Rensselaer Polytechnic Institute
Scientific Computation
Research Center

PCMS: A Geometry and Discretization Aware Multi-physics Coupling Tool for Fusion Devices

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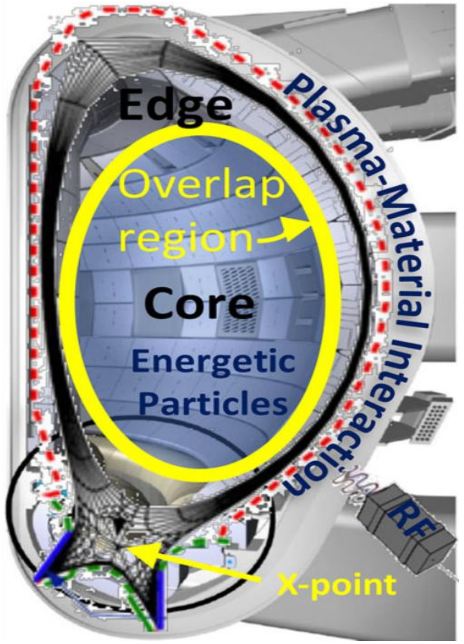
Motivation



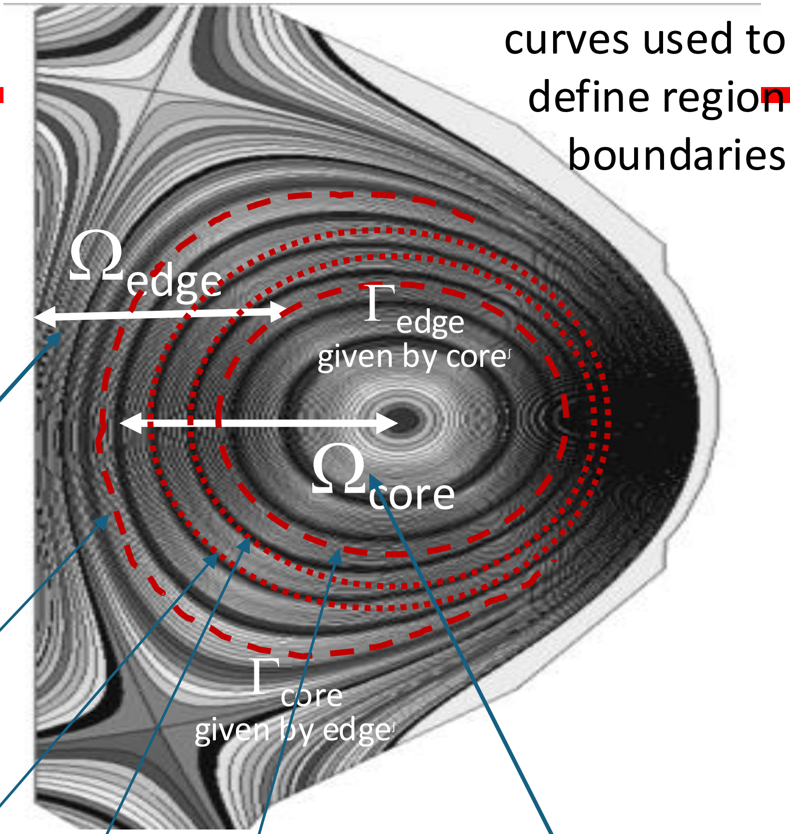
Range of Computational Methods Necessary For Understanding Physics and Pilot Plant Design

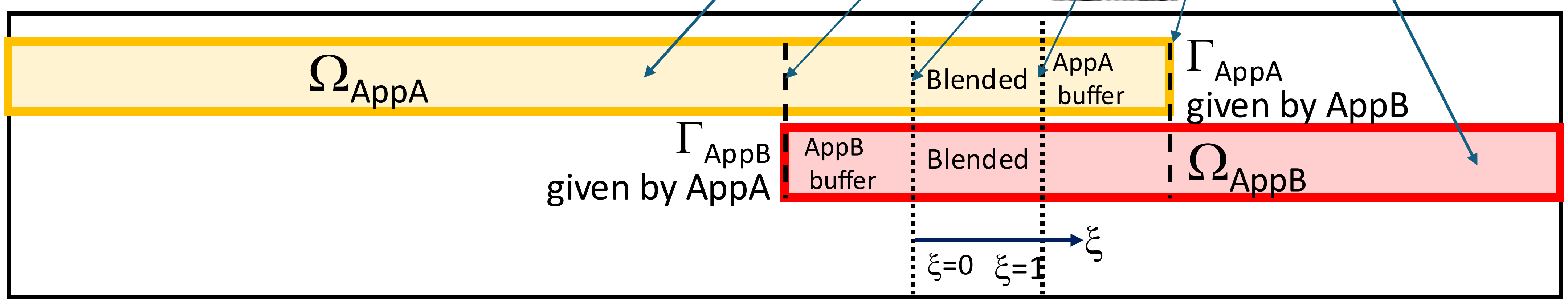
- Plasma facing materials:
  - Molecular dynamics (material evolution)
  - Finite element (heat transfer, structural design)
  - Kinetic Monte Carlo (wall interactions)
- Plasmas (solve Boltzmann and Maxwell's equations):
  - Particle-in-cell: often 5D gyrokinetic
  - Continuum: often magnetohydrodynamics, or 5D gyrokinetic
- Etc.

How can we leverage decades of specialized physics code development to analyze coupled phenomena across engineering and physics simulations for whole device and plant models?

Concurrent Coupling

- Each application solves its model(s) over a portion of the domain.
- The domains overlap: The overlap can include three subregions
  - The blended region in which the fields are coupled based on a field blending strategy
  - A buffer region for Application A (edge) in which the “right” end boundary conditions are determined by Application B (core) and/or source terms added
  - A buffer region for Application B (core) in which the “left” end boundary conditions are determined by Application A (edge) and/or source terms added





Fusion Coupling Has Many Challenges

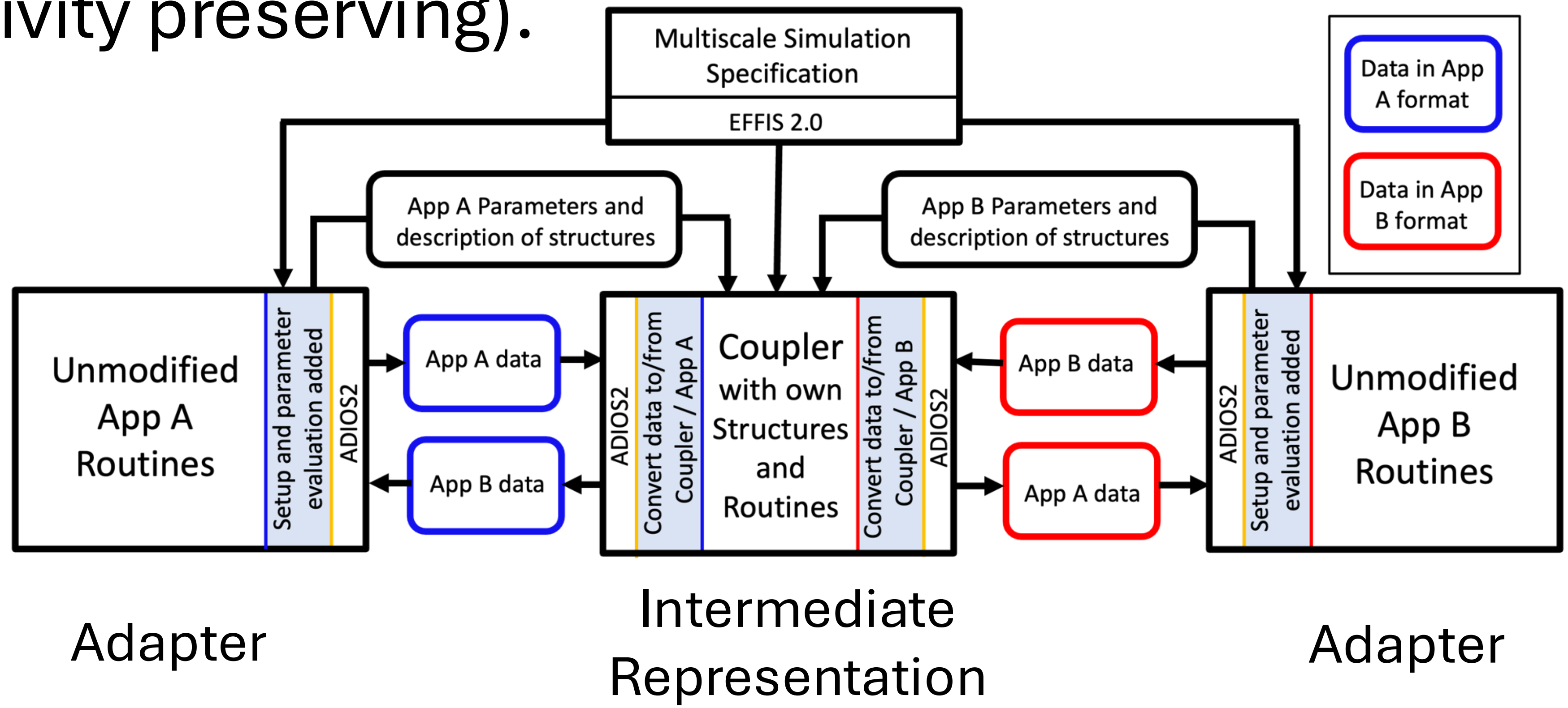
- Multitude of field following and radial coordinate systems.
- Field data stored in application dependent combinations of real and Fourier space.
- Both structured and unstructured meshes.
- Field data distributed with varying partitioning schemes and distributed data structures.
- Must run on exascale supercomputers.

Generalized Coupler Requirements

- Do not modify existing data structures or algorithms.
- Make effective use of exascale computing systems.
- Efficiently handle data and coordinate transformations.
- Perform efficient operations with structured and unstructured meshes.
- Handle parallel coordination and communication of distributed field data.

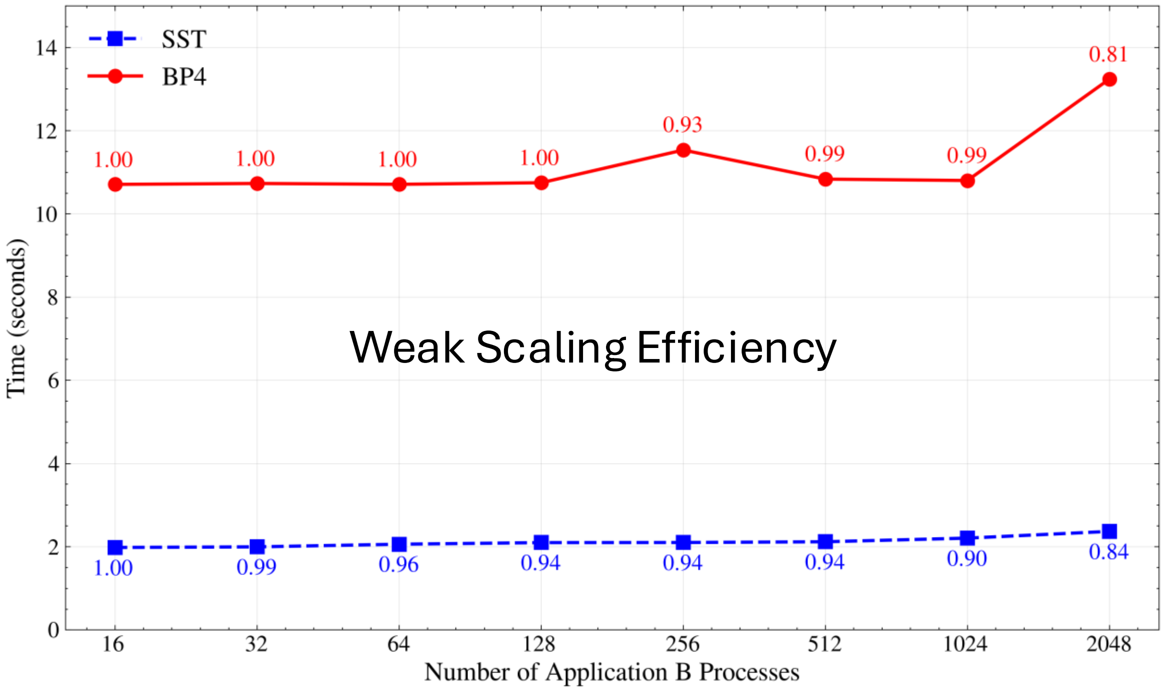
Parallel Coupler for Multimodel Simulations

1. Distributed Control: scalably handle sending data between partitioned simulations.
2. Physics Preserving Field Mapping: map between fields accounting for physics constraints (e.g., conservation, div. free, positivity preserving).

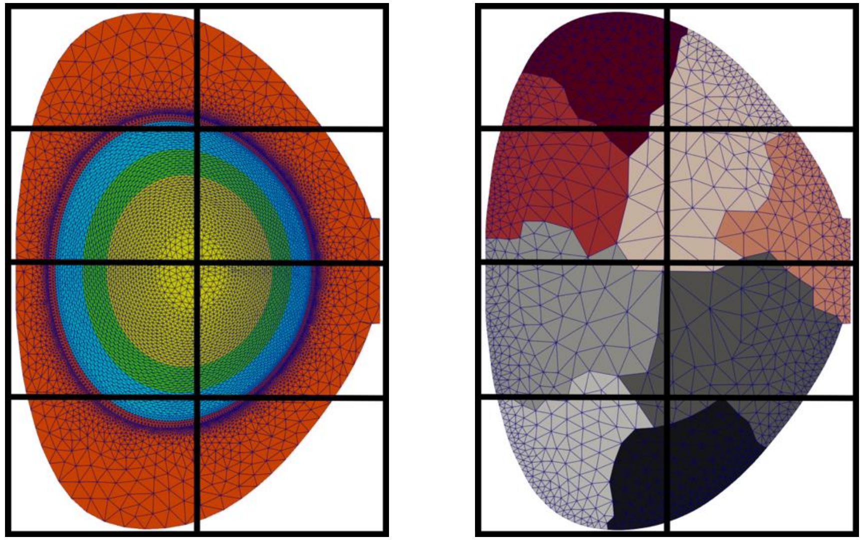


Distributed Control of Unstructured Field Information

- Use a third "trivial" partition to coordinate data transfers between the applications.
- Coupling demonstrated weak scaling on Frontier.



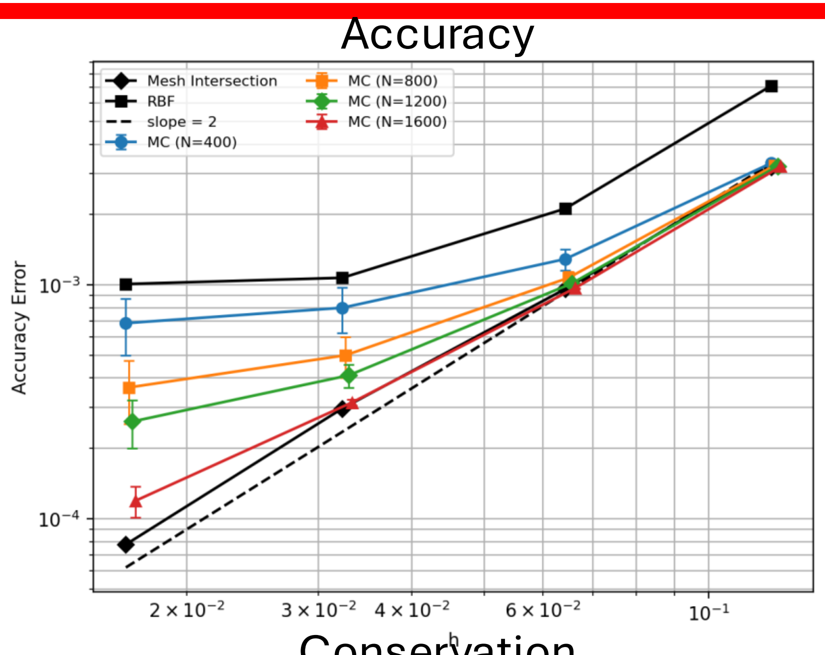
PCMS weak scaling on up to 260 nodes (256 nodes for application B and two nodes each for the coupler and application A)

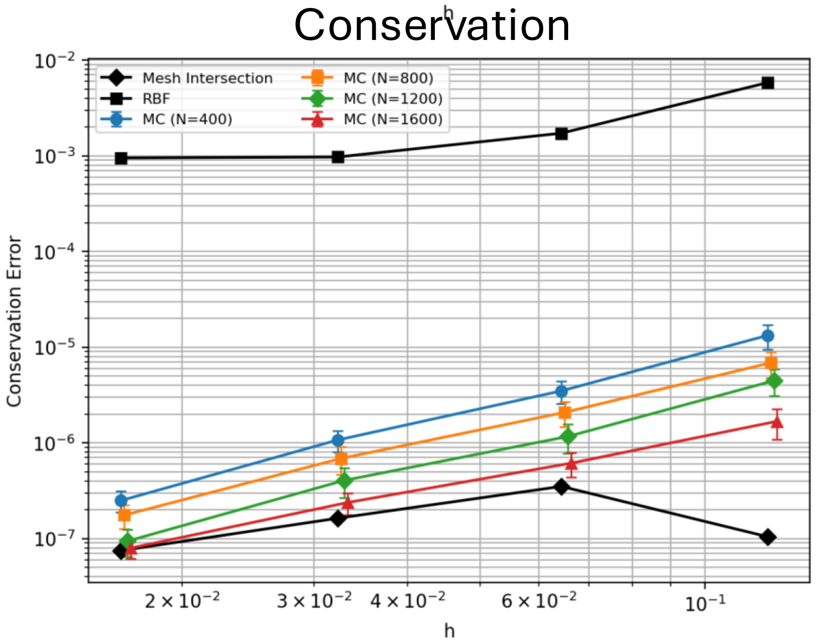


Unstructured mesh colored by its graph partition to eight processes (left). Field-following mesh colored by its classification-based partition to four processes (right). Each mesh is overlaid with a rendezvous partition (black grid)

GPU Accelerated Field Mapping Methods

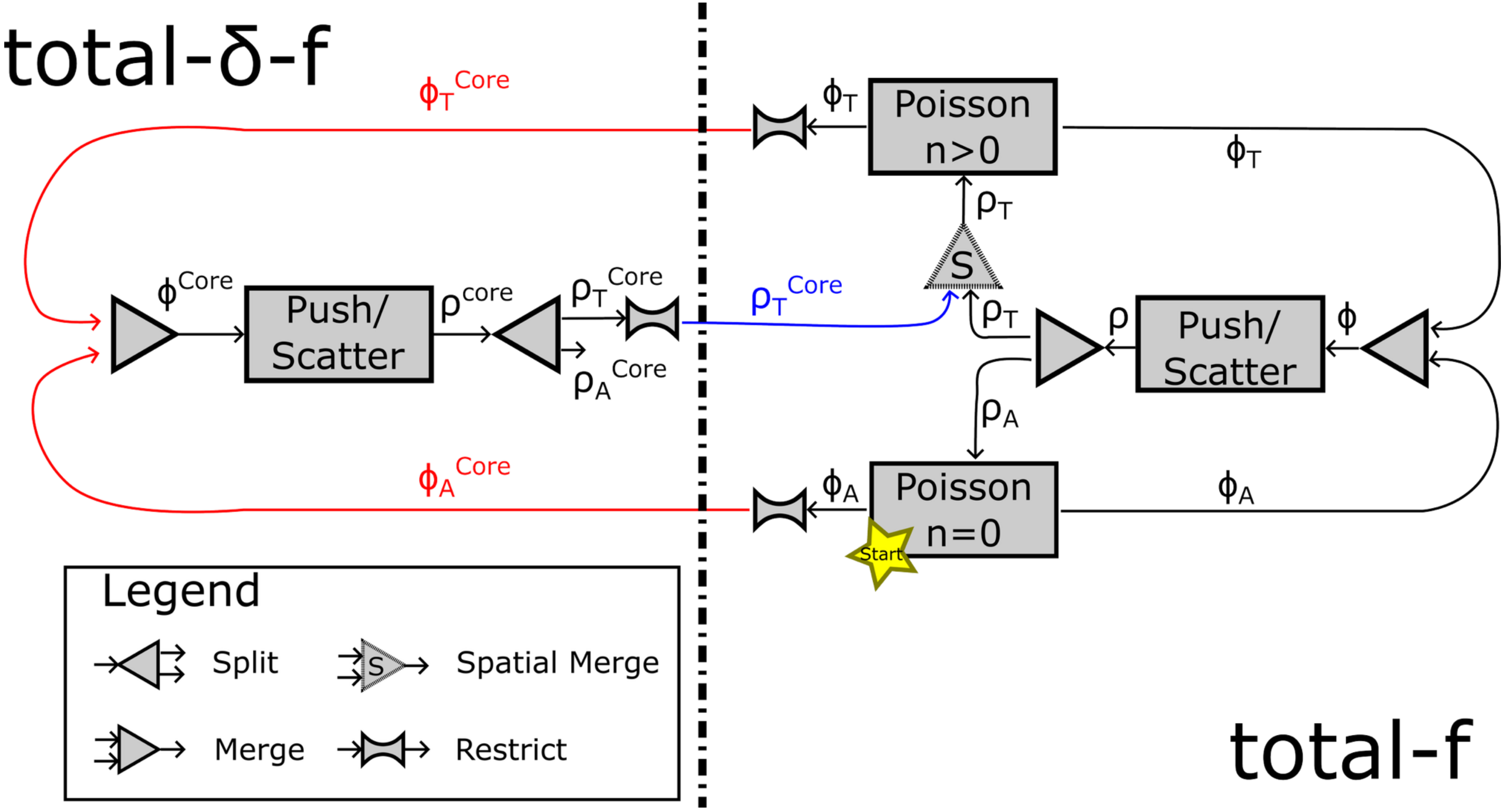
- Conservative mesh intersection methods:
  - Uses full details of discretization and shape function definitions
  - Provides highest quality field transfer, requires less parameter tuning
  - Challenging to extend to high-dimensions
- Conservative Monte Carlo methods:
  - Provides fully conservative transfer without requiring source discretization or shape function definitions (only requires fields can be evaluated)
  - Extensible to high-dimensions
- Local Weighted Polynomial Fitting (RBF/SPR):
  - Extensible to high-dimensions (demonstrated)
  - Treats all target points independently
  - Not conservative
- Acceleration structures for point localization
- Coordinate transformations





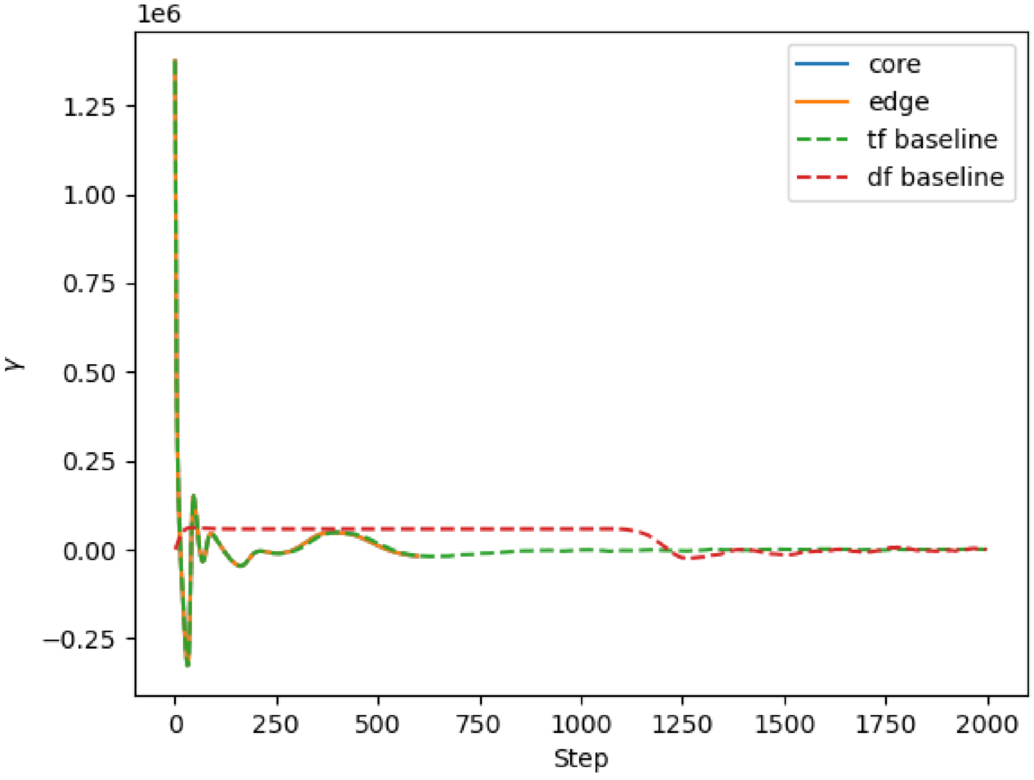
Core-Edge Integrated Gyrokinetic PIC Simulations

Electrostatic, adiabatic electron, no collisions

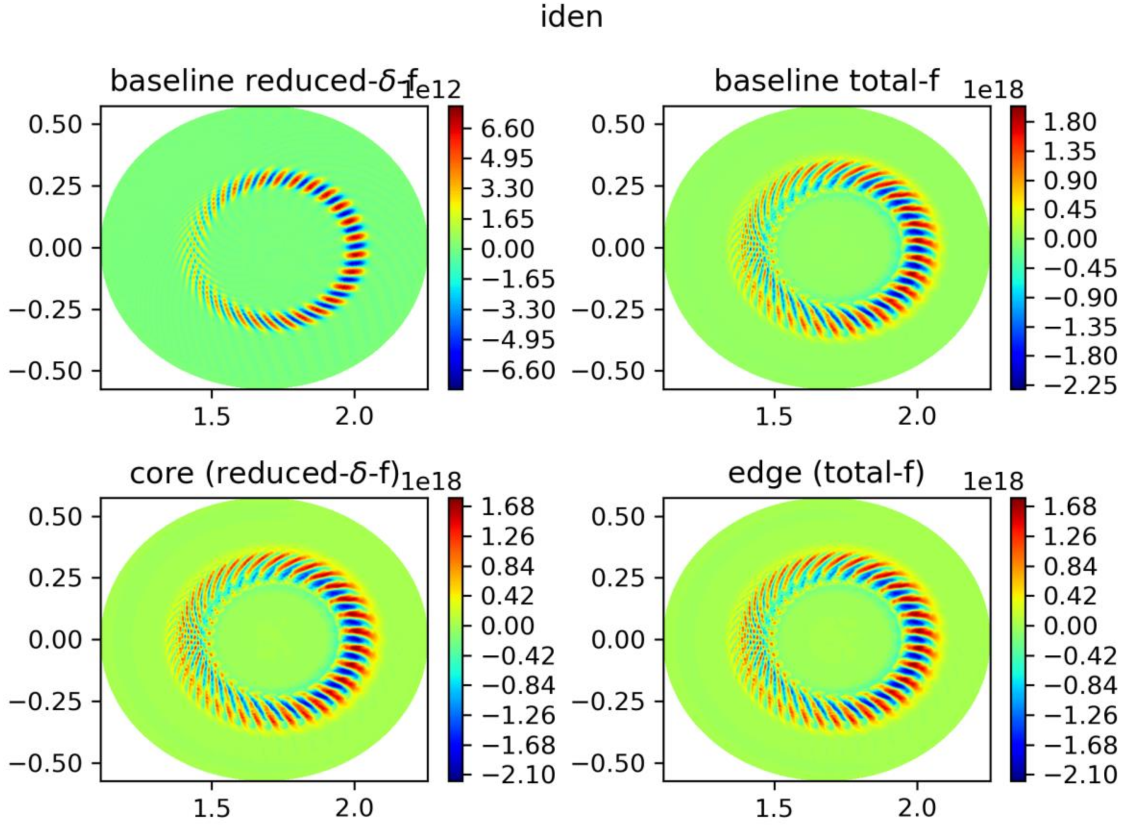


Core-Edge Integrated Gyrokinetic PIC Simulations

Turbulence Growth Rate



Ion Density, step 600



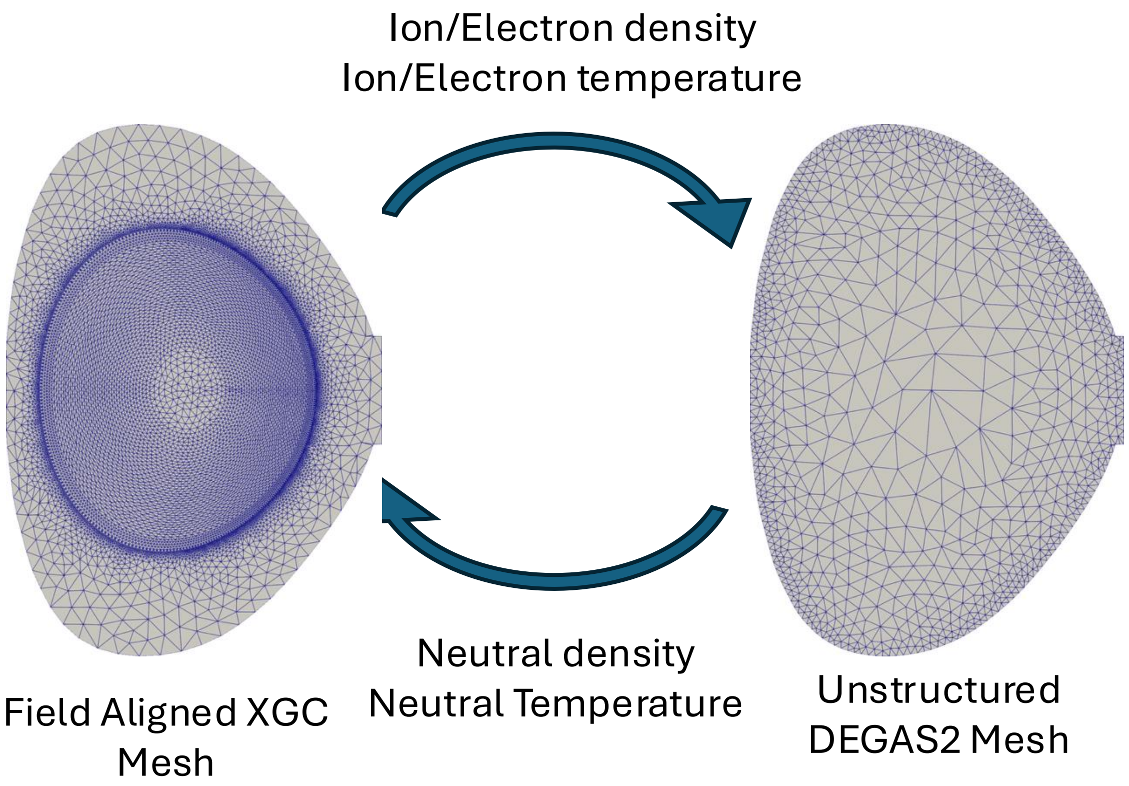
Ion density field on cyclone ITG

Coupled Neutral Particles and Gyrokinetic Plasmas

- Atomic and molecular neutral particle reactions represent key sources and sinks in plasma.
- Want to couple Monte Carlo neutral code with gyrokinetic plasma code to evolve the neutral distribution function along with charged particles.

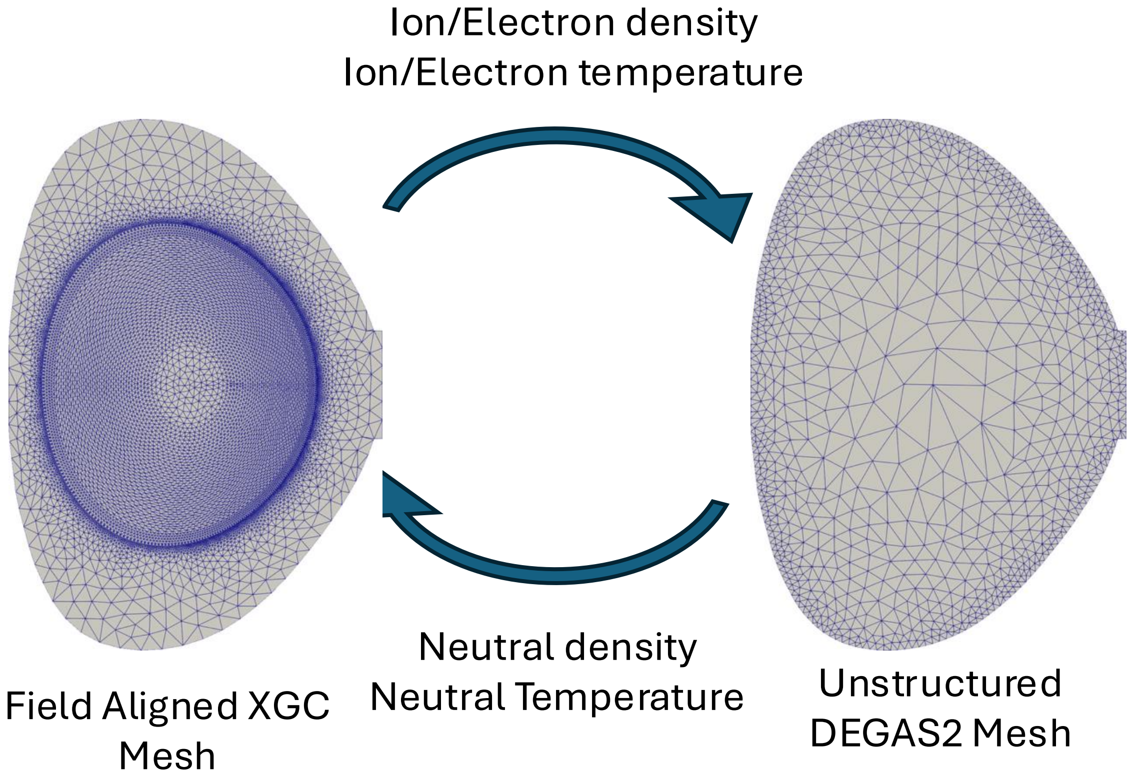
Key Challenge:

- Appropriate discretizations for plasmas and neutrals are very different
  - XGC uses a field-aligned unstructured mesh.
  - Degas2 does not require field alignment, want to have large elements in core



Coupling Setup

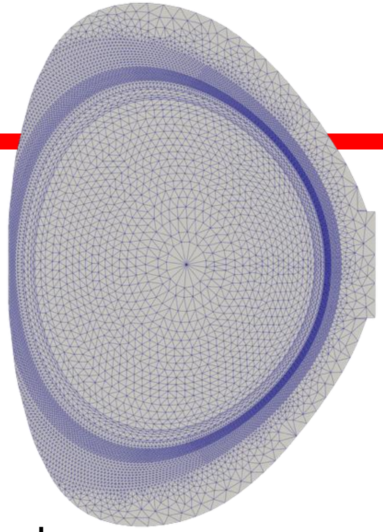
- LTX geometry
- Total-f XGC simulation
- Couple every 10 XGC timesteps
- Degas2 evolves neutral particles



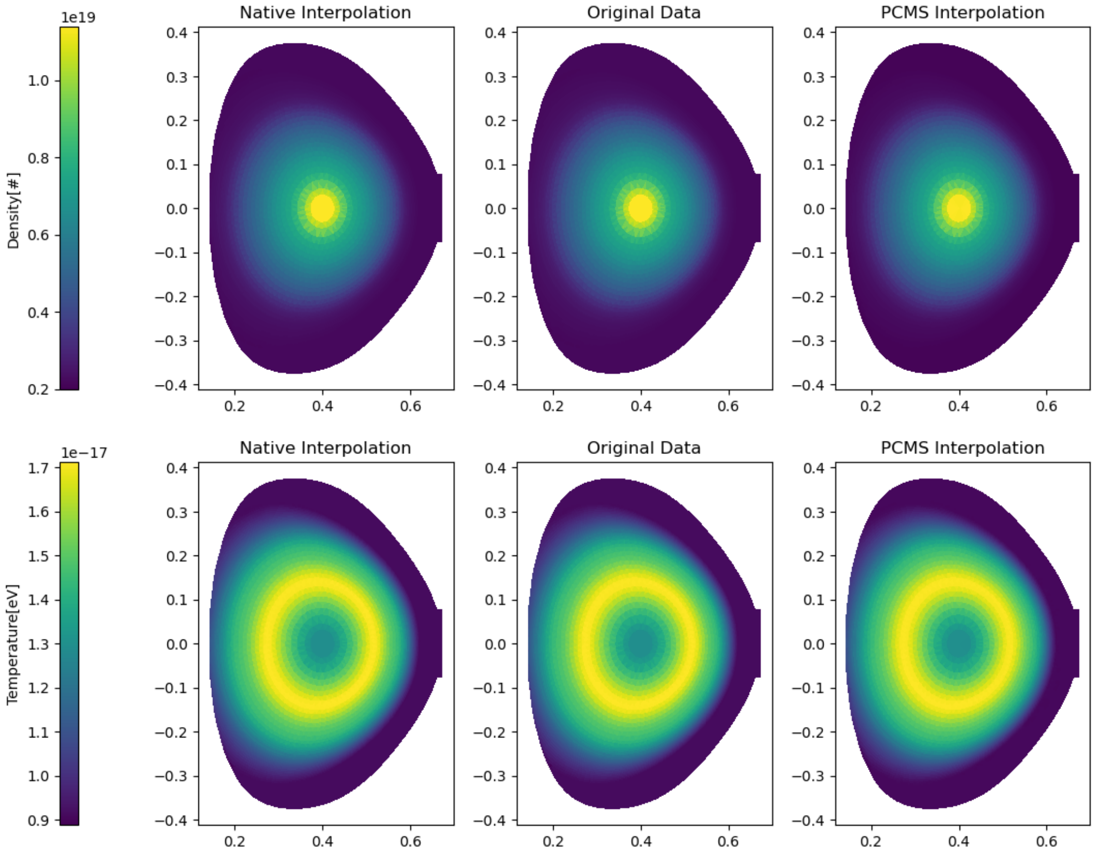
Verification: Same Mesh

- Compare nodal averaging to PCMS-based interpolation with same mesh.

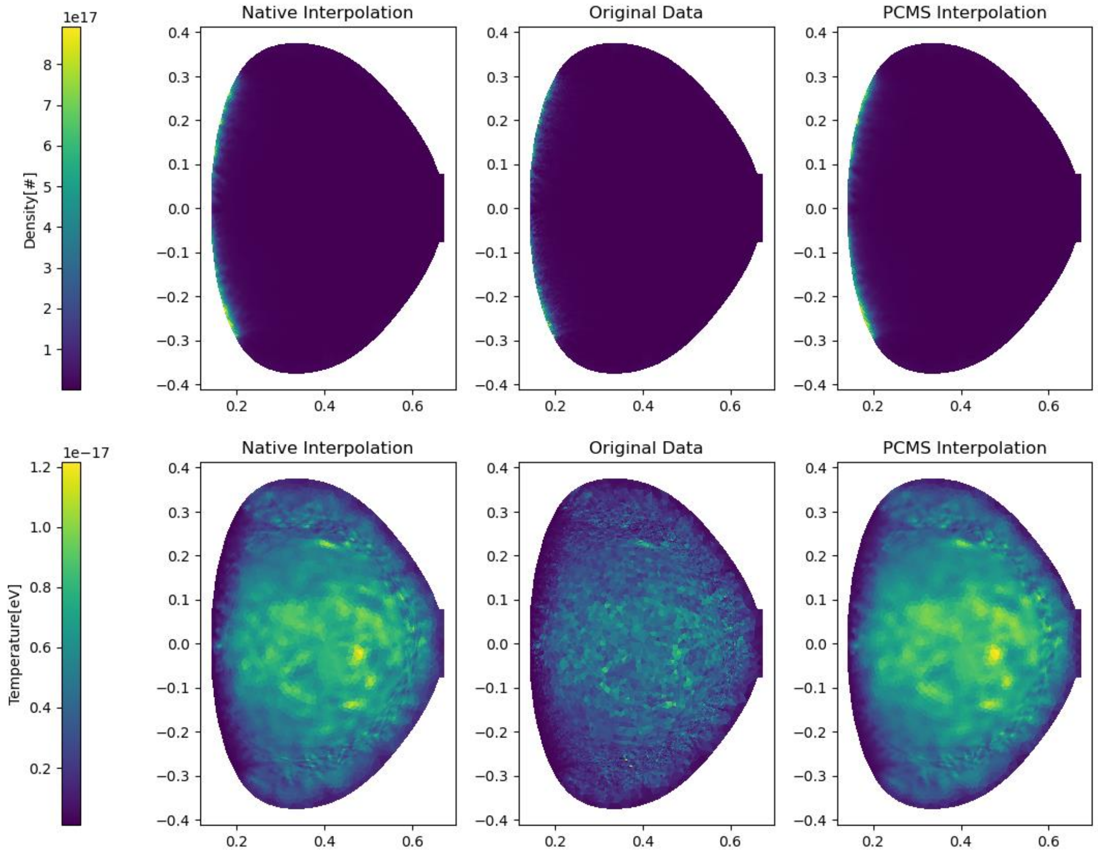
19,215 Elements
9,703 Vertices



Ions



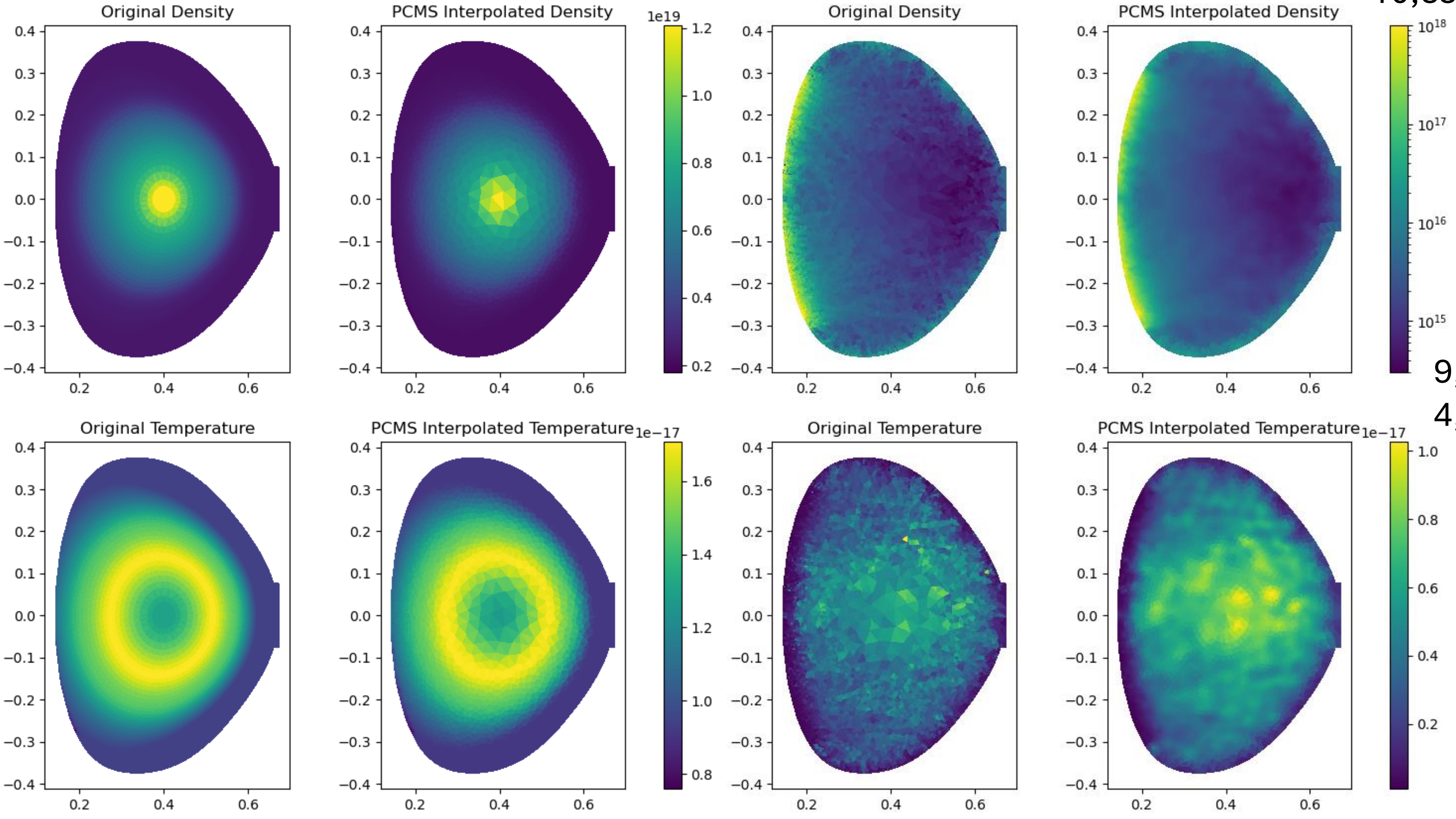
Neutrals



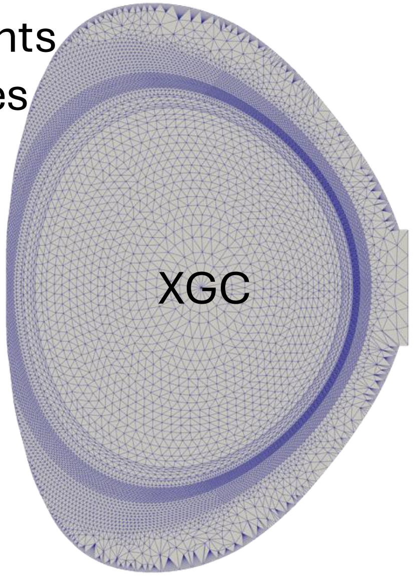
Different Mesh Comparison

Ions

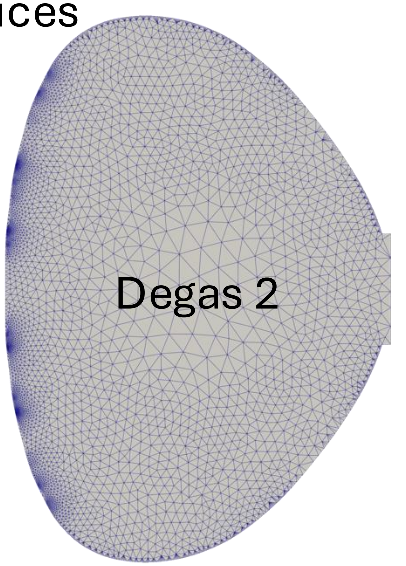
Neutrals



19,842 Elements
10,334 Vertices



9,104 Elements
4,966 Vertices

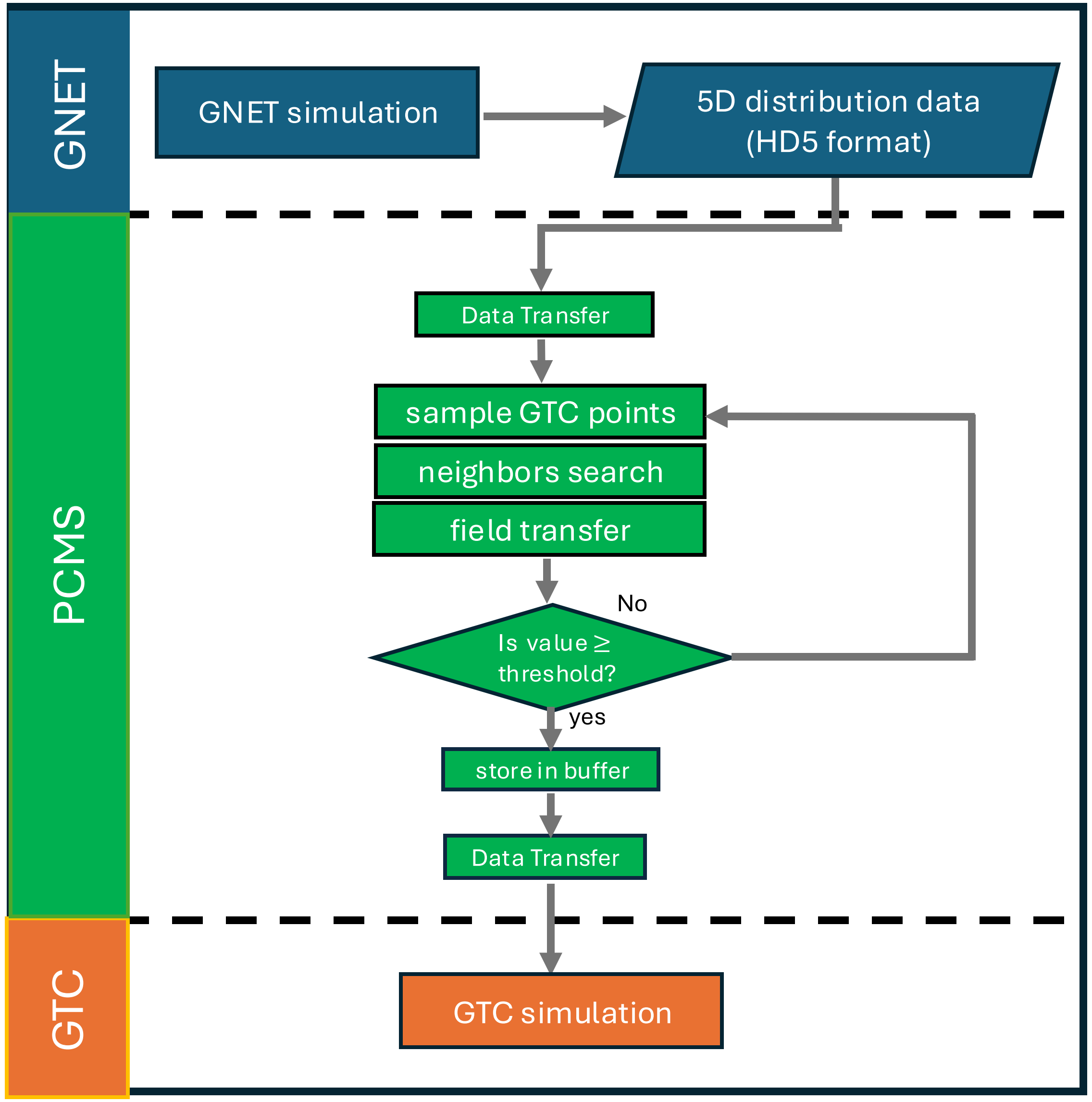


Distribution Function Coupling of Energetic Particles and Plasmas

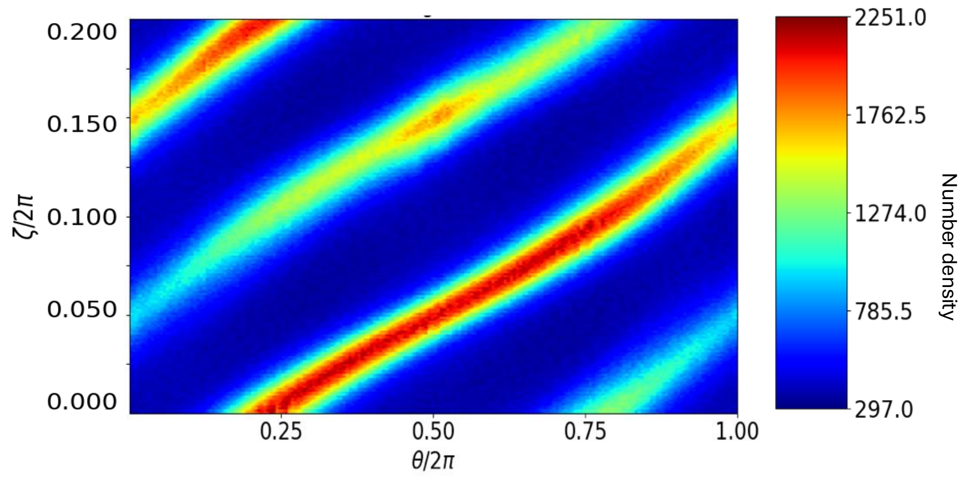
- GNET models fast ions using $[\rho, \theta, \zeta, E, p]$ as coordinates
- GTC used for gyrokinetic plasma microturbulence using : $[\psi,\ \theta,\ \zeta,\ v_{||}, \mu]$ as coordinates
- GNET and GTC are coupled through the 5D distribution function

Key Challenge:

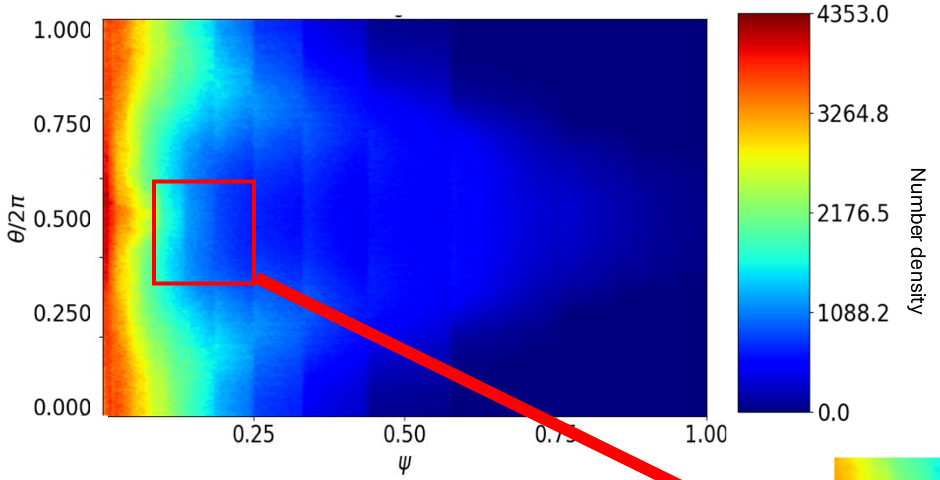
- Coupling requires (moment preserving) transfer of 5D fields



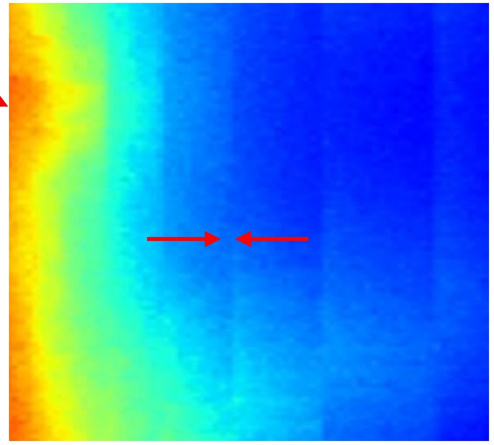
Results: Initial Approach

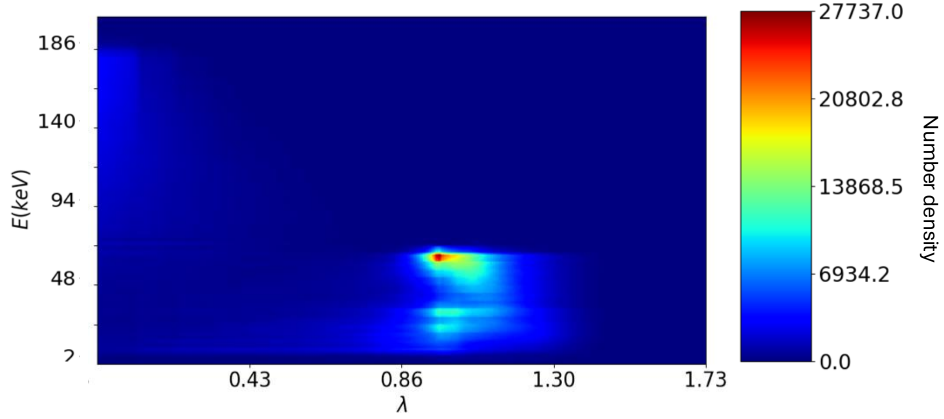


$\zeta - \theta$ plane

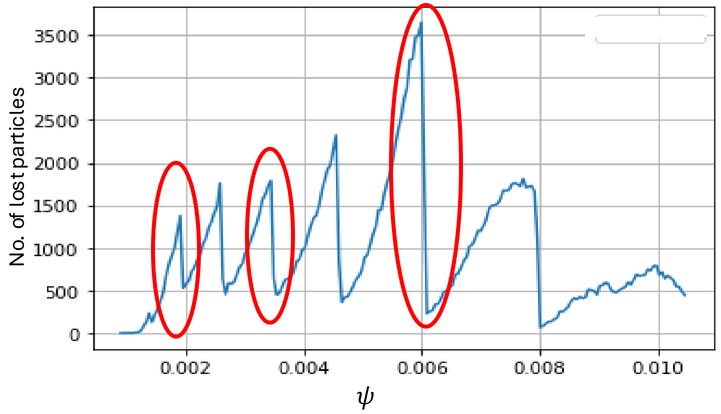


$\theta - \psi$ plane



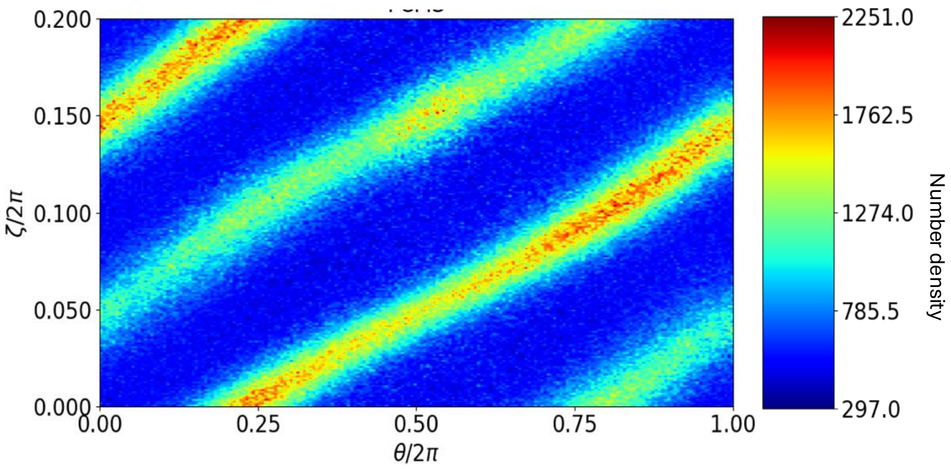


$\mathrm{E} - \lambda$ plane

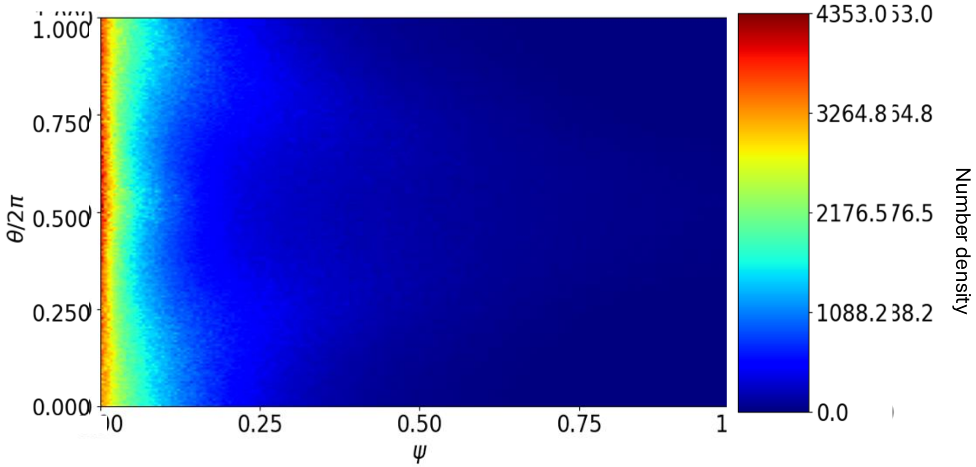


No. of lost particles vs ψ

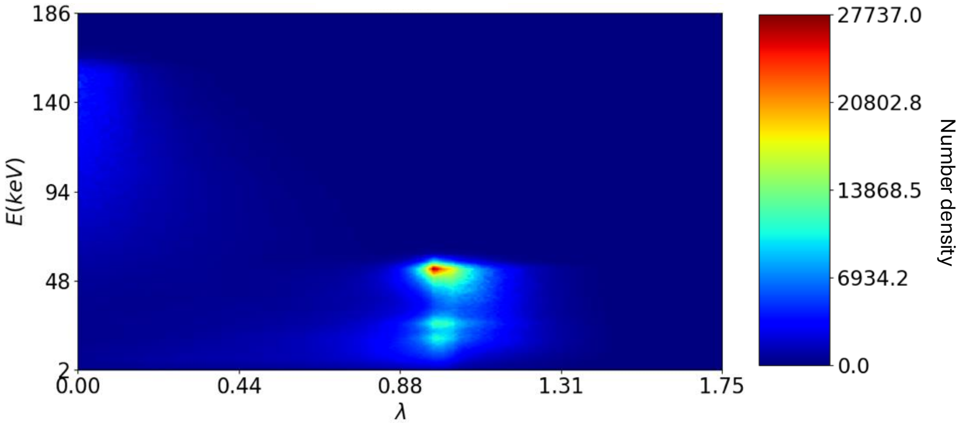
Results: Our Approach



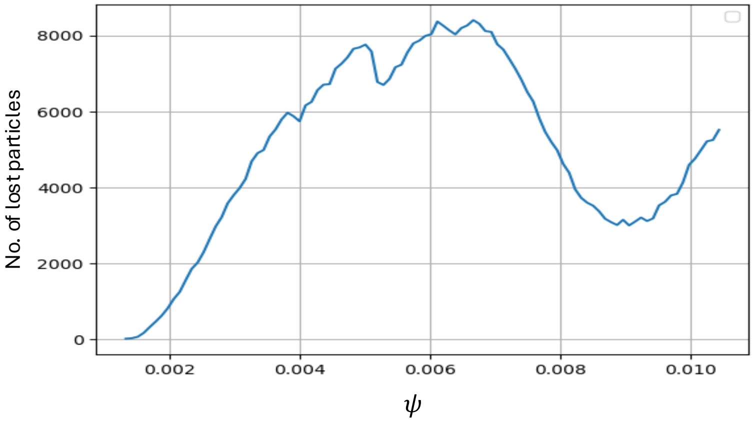
$\zeta - \theta$ plane



$\theta - \psi$ plane



$\mathrm{E} - \lambda$ plane



No. of lost particles vs ψ

Summary

- PCMS provides capabilities to make tight coupling of fusion simulations easier.
  - Effective field and coordinate transformations for fusion codes
  - Handle wide range of distributed fields

- **Future Work**
  - Integration with SUNDIALS for automatic stable coupling timestep selection (using SUNDIALS)
  - Support for linking physics models to AI/ML tensors
  - Lifting operators for mapping low-dimensional fields to higher-dimensional fields (e.g., axisymmetric solve to 3D)

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