geometry import domains
2  domain = domains.HollowTorus(a1=.05, sfl=True, tor_period=1)
3  domain.show()
✓ 1.0s
```
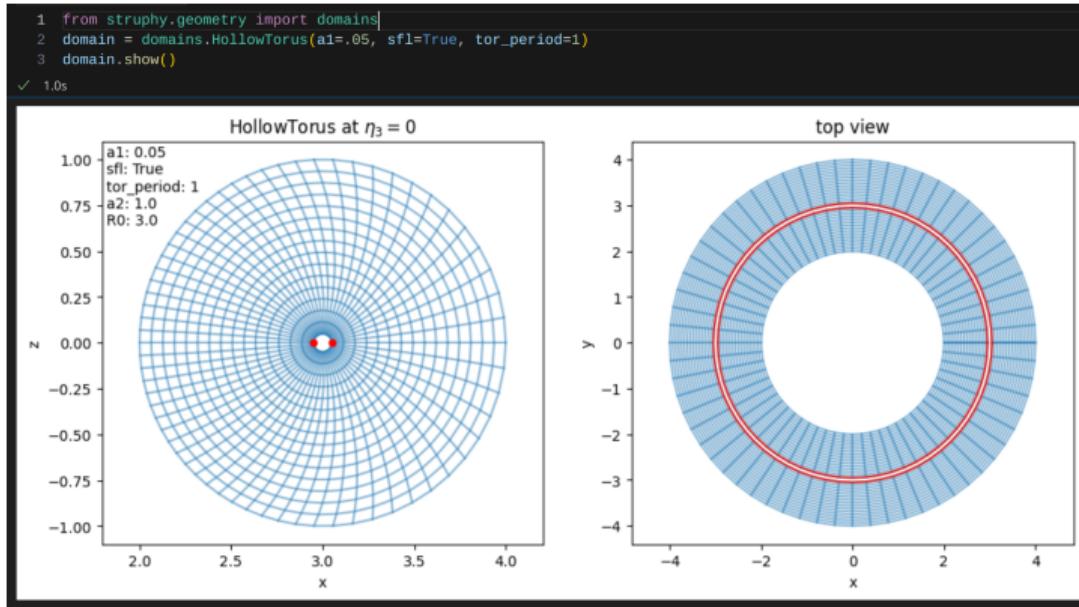
3. Add a new model yourself via the `StruphyModel` abstract base class

What a `StruphyModel` **looks like 1/2**

1. Inherit abstract base class:

```python
class VlasovMaxwellOneSpecies(StruphyModel):
    r'''Vlasov-Maxwell equations for one species.
```

2. Define species (i.e variables) and corresponding data structures in memory:

```python
@staticmethod
def species():
    dct = {'em_fields': {}, 'fluid': {}, 'kinetic': {}}

    dct['em_fields']['e_field'] = 'Hcurl'
    dct['em_fields']['b_field'] = 'Hdiv'
    dct['kinetic']['ions'] = 'Particles6D'
    return dct
```

3. Add propagators (push variables $t \rightarrow t + \Delta t$):

```python
@staticmethod
def propagators_dct():
    return {propagators_fields.Maxwell: ['e_field', 'b_field'],
            propagators_markers.PushEta: ['ions'],
            propagators_markers.PushVxB: ['ions'],
            propagators_coupling.VlasovAmpere: ['e_field', 'ions']}
```

What a `StruphyModel` looks like 2/2

4. Pass keyword arguments from parameter file to propagators:

```python
# set keyword arguments for propagators
self._kwargs[propagators_fields.Maxwell] = {'solver': params_maxwell}

self._kwargs[propagators_markers.PushEta] = {'algo': algo_eta,
                                             'bc_type': ions_params['markers']['bc']['type']}

self._kwargs[propagators_markers.PushVxB] = {'algo': algo_vxb,
                                             'scale_fac': 1./self._epsilon,
                                             'b_eq': b_backgr,
                                             'b_tilde': self.pointer['b_field']}

self._kwargs[propagators_coupling.VlasovAmpere] = {'c1': self._alpha**2/self._epsilon,
                                                   'c2': 1./self._epsilon,
                                                   'solver': params_coupling}

# Initialize propagators used in splitting substeps
self.init_propagators()
```

The propagators are the building blocks of each model. They can be combined to design new models. There are currently 41 propagators coded in Struphy. New propagators can be added through the `Propagator` abstract base class.

What is the purpose of Struphy?

1. Provide a fast, easy-to-use `Python` framework for plasma physics PDEs

2. Bring to practice the newest numerical algorithms (3D realistic scenarios)

3. Provide maintainable, understandable and accessible code

4. Compound the programming of researchers

5. Teach important software development skills

6. Enthuse students for plasma physics simulations

7. Spread the open-source paradigm in the academic community

Current developers

- Dominik Bell (PhD) - energy-conserving δf-methods (with Eric, Martin)
- Valentin Carlier (PhD) - variational MHD (with Martin)
- Ori Saporta-Katz (nt-Tao fusion startup) - MHD in time-varying backgrounds
- Yingzhe Li (Post-doc) - 6D Vlasov astrophysics hybrid model (with Eric)
- Max Lindqvist (ACH) - domain cloning, Struphy-Psydac integration (with Roman)
- Nathan Marín (PhD) - quasi-inter-/histopolation, shear-Alfvén preconditioning
- Byung-Kyu Na (PhD) - MHD-drift-kinetic hybrid models (with Xin)
- Philipp Thalhofer (Master) - quasi-neutral fluids with Lagrange multiplier (Omar)
- Matilde Tozzi (Master) - using the `pyAmrex` backend in Struphy (with Eric)

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Struphy data structures

- Particle data structures: 2D `numpy` arrays with communication buffer

- Grid data structures: `Stencil`-format from `psydac` with ghost regions

- Use of matrix-free operators (only `dot` product needed)

- All Struphy models are implemented in 3D configuration space

- Lower-dim. simulations can be carried out by setting `Nel = [128, 128, 1]`

- Velocity dimensions can range from 0-3 (at present)

- Domain decomp., domain cloning and MPI comm. happens under the hood

Particle data structures

Domain decomposition
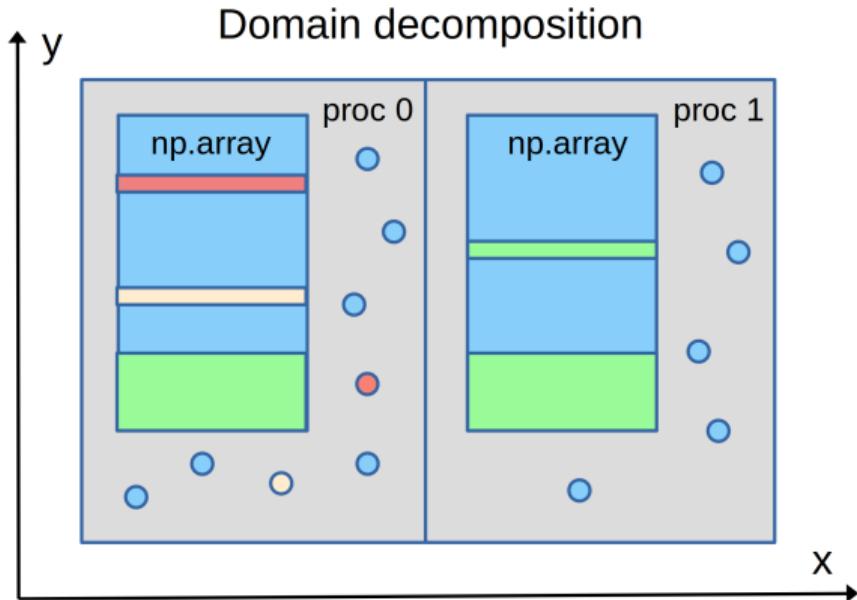
→ each row is a marker

→ columns are marker attributes

→ buffer (green) to manage load imbalance

Particle data structures

Domain decomposition

sorting → sorting with certain frequency

→ boundary conditions: periodic, reflect, remove

→ more info in the `Particles` abstract base class
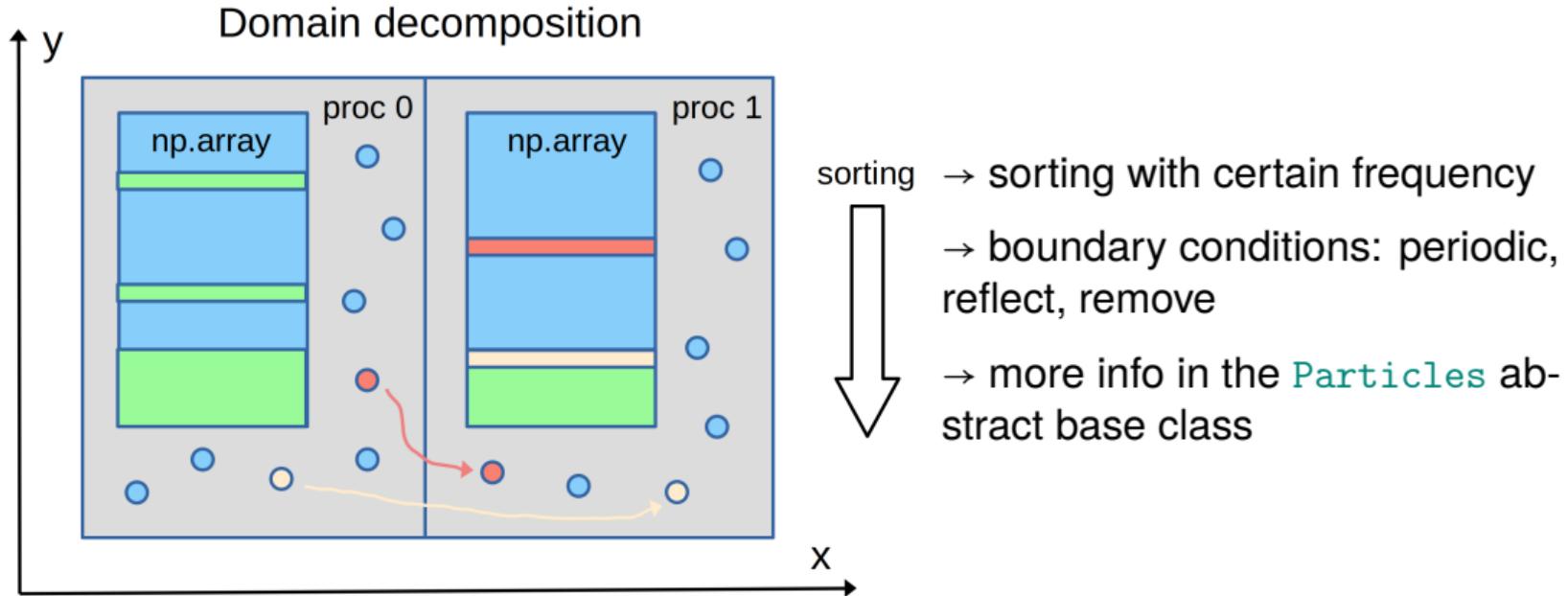
Grid data structures

Struphy uses the grid data structures provided by `psydac`:
https://github.com/pyccel/psydac
`psydac` main developers: <u>Yaman Güclü</u> (NMPP) and <u>Said Hadjout</u> (former student).

- `StencilVectorSpace`
- `StencilVector` holds the FE coefficients (or other grid data)
- `StencilMatrix` operators on `StencilVector`
- `LinearOperators` are used for matrix-free operations
- particle-to-grid accumulation into `StencilMatrix` or `StencilVector`

These objects have MPI communication via ghost regions.

StencilVector

Global StencilVector of size N

Three processes (global indexing)

rank 0   rank 1   rank 2

MPI communication (update ghost regions)
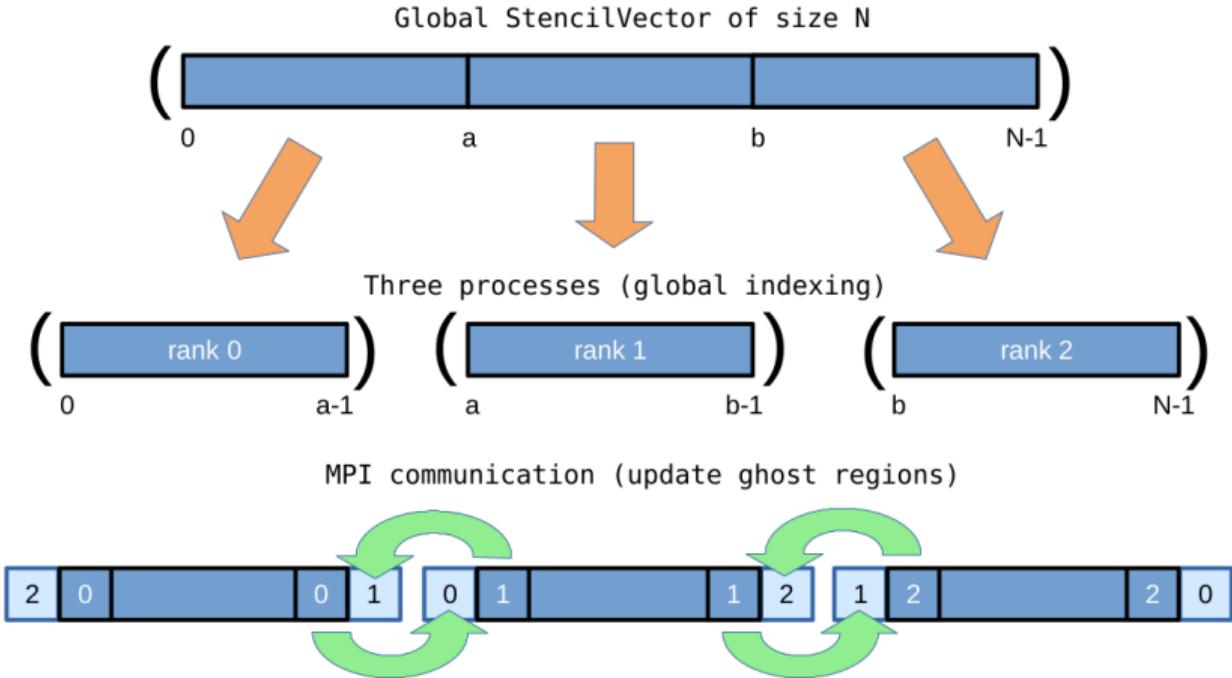
StencilMatrix
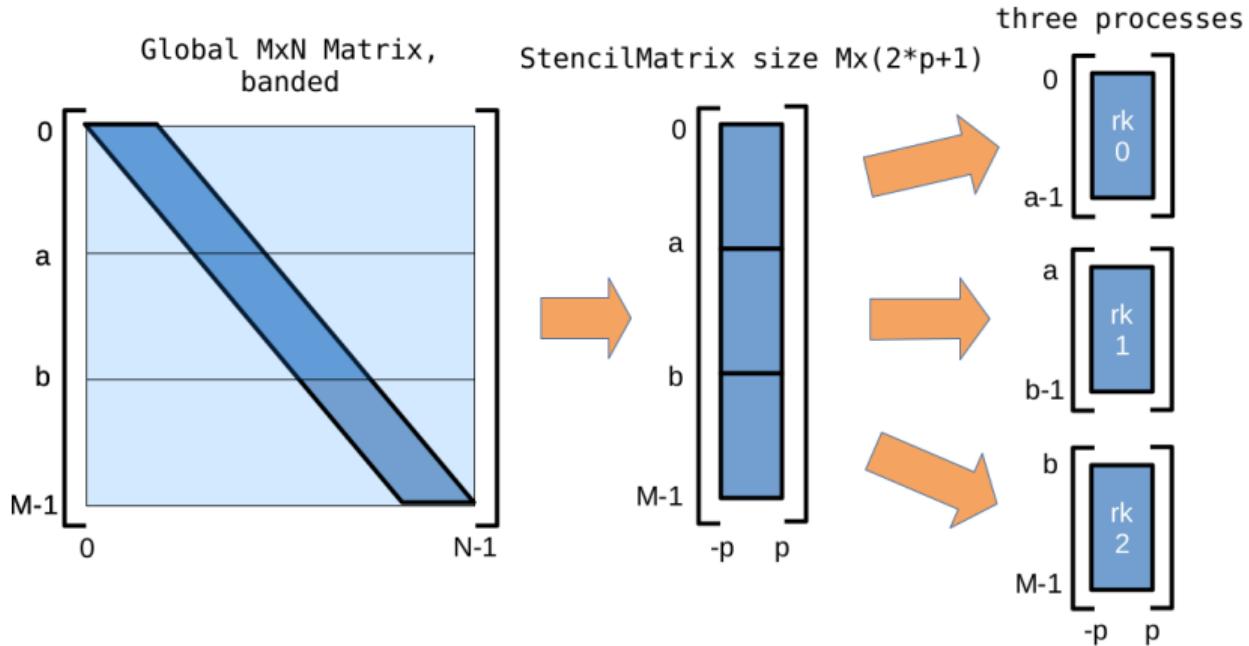
Boundary conditions: periodic, hom. Dirichlet, Neumann (traces of de Rham spaces)

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Lagrangian methods: PIC

Discretization of conservation laws of the form

$$\partial_t f + \nabla_q \cdot (G(f)\, f) = S(f) \qquad q \in \Omega \subset \mathbb{R}^n ,$$

where $\Omega \subset \mathbb{R}^n$ open, some (curvilinear) coordinates $q \in \Omega$ and $G(f)$ a (nonlinear) flow velocity.

$$f \approx f_h(t, q) = \frac{1}{N} \sum_{k=1}^{N} w_k(t)\, \delta(q - q_k(t)) .$$

System of ODEs (here for incompressible flow $\nabla_q \cdot G = 0$):

$$\dot{q}_k = G(t, f_h) \qquad\qquad q_k(0) = q_{k0} ,$$

$$\dot{w}_k = \frac{1}{s(t = 0, q_{k0})}\, S(f_h) \qquad w_k(0) = \frac{f(t = 0, q_{k0})}{s(t = 0, q_{k0})} .$$
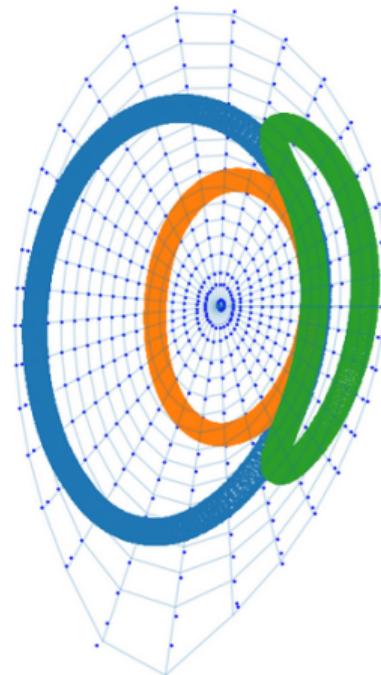
6D Vlasov orbits in EQDSK equilibrium

Finite element exterior calculus (FEEC)

$$u \approx u_h = \sum_{i=1}^{M} u_i \Lambda_i \quad \in V_h \,,$$

where $\Lambda_i \in V$ are linearly independent basis functions, $(u_i)_i \in \mathbb{R}^M$ are FE coefficients.

Finite element exterior calculus (FEEC)

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where $\Lambda_i \in V$ are linearly independent basis functions, $(u_i)_i \in \mathbb{R}^M$ are FE coefficients.

- $\Pi_0 : H^1(\Omega) \to V_h^0, \quad \Pi_1 : H(\mathrm{curl}, \Omega) \to V_h^1, \quad \Pi_2 : H(\mathrm{div}, \Omega) \to V_h^2, \quad \Pi_3 : L^2(\Omega) \to V_h^3$

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- $\mathrm{curl}\,\mathrm{grad} = 0, \qquad \mathrm{div}\,\mathrm{curl} = 0$

Finite element exterior calculus (FEEC)

Arnold, D., Falk, R., Winther, R.: Finite element exterior calculus: from Hodge theory to numerical stability. Bulletin of the American mathematical society, 47(2): 281-354, (2010).

$$
\begin{array}{ccccccc}
H^1(\Omega) & \xrightarrow{\text{grad}} & H(\text{curl}, \Omega) & \xrightarrow{\text{curl}} & H(\text{div}, \Omega) & \xrightarrow{\text{div}} & L^2(\Omega) \\
\downarrow{\scriptstyle \Pi_0} & & \downarrow{\scriptstyle \Pi_1} & & \downarrow{\scriptstyle \Pi_2} & & \downarrow{\scriptstyle \Pi_3} \\
V_h^0 & \xrightarrow{\text{grad}} & V_h^1 & \xrightarrow{\text{curl}} & V_h^2 & \xrightarrow{\text{div}} & V_h^3
\end{array}
$$

$$
u \approx u_h = \sum_{i=1}^{M} u_i \Lambda_i \quad \in V_h \,,
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- $\text{curl}\,\text{grad} = 0 \,, \qquad \text{div}\,\text{curl} = 0$

- $\Pi_1 \text{grad} = \text{grad}\,\Pi_0 \,, \qquad \Pi_2 \text{curl} = \text{curl}\,\Pi_1 \,, \qquad \Pi_3 \text{div} = \text{div}\,\Pi_2$

Geometric DOFs and B-splines

0-form   1-form   2-form   3-form

$\int$ $\iint$ $\iiint$
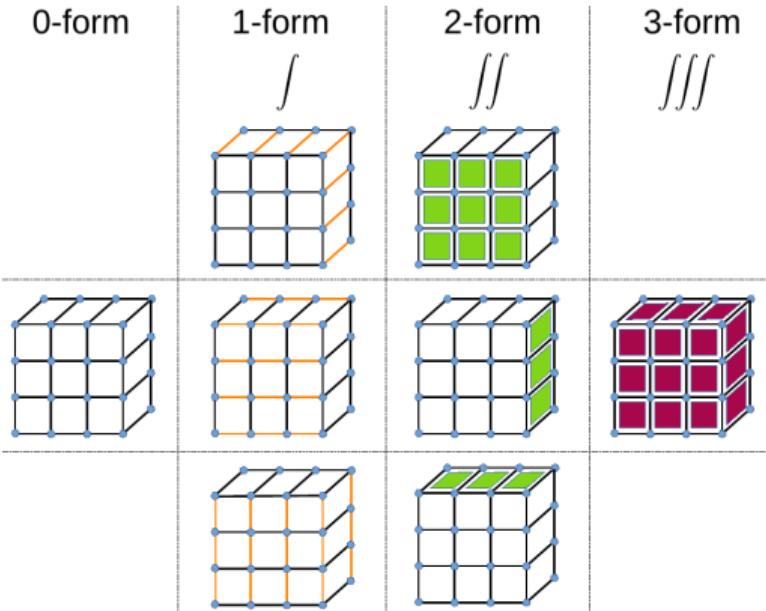
Point values, edge, face and volume integrals
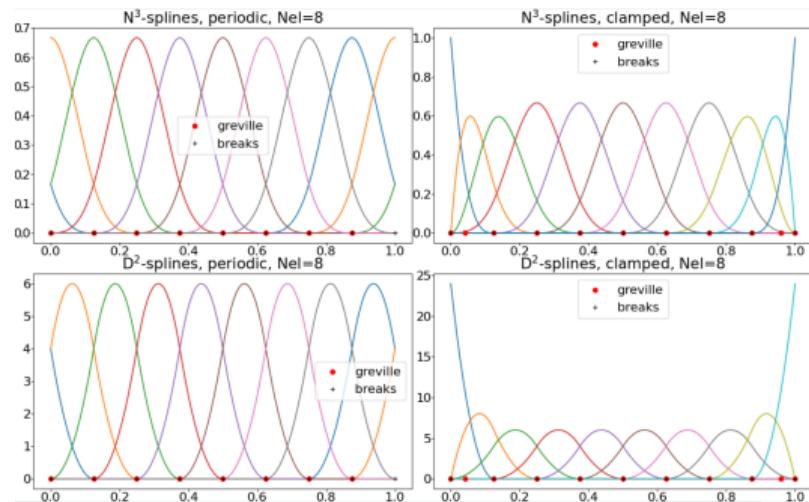
High-order B-splines, tensor product:

$$\Lambda_{ijk}^{1,1}(\mathbf{x}) = D_i^{p-1}(x)N_j^p(y)N_k^p(z)$$

Polar splines at magnetic axis

- Polar spline framework for discrete differential forms

  Toshniwal et. al., Comput. Meth. Appl. Mech. Engrg. **376**, 113576 (2021)

- 3 new $\mathcal{C}^1$-continuous polar splines around pole
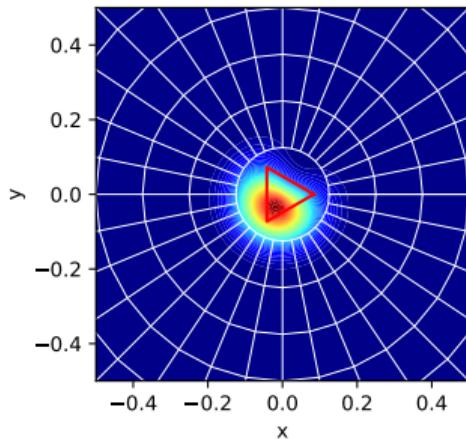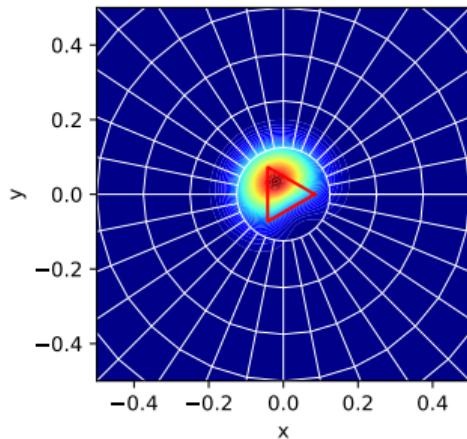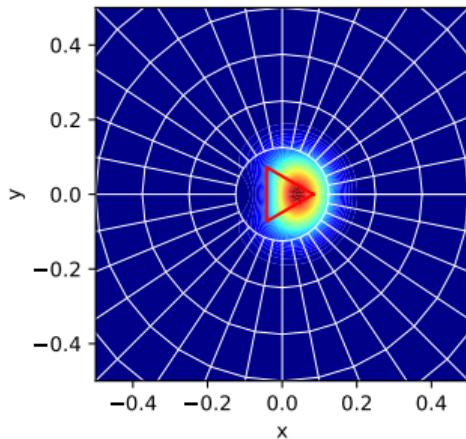
- Polar sub-spaces $\overline{V}_h^n \subset V_h^n$ contain C^0-functions on mapped domain

Wave-particle resonances

- Study coupling of energetic particles to waves

- Current focus on MHD-kinetic hybrid models

- An improved particle sorting algorithm for nearest neighbour search is being implemented

 → completely mesh-free methods (direction SPH)

Nonlinear Landau damping with geometric PIC

full, linear MHD, nonlinear coupling to drift-kinetic eq. use of binomial filter:

Radial velocity and magnetic field:
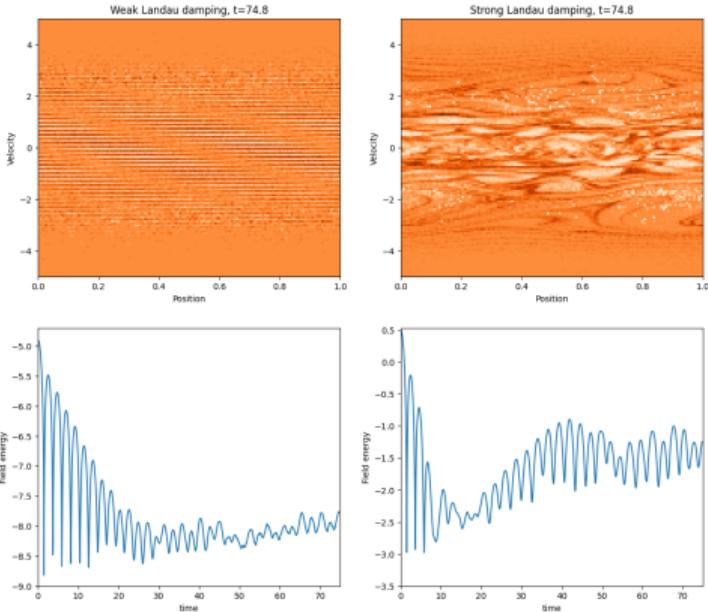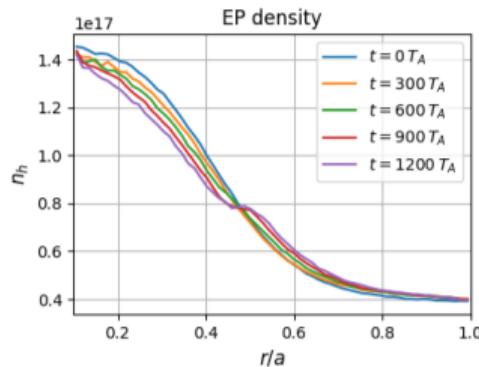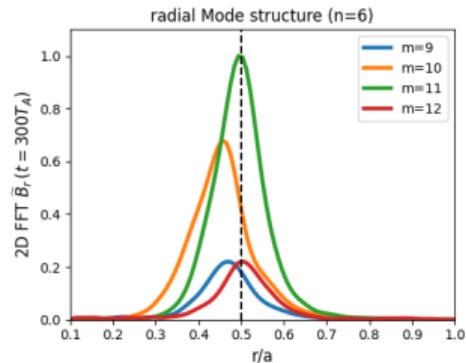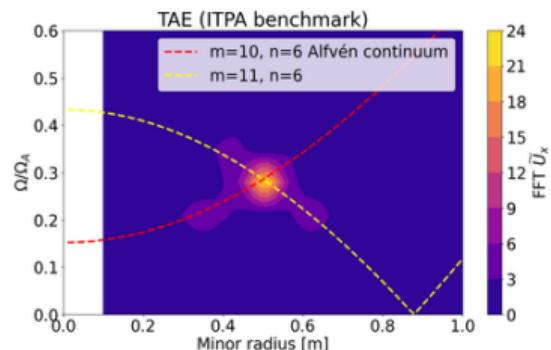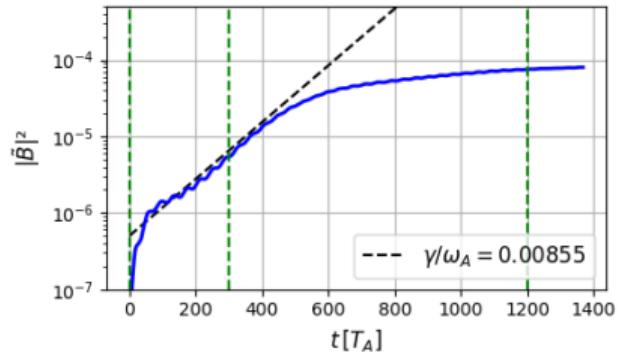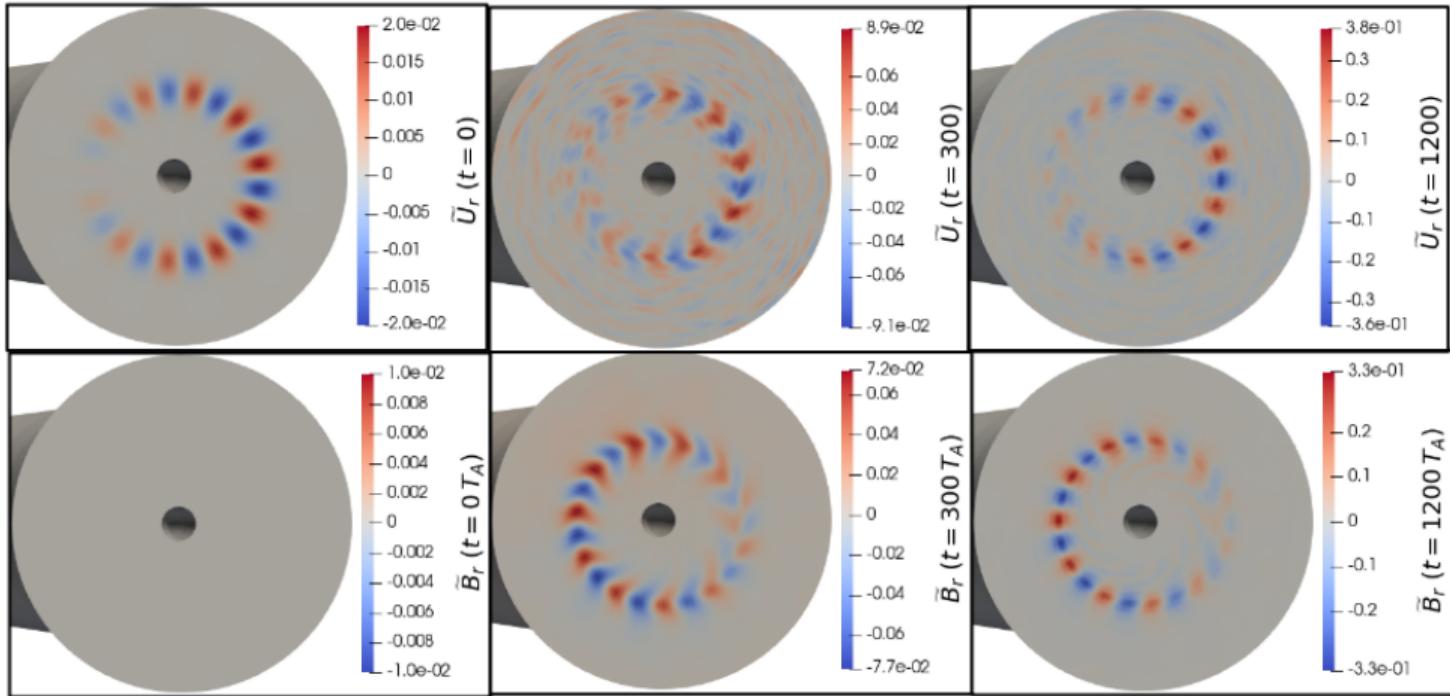
TAE benchmark (courtesy of Byung-Kyu Na) 3/3

Zonal flows? Contact: byungkyu.na@ipp.mpg.de
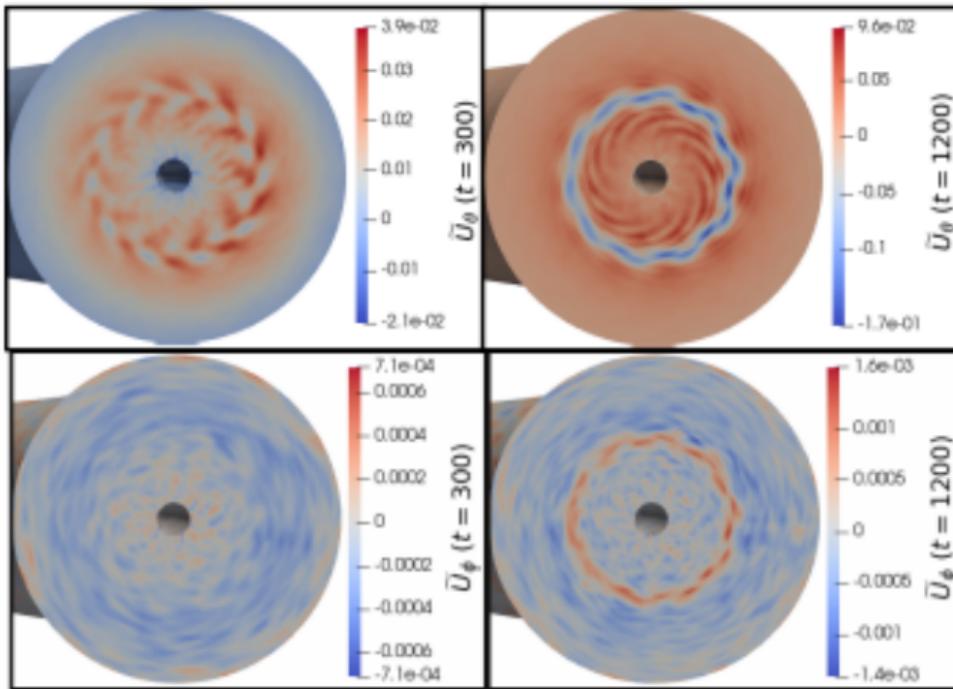
Variational MHD (courtesy of Valentin Carlier)

full nonlinear MHD with geometric conservation laws. Contact: Valentin.Carlier@ipp.mpg.de
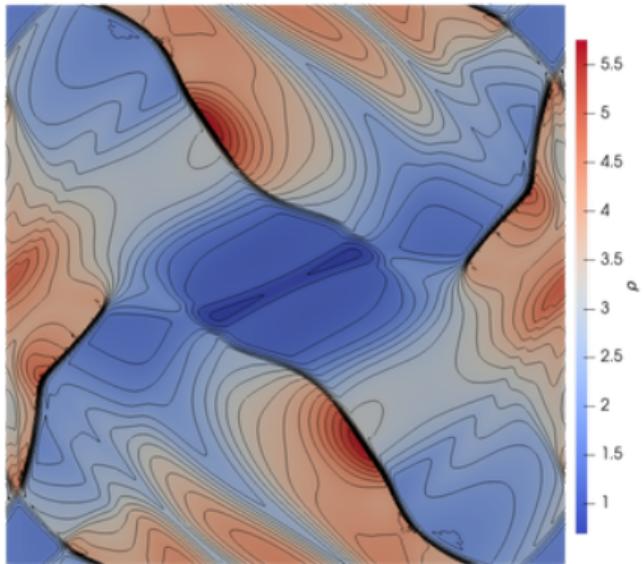
Orszag-Tang vortex
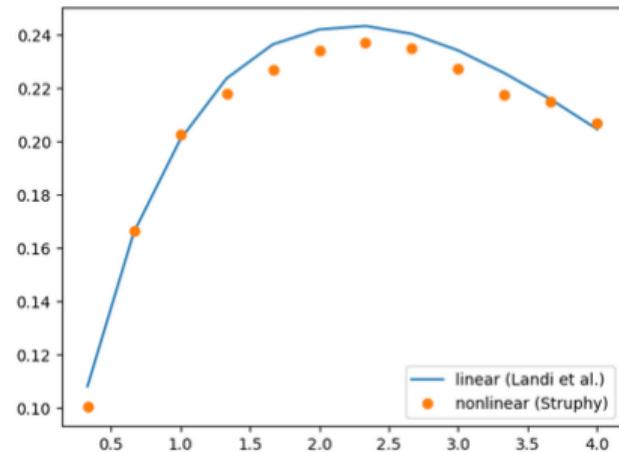
Current sheet instability

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Installing Struphy

- Virtual environment:

```
python -m venv env
source env/bin/activate
```

- Current (stable) version:

```
pip install struphy
struphy compile
```


https://struphy.pages.mpcdf.de/
struphy/index.html

- Install from source:

```
git clone https://gitlab.mpcdf.mpg.de/struphy/struphy.git
cd struphy
pip install -e .
struphy compile
```

Get in touch

- Google `struphy`
- Documentation: `https://gitlab.mpcdf.mpg.de/struphy/struphy`
- Repository: `https://gitlab.mpcdf.mpg.de/struphy/struphy`
- Ticket system: `https://gitlab.mpcdf.mpg.de/struphy/struphy/-/issues`
- Developer's channel: `https://chat.gwdg.de/channel/struphy-developers`
- Follow Struphy on LinkedIn: `https://www.linkedin.com/company/struphy/`
- Main contacts:
  - Eric Sonnendrücker
  - Xin Wang
  - myself