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FÜR PLASMAPHYSIK

Technical overview of the GENE-X code

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EUROfusion

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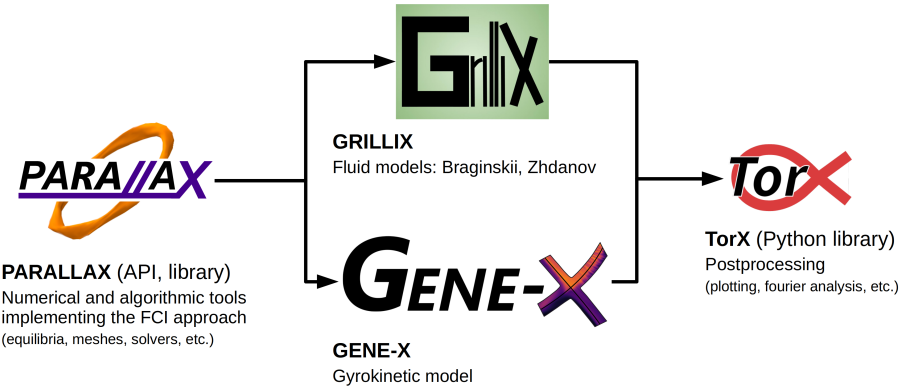
The PARALLAX Code Family

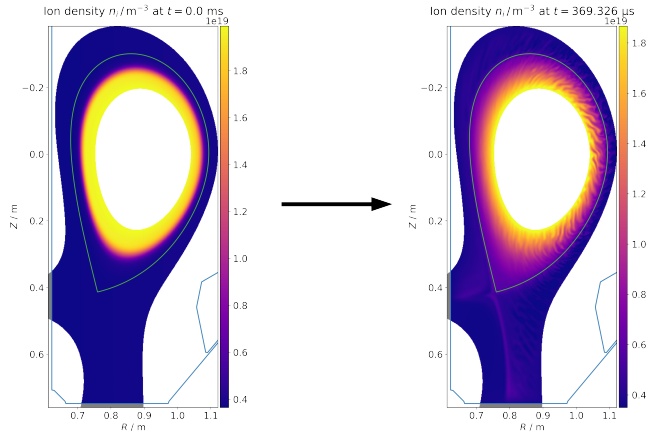


In a Nutshell

GENE-X is a gyrokinetic code to simulate plasma turbulence in **X-point geometries**.

Features:

- global
- non-linear
- full-f
- electromagnetic
- collisional



Equations solved by the code I

$$\frac{\partial f_\alpha}{\partial t} + v_{||}\frac{\mathbf{B}^*}{B^*_{||}}\cdot\nabla f_\alpha + \frac{c}{q_\alpha B^*_{||}}\mathbf{b}\times(\mu\nabla B + q_\alpha\nabla\phi_1)\cdot\nabla f_\alpha$$
$$- \frac{\mathbf{B}^*}{m_\alpha B^*_{||}}\cdot(\mu\nabla B + q_\alpha\nabla\phi_1)\frac{\partial f_\alpha}{\partial v_{||}} - \frac{q_\alpha}{m_\alpha c}\frac{\partial A_{1,||}}{\partial t}\frac{\partial f_\alpha}{\partial v_{||}} = C_\alpha(f_\alpha).$$

`timestep`
`operators/op_rhs_vlasov_static`
`operators/op_rhs_vlasov_dynamic`
`operators/collisions`

- $\alpha\ldots$ particle species. (electrons + ions)
- $v_{||}\ldots$ parallel velocity
- $\mu\ldots$ magnetic moment

Equations solved by the code II

$$-\nabla\cdot\left(\sum_\alpha \frac{m_\alpha c^2 n_{0,\alpha}}{B^2}\nabla_\perp\phi_1\right) = \sum_\alpha q_\alpha \int f_\alpha \,\mathrm{d}W,$$

$$-\Delta_\perp A_{1,||} = 4\pi\sum_\alpha \frac{q_\alpha}{c}\int v_{||} f_\alpha \,\mathrm{d}W,$$

$$-\left(\Delta_\perp + 4\pi\sum_\alpha \frac{q_\alpha^2}{m_\alpha c^2}\int v_{||}\frac{\partial f_\alpha}{\partial v_{||}}\,\mathrm{d}W\right)\frac{\partial A_{1,||}}{\partial t} = 4\pi\sum_\alpha \frac{q_\alpha}{c}\int v_{||}\left(\frac{\partial f_\alpha}{\partial t}\right)^\star \mathrm{d}W.$$

operators/field_solve_operators/op_solve_qn_eq

operators/op_mom_maxwells_eq

operators/field_solve_operators/op_solve_amps_law

operators/field_solve_operators/op_solve_ohms_law

operators/op_mom_ohms_law

Data structure

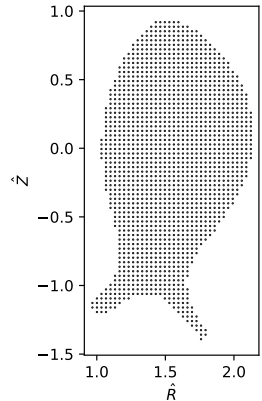
- The distribution function f_α is stored on a 5D+species grid $(RZ, \varphi, v_{||}, \mu, \alpha)$
- The electrostatic potential ϕ_1, parallel electromagnetic vector potential $A_{1,||}$ and parallel electric field $E_{1,||} = \partial A_{1,||}/\partial t$ are stored on a 3D grid (RZ, φ)
- Also moments (results of $\mathrm{d}W$ integrals) are 3D
- We have implemented types that contain this data + handle the pack/unpack to/from 1D for MPI exchange:
  `datastructures/data_storage_5d`
  `datastructures/data_storage_2d`
- All relevant data of the simulation is stored in `state_vector`
- All operations done on data are implemented in `operators`
- The state vector keeps its data encapsulated to prevent global access. Operators are applied via e.g. `state_vector%apply(op_rhs_vlasov_static)`

Dimensions

- RZ - Cartesian but unstructured 2D grid (see figure right)
- φ - angle dimension - uniform
- $v_{||}, \mu$ - velocity space - uniform 2D Cartesian
- α - species - parameter

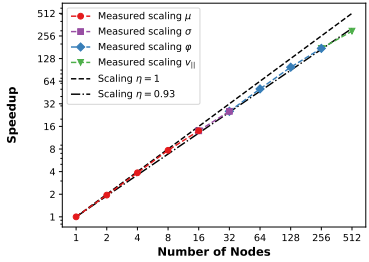
Conventions in the code:

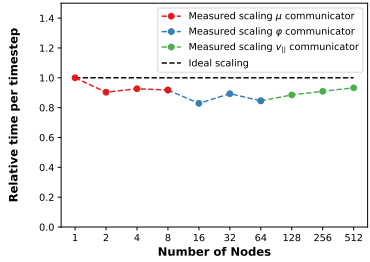
- Loop indices `i, k, l, m, n` for $RZ, \varphi, v_{||}, \mu, \alpha$
- `lb` and `ub` - 5D arrays with lower and upper bound - **with MPI ghosts**
- `lb_stripped` and `ub_stripped` - 5D arrays with lower and upper bound - **no MPI ghosts**



Parallelization

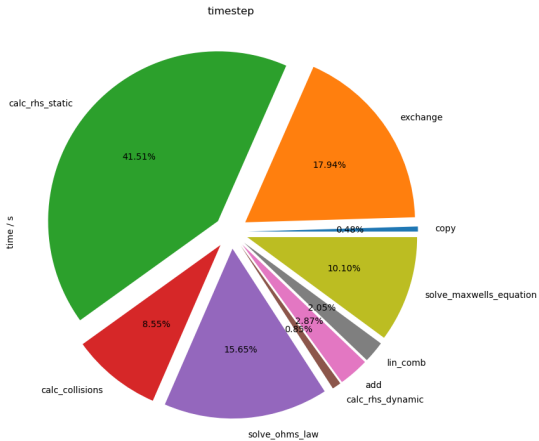
- Hybrid MPI+OMP. MPI in $\varphi, v_{||}, \mu, \alpha$. OMP in RZ
- Typical problem size approx. $(RZ, \varphi, v_{||}, \mu, \alpha)$ = $(200000, 32, 80, 20, 2)$
- Latest production runs on Raven supercomputer (MPCDF)
  320 nodes - 72 cores. 640 MPI procs, 36 cores for OMP.
  MPI decomposition e.g. $(RZ, \varphi, v_{||}, \mu, \alpha)$ = $(1, 16, 2, 10, 2)$.
- Good strong (left) + weak (right) scaling





Performance

Example for recent production run with $(RZ, \varphi, v_{||}, \mu, \alpha) = (200000, 32, 80, 20, 2)$



Wall-clock time: approx 2.6 s
(configuration given on last slide)

Intensity ranking:

1. `op_rhs_vlasov_static`
2. `field_solve_operators`
3. MPI `exchange`
4. `collisions`

Interface to PARALLAX

- `mesh/mesh_5d` contains all calls to PARALLAX library routines
- Important tasks: create equilibrium (magnetic field), create 2D RZ mesh (with multigrid), create elliptic solver (mGMRES)
- PARALLAX has 3 types of points: inner + boundary + ghost
- Currently GENE-X has 2 types: inner + ghost (contains PARALLAX boundary)
- Currently **no** MPI decomposition in RZ

Re-ordering of the unstructured mesh

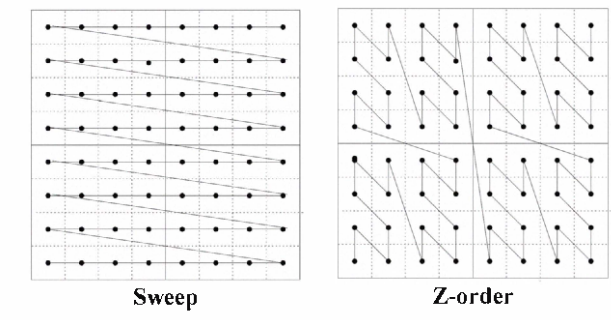
- Implemented in PARALLAX

```
call this%multigrid_3d(k)%init(..., reorder_size=X)
```

- However, we use `X=0` - **no** reordering so far
- Reordering would change the order of inner + boundary + ghost points

What is reorder?

https://en.wikipedia.org/wiki/Z-order_curve



May increase performance for stencil heavy operations.

Why reorder?

- Performance limited by memory access - bottleneck `op_rhs_vlasov_static`
- Finite difference stencils in RZ - because dimension is unstructured, neighbor search is needed
- Finite difference stencils in φ require CSR matrix-vector dot product - involves stencil in RZ due to interpolation
- Effect of reordering on PARALLAX elliptic solvers expected (may dig out details)
- Question: do all code parts **profit** from reordering?

Code Infrastructure

- Program for code benchmarks of individual operators is available `benchmarks/benchmark_operators` (field solvers not included so far)
- Workflow: protected master on Gitlab - branch out for new feature, merge request ASAP when ready to avoid conflicts (CI/CD)
- Unit tests are performed automatically when pushing to Gitlab. These may take a while due to the slurm queue. Best run tests manually before pushing to identify errors earlier
- New functions, subroutines require new tests if not covered by existing tests or if isolated feature
- Code review before merge to double check bugs
- PARALLAX coding standards available

Open questions: Code access? Runners for unit tests?

Summary

Current Status

- Bottleneck is memory access
- `op_rhs_vlasov_static` is most intense part of the code
- RZ dimension is unstructured
- Morton Z-reordering implemented in PARALLAX for RZ dimension
- Benchmark program for individual code parts available

Contact

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Todos

- Main goal: performance optimization of `op_rhs_vlasov_static`
- Enable reordering by fixing handling of boundary/ghost cells
- Identify other changes needed to enable reorder
- Benchmark effect on `op_rhs_vlasov_static` and other code parts (maybe add field solver benchmark?)