MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

STRUPHY

domain cloning and profiling with pylikwid

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EUROfusion

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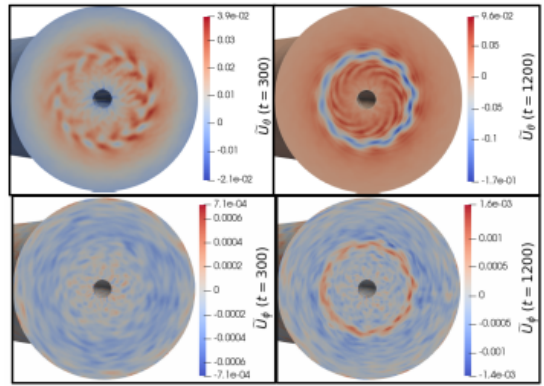
StruPhy: Structure-Preserving Hybrid Codes

- Solution of PDEs using Geometric Finite Element Exterior Calculus (FEEC) and Particle-in-Cell (PIC) methods in 3D
- Features a growing list of PDE models applicable to a variety of mapped domains
- Open-source and can be installed on any architecture
- Written in **Python**, kernels traslated to C/Fortran with `pyccel`



Zonal flow components of a toroidal Alfvén eigemode

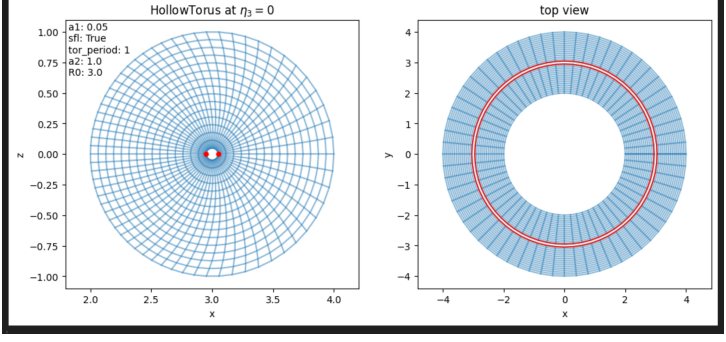
Why Python? - Philospohy of Struphy development

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

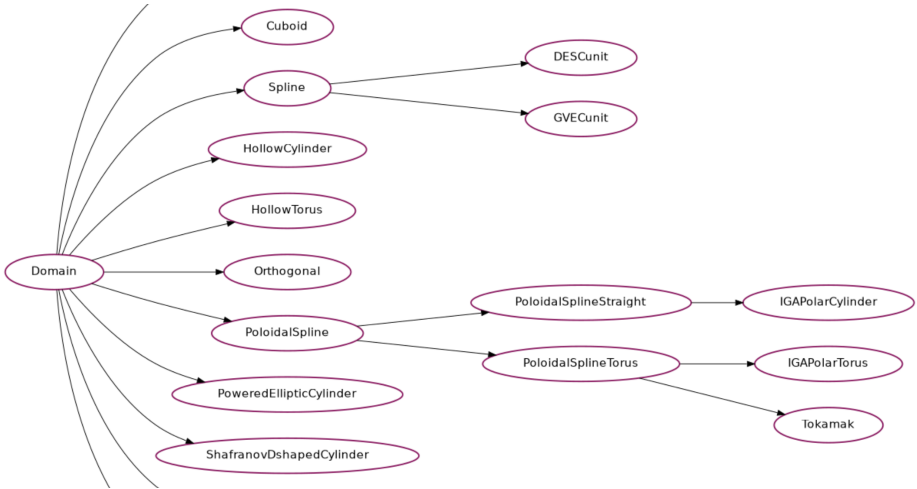
How Struphy works

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

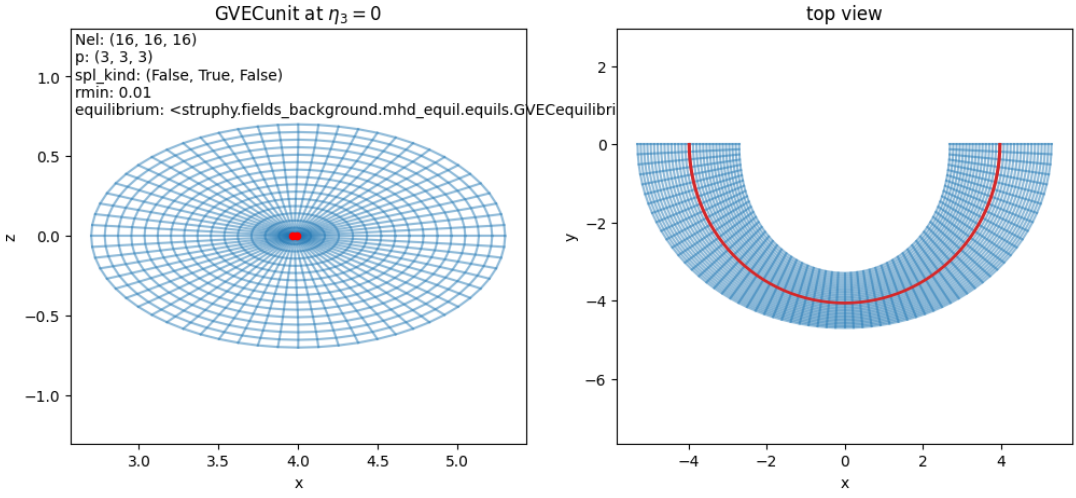
```
1 from struphy.geometry import domains
2 domain = domains.HollowTorus(a1=.05, sf1=True, tor_period=1)
3 domain.show()
✓ 1.0s
```



`StruphyModel` can be launched in curvilinear coordinates



Grid example: from GVEC output



Struphy Models

Struphy features a variety of plasma models for different physics scenarios

- **Fluid models**: `LinearMHD`, `LinearExtendedMHDuniform`, `ColdPlasma`, `VariationalMHD`, `ViscoresistiveMHD`, `ViscousFluid`
- **Kinetic models**: `VlasovAmpereOneSpecies`, `VlasovMaxwellOneSpecies`, `LinearVlasovAmpereOneSpecies`, `DriftKineticElectrostaticAdiabatic`
- **Fluid-kinetic hybrid models**: `LinearMHDVlasovCC`, `LinearMHDVlasovPC`, `LinearMHDDriftkineticCC`, `ColdPlasmaVlasov`
- **Toy models**: `Maxwell`, `Vlasov`, `GuidingCenter`, `ShearAlfven`, `VariationalPressurelessFluid`, `VariationalBarotropicFluid`, `VariationalCompressibleFluid`, `Poisson`, `DeterministicParticleDiffusion`, `RandomParticleDiffusion`

The `LinearMHDDriftkineticCC` model will be used for profiling

Struphy propagators

Propagators are the main building blocks of Struphy models, a large list are available

- **Field propagators**: `Maxwell` , `OhmCold` , `JxBCold` , `ShearAlfven` , `ShearAlfvenB1` , `Hall` , `Magnetosonic` , `MagnetosonicUniform` , `FaradayExtended` , `CurrentCoupling6DDensity` , `ShearAlfvenCurrentCoupling5D` , `CurrentCoupling5DDensity` , `ImplicitDiffusion` , `VariationalMomentumAdvection` , `VariationalDensityEvolve` , `VariationalEntropyEvolve` , `VariationalMagFieldEvolve` , `VariationalViscosity` , `VariationalResistivity` , `TimeDependentSource` , `AdiabaticPhi`
- **Particle propagators**: `PushEta` , `PushVxB` , `PushEtaPC` , `PushGuidingCenterBxEstar` , `PushGuidingCenterParallel` , `PushVinEfield` , `StepStaticEfield` , `PushDeterministicDiffusion` , `PushRandomDiffusion`
- **Particle-field coupling propagators**: `VlasovAmpere` , `EfieldWeights` , `EfieldWeightsImplicit` , `EfieldWeightsDiscreteGradient` , `EfieldWeightsAnalytic` , `PressureCoupling6D` , `CurrentCoupling6DCurrent` , `CurrentCoupling5DCurlb` , `CurrentCoupling5DGradB`

The propagators for `LinearMHDDriftkineticCC` are marked in red

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LIKWID

- LIKWID (Like I Knew What I'm Doing) is a performance monitoring and benchmarking tool for multi-core processors.
- Developed to simplify the access to performance counters on modern processors.
- Selected tools
  - `likwid-topology` : print thread, cache and NUMA topology.
  - `likwid-perfctr` : configure and read out hardware performance counters.
  - `likwid-pin` : pin your threaded application.
  - `likwid-mpirun` : Wrapper to start MPI and Hybrid MPI/OpenMP applications.

Pylikwid - python marker API

- Python wrapper for LIKWID, access to LIKWID marker API directly in Python scripts.
- `likwid-perfctr -C 0 -g MEM_DP -m python test.py`

```
# test.py
import pylikwid
import numpy as np
pylikwid.markerinit()
pylikwid.markerthreadinit()
N = 100_000
a = np.random.random((N,1))
b = np.random.random((N,1))
c = np.random.random((N,1))
pylikwid.markerstartregion("RegionID")
d = a + b * c
pylikwid.markerstopregion("RegionID")
pylikwid.markerclose()
```

Pylikwid - Struphy implementation

- `ProfilingConfig`: Singleton class for managing global profiling settings.
- `ProfileManager`: Manages profiling regions, collects data across MPI processes, and saves profiling results for analysis.

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```
config = ProfilingConfig()
config.likwid = args.likwid # Turn on likwid profiling with --likwid
# ...
for propagator in self.propagators:
    prop_name = type(propagator).__name__
    with ProfileManager.profile_region(prop_name):
        propagator(dt)
```

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```
struphy run LinearMHDDriftkineticCC --mpi 32 --likwid
```

- Profiling with `pylikwid` integration to the weekly scheduled CI using private runners (in progress).

Profiling on Raven - `LinearMHDDriftkineticCC`

Particle propagators

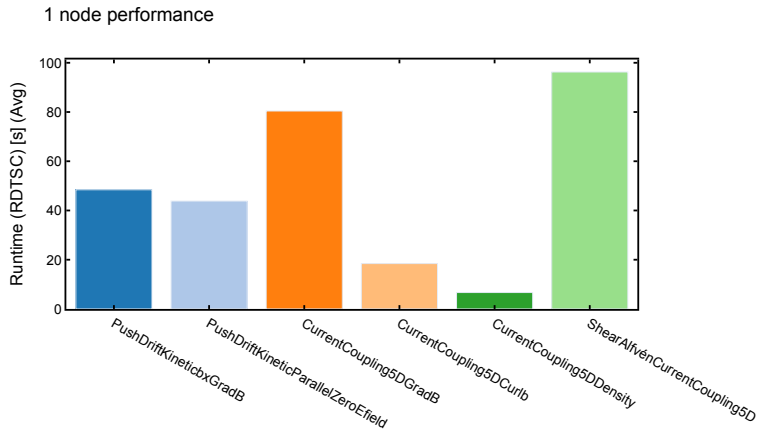
- `PushGuidingCenterBxEstar`
- `PushGuidingCenterParallel`

Particle-field coupling propagators

- `CurrentCoupling5DCurlb`
- `CurrentCoupling5DGradB`

Field propagators

- `ShearAlfvenCurrentCoupling5D`
- `CurrentCoupling5DDensity`



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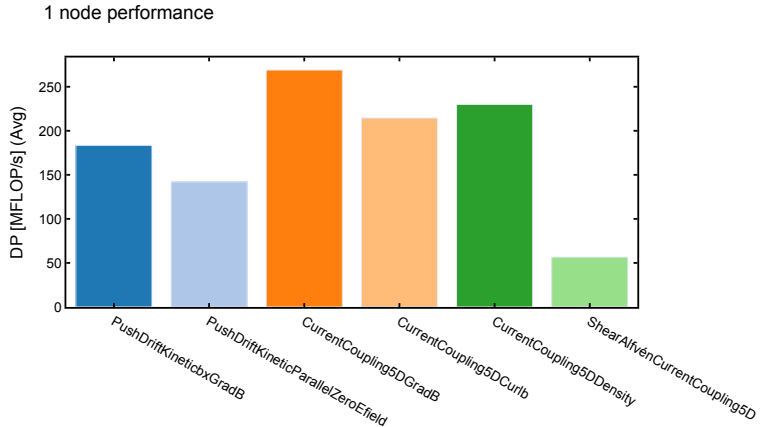

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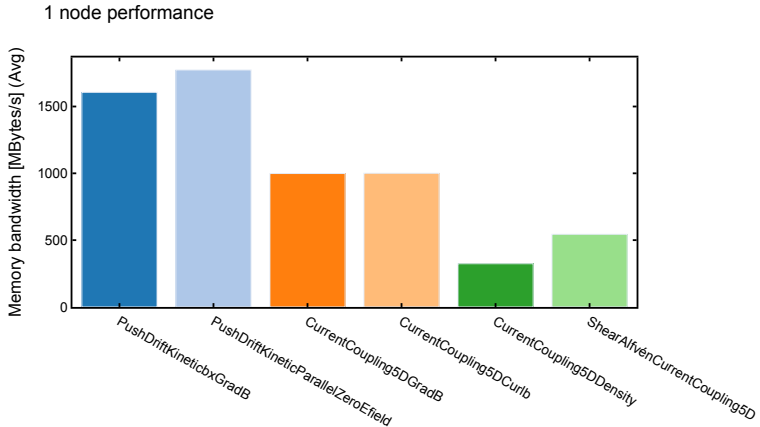

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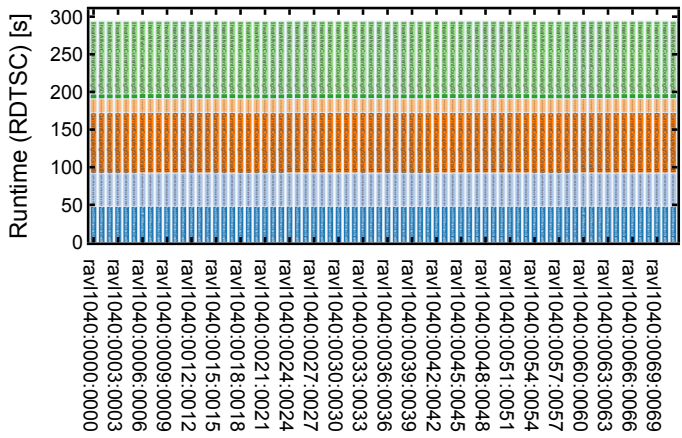

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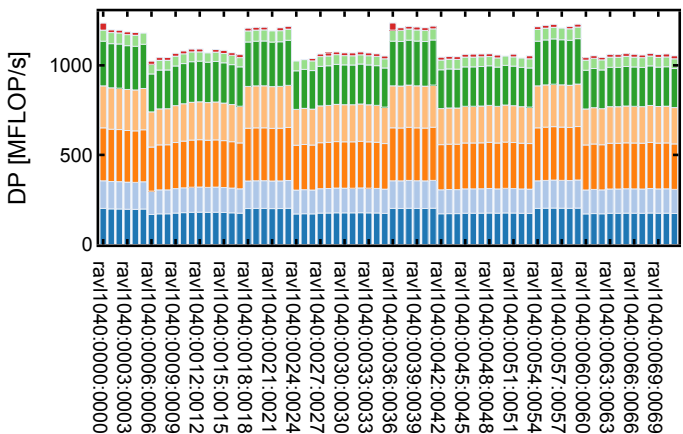

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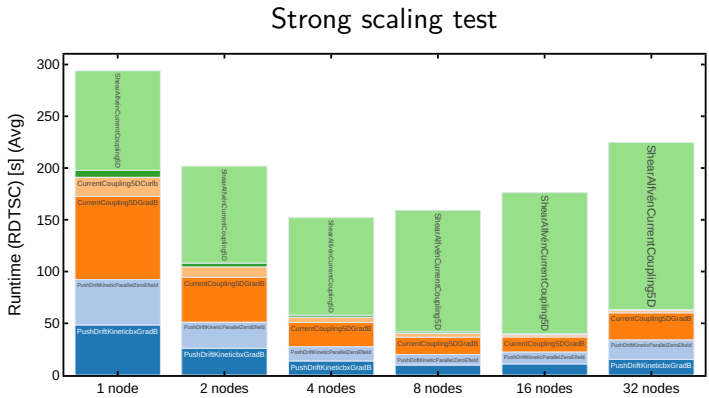

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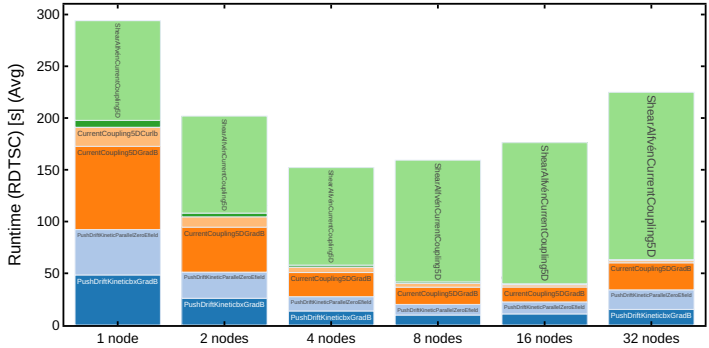
Strong scaling test



Next: Improve scaling of the particle propagators

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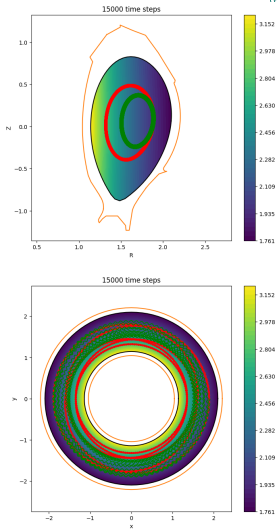
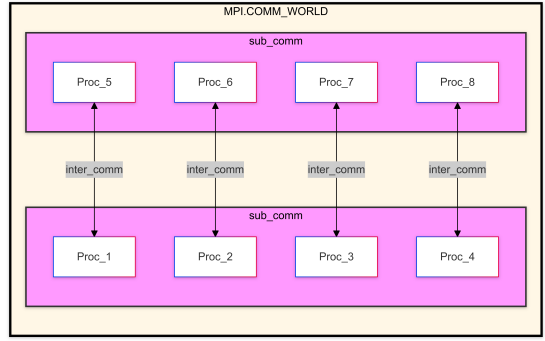
Domain Cloning

- $N_{\text{particles}}$ are evenly distributed among N_{clones} clones.
- Each clone independently calculates the charge density, summed across all clones.
- Field equations are solved separately within each clone.
- Particles propagate independently within the clones.
- Grid resolution decoupled from the number of processing elements, allowing for more MPI tasks than the number of toroidal grid points.



Domain Cloning - Communicators

- Additional communicators are initialized.
- `sub_comm`: within clones.
- `inter_comm`: between clones.
- Implementation: `sub_comm` replaces `MPI.COMM_WORLD` in the model, `inter_comm` is called after particle accumulation.




```
inter_comm.Allreduce(MPI.IN_PLACE, data_array, op=MPI.SUM)
data_array /= Nclones
```

Domain Cloning - `LinearMHDDriftkineticCC`

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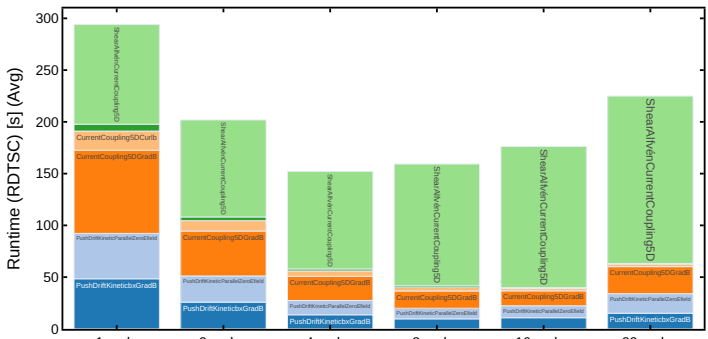
Scaling without domain cloning



Domain Cloning - `LinearMHDDriftkineticCC`

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- `CurrentCoupling5DGradB`

Field propagators

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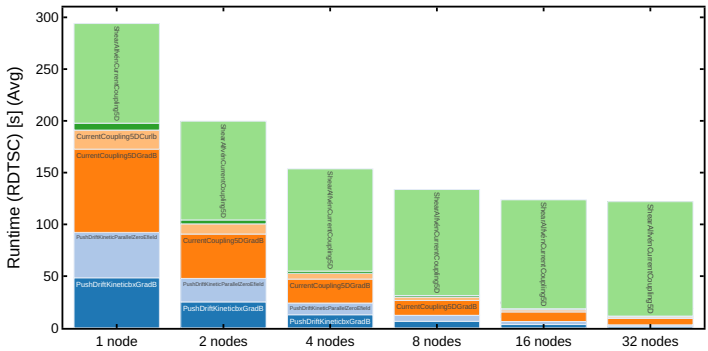
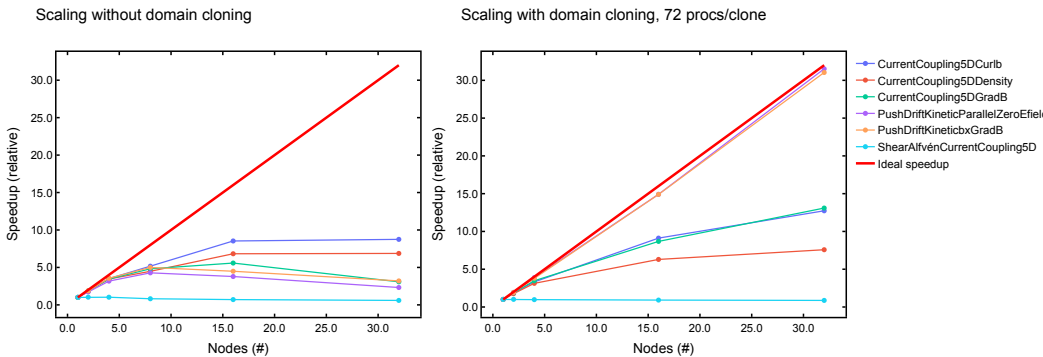
- `CurrentCoupling5DDensity`

Scaling with domain cloning, 72 procs/clone



Domain Cloning - `LinearMHDDriftkineticCC`



Conclusion: Particle propagators scale well using domain cloning.

Summary

- **Struphy**: Python-based, structure-preserving hybrid simulation framework for plasma physics.
- **Profiling**: Pylikwid integration provides detailed performance metrics, easily accessible for users.
- **Domain Cloning**: Enables scalable simulations of the particle propagators.
- **In progress**: Interface to PETSc

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

- 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:
  - Stefan Possander
  - Eric Sonnendrücker
  - Xin Wang