Lawrence Livermore National Laboratory

High-Order, Finite Volume Discretization of Gyrokinetic Vlasov-Poisson Systems on Mapped Grids

Applied Mathematics Principal Investigators Meeting

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We are developing advanced numerical methods for the kinetic simulation of fusion edge plasmas

Motivating Office of Science application:
Simulation of tokamak edge plasmas

- Prediction of edge turbulence is essential for understanding phenomena governing plasma confinement
- Simulation of edge turbulence requires kinetic models
- Kinetic models have been successfully used for core simulation for several years (GS2, GENE, GYRO), but the solution of edge models presents different algorithmic challenges
- A collaboration between ASCR and OFES has been established to create a continuum edge code

Goal of this AMR project: Develop the numerical algorithms needed to solve kinetic edge equations

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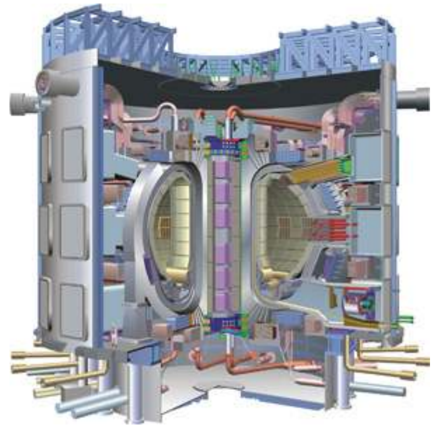
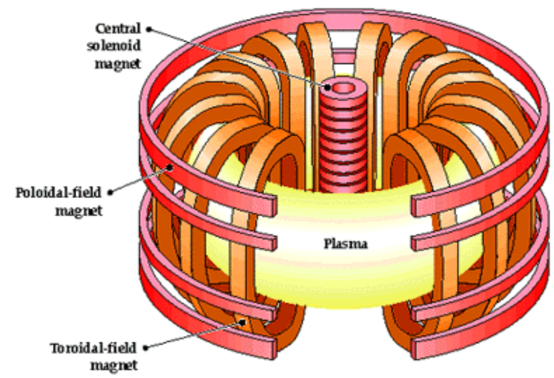




A gyrokinetic turbulence model can be developed as a nonlinear conservation law in a special coordinate system

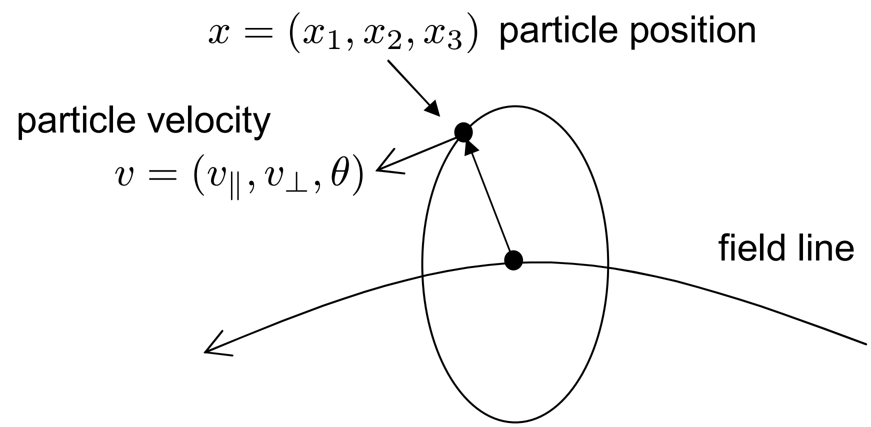
Gyrokinetic turbulence models predict particle distributions f(x,v) by neglecting the phase and frequency of the particle gyromotion about field lines.

Reduces the number of independent variables from 6 to 5 (plus time).

Accomplished by solving in an asymptotically constructed coordinate system, not just by "averaging out" the gyrophase θ

Gyrocenter coordinates:

- Distribution functions are symmetric in gyrophase
- Magnetic moment $\mu = mv_\perp^2/2B$ is a constant of the motion



Vlasov:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{\boldsymbol{R}}\boldsymbol{\nabla}_{\boldsymbol{R}} f + \dot{v}_\parallel \frac{\partial}{\partial v_\parallel} f = 0$$

Liouville theorem:

$$\boldsymbol{\nabla}_{\boldsymbol{R}} \cdot \left(\dot{\boldsymbol{R}} B_\parallel^*\right) + \frac{\partial}{\partial v_\parallel}\left(\dot{v}_\parallel B_\parallel^*\right) = 0$$

Conservative Vlasov:

$$\frac{\partial (B_\parallel^* f)}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{R}} \cdot \left(\dot{\boldsymbol{R}} B_\parallel^* f\right) + \frac{\partial}{\partial v_\parallel}\left(\dot{v}_\parallel B_\parallel^* f\right) = 0$$

The gyrokinetic system is closed by the evaluation of the phase space velocities and the solution of a modified Poisson equation

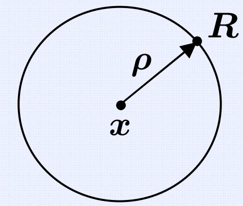
The ion contribution to the charge density in the gyrokinetic Poisson equation is comprised of two parts:

$$\epsilon_0 \nabla^2 \Phi(\boldsymbol{x}) = e\left[n_e(\boldsymbol{x}) - Z_i\left(\bar{n}_i(\boldsymbol{x}) + \widetilde{n}_i(\boldsymbol{x})\right)\right]$$

- Gyrocenter density (gyrophase independent)

$$\bar{n}_i(\boldsymbol{x}) = \int f_i(\boldsymbol{R}, v_\parallel, \mu, t)\,\delta(\boldsymbol{R} - \boldsymbol{x} + \boldsymbol{\rho})\,B_\parallel^\star\, d\boldsymbol{R}\,dv_\parallel\,d\mu\,d\theta$$

- Polarization density (gyrophase dependent) $\widetilde{n}_i(\boldsymbol{x})$



Key parameter:

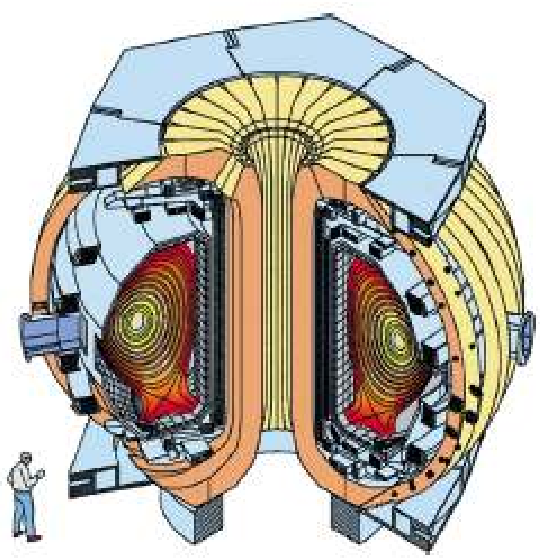
$k_\perp \rho$

= number of perpendicular wavelengths per gyroradius

In the long wavelength limit $k_\perp \rho \ll 1$ the gyrokinetic Poisson equation is

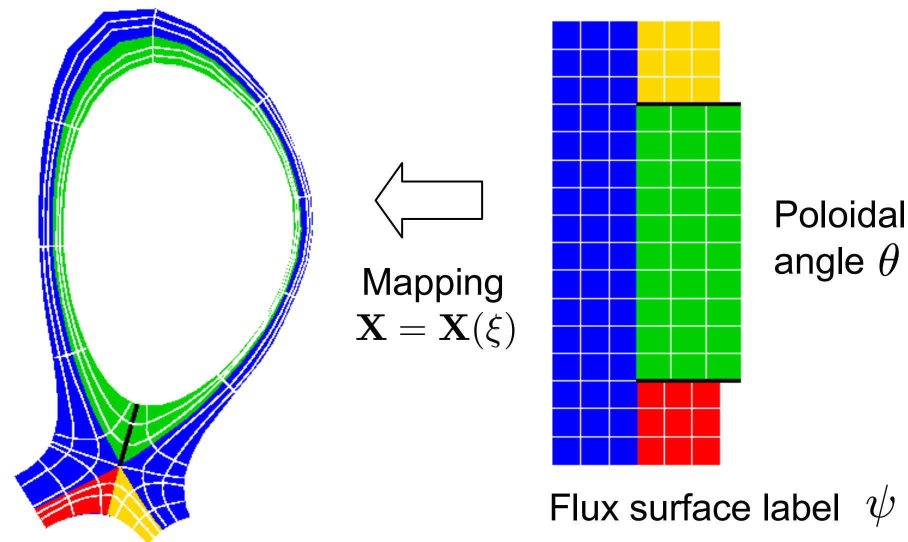
$$\boldsymbol{\nabla} \cdot \left\{\left[\epsilon_0 \boldsymbol{I} + \frac{\bar{n}_i}{B^2}\left(\boldsymbol{I} - \vec{\boldsymbol{b}}\vec{\boldsymbol{b}}^T\right)\right]\boldsymbol{\nabla}\Phi\right\} = n_e - Z_i \bar{n}_i, \qquad \vec{B} = B\vec{b}$$

The magnetic field defines a multiblock coordinate system in tokamak edge geometries



- The equilibrium magnetic field determines a mapping from physical to computational coordinates
- Resulting alignment with flux surfaces facilitates accommodation of strong anisotropies in discretization

In 2D: A poloidal slice of the plasma edge can be mapped to a multiblock, locally rectangular grid



Physical coordinates: $\mathbf{X}$

Computational coordinates: $\xi = (\psi, \theta)$

In 3D: A toroidal component is added

We are pursuing a comprehensive approach to the development of algorithms addressing multiple requirements

Requirements:

- Conservation
- Low-dissipation advection
- Preservation of distribution function positivity
- Efficient resolution of a large phase space
- Robust for high anisotropy
- Efficient implicit solves

Numerical methodologies:

- Finite volume discretizations applied to conservative formulations of hyperbolic and elliptic operators
- High-order discretization
- Limiters
- Mapped, multiblock grids
- Preconditioned iterative methods

We have developed a systematic strategy for 4th-order finite volume discretization on mapped grids

Cartesian computational grid control volumes:

$$V_{\mathbf{i}} = [(\mathbf{i} - \frac{1}{2}\mathbf{u})h, (\mathbf{i} + \frac{1}{2}\mathbf{u})h] \ , \ \mathbf{i} \in \mathbf{Z}^D \ , \ \mathbf{u} = (1, 1, \dots, 1)$$

Smooth mapping to physical coordinates:

$$\mathbf{X} = \mathbf{X}(\xi) \ , \ \mathbf{X} : [0,1]^D \rightarrow \mathbf{R}^D$$

$$\int_{X(V_{\mathbf{i}})} \nabla_{\mathbf{x}} \cdot \vec{F} d\mathbf{x} = \sum_{\pm = +,-} \sum_{d=1}^{D} \pm \int_{A_d} (\mathbf{N}^T \vec{F})_d dA_\xi$$

where $\mathbf{N}_{p,q} \equiv det((\nabla_\xi \mathbf{X})(p|\mathbf{e}^q))$, in which $A(p|v)$ denotes the matrix obtained by replacing the p^{th} row of the matrix A by the vector v.

Key elements: The average of products is obtained by the repeated application of

$$\langle fg \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \langle f \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \langle g \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{12} G_0^{\perp,d} \left(\langle f \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \right) \cdot G_0^{\perp,d} \left(\langle g \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \right) + O(h^4).$$

where $G_0^{\perp,d} =$ second-order accurate centered difference of $\nabla_\xi - \mathbf{e}^d \frac{\partial}{\partial \xi_d}$ and $\langle q \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = \frac{1}{h^{D-1}} \int_{A_d} q(\xi) dA_\xi + O(h^4)$

and fourth-order averages are computed using face-centered pointwise values via

$$\langle f \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} = f_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{24} \sum_{d' \neq d} \frac{\partial^2 f}{\partial \xi_{d'}^2} |_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + O(h^4).$$

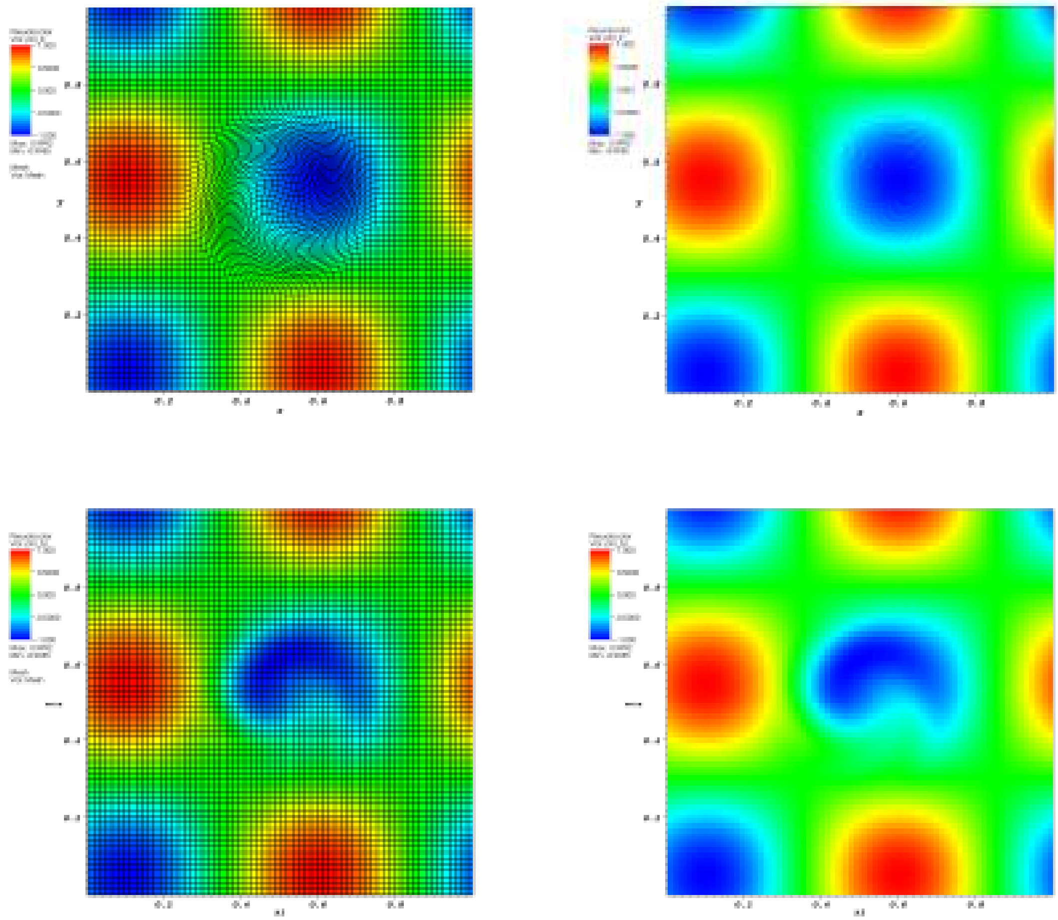
- Use to compute the face averages $\left\langle \mathbf{N}^T \vec{F} \right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^\mathbf{d}}$
- Use Poincaré Lemma to derive high-order estimates of $\left\langle \mathbf{N}^T \right\rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^\mathbf{d}}$ such that the cell-averaged $\nabla_{\mathbf{x}} \cdot \vec{F} = 0$ for constant $\vec{F}$

Application of the mapped grid finite volume discretization to an advection test problem

Physical coordinates

MappedAdvect.mov

Computational coordinates



Example mesh from D. Calhoun and R. LeVeque, Proceedings of the Chicago Workshop on Adaptive Mesh Refinement Methods, 2003.

We are developing high-resolution discretizations for the gyrokinetic Vlasov equation

- The gyrokinetic Vlasov equation describes advection by a phase space velocity field that is a nonlocal function of the distribution function f :

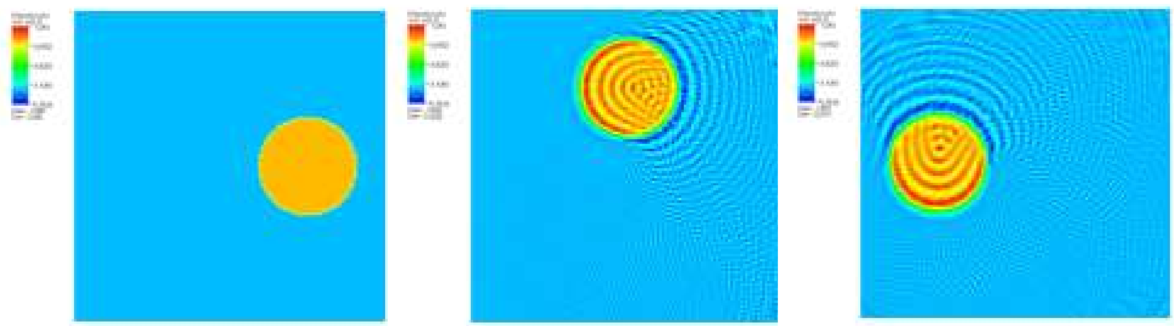
$$\frac{\partial f}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{R}} \cdot \left(\dot{\boldsymbol{R}}(f) f \right) + \frac{\partial}{\partial v_{\|}} \left(\dot{v}_{\|}(f) f \right) = 0$$

- Dependence of the phase space velocities $\dot{\boldsymbol{R}}$ and $\dot{\boldsymbol{v}}_{\|}$ on f is through the Poisson solve
- To obtain a high-order discretization that is robust for this highly nonlinear system, we combine
  - fourth-order, multidimensional, flux-corrected transport (FCT) spatial discretization
  - fourth-order Runge Kutta time integration
- Based on a new PPM limiter
  - Preserves fourth-order accuracy where solution is smooth (does not reduce accuracy at smooth extrema like classical FCT and PPM)
  - Can be combined with an FCT multidimensional limiter (Zalesak) to preserve distribution function positivity

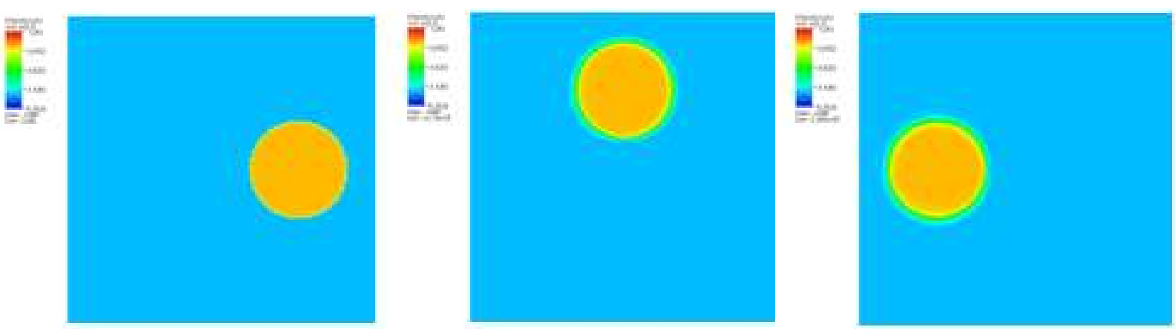
The new PPM limiter combined with an FCT limiter preserves positivity while maintaining 4th order accuracy

Test problem: Advection of a circle in solid-body rotation

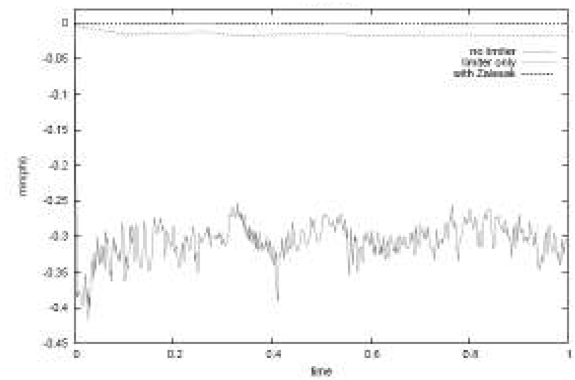
Without limiter:



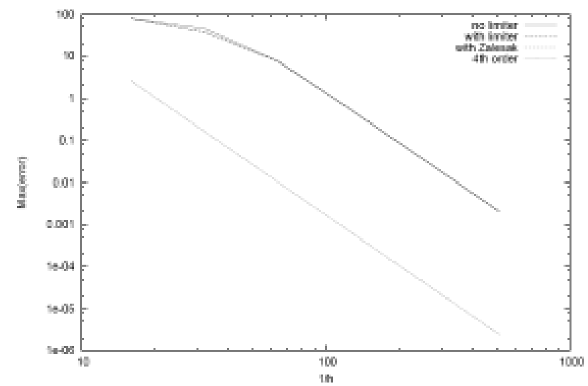
With limiter:



Min vs. time for circle in solid-body rotation test problem



Convergence for Gaussian (smooth solution) test problem



We have added hyperviscosity to the hyperbolic discretization

- Central discretizations require artificial dissipation for stability for variable coefficient & nonlinear problems
- Our high-order physical-space hyperviscosity:

$$\mu h^5 \nabla_{\mathbf{x}}^6 u = \mu h^5 \sum_{\pm=+,-} \sum_{d=1}^{D} \sum_{s=1}^{D} \pm \langle J^{-1} (\mathbf{N}^T \mathbf{N})_{ds} \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d} \langle \frac{\partial}{\partial \xi_s} \nabla_{\mathbf{x}}^4 u \rangle_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}^d}$$

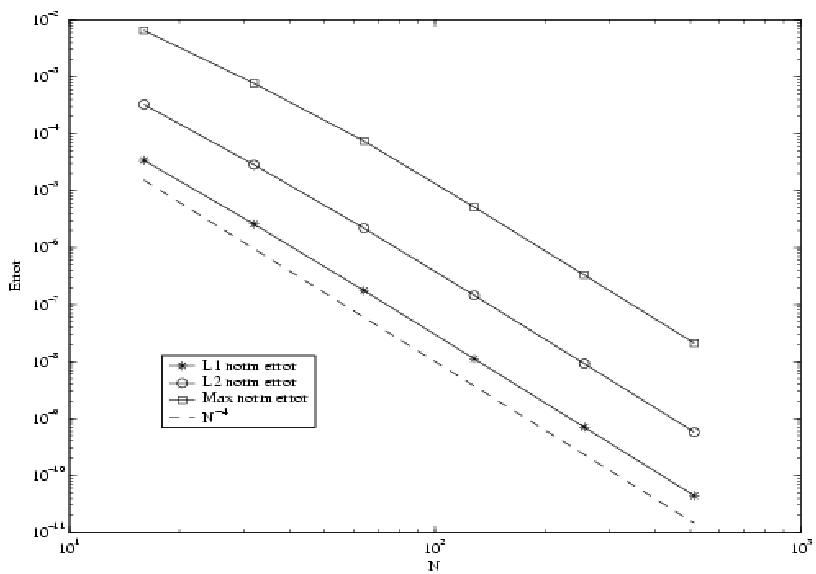
  - Ensures free-stream preservation
  - Is Kreiss dissipative on uniform grids
- Open question: value of the viscosity coefficient μ ?
  - Exploring matrix-free Arnoldi iteration on semi-discrete operator
    - determines approximate limiting eigenvalues

4^{th}-order accuracy of the gyrokinetic Poisson discretization has been obtained on core equilibrium geometries

Given Φ, use high accuracy quadrature to manufacture ρ such that

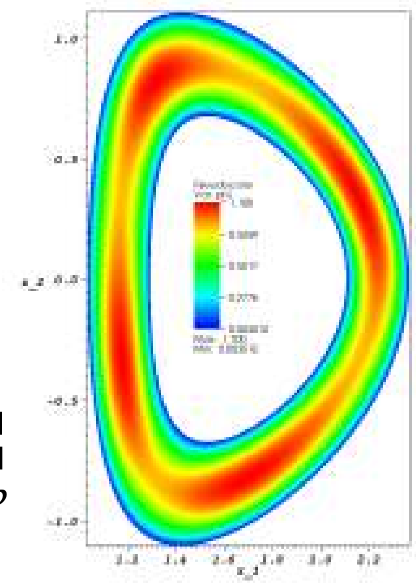
$$\nabla \cdot \left\{ \left[\epsilon_0 \boldsymbol{I} + \frac{n_i}{B^2} \left(\boldsymbol{I} - \vec{\boldsymbol{b}}\vec{\boldsymbol{b}}^T \right) \right] \nabla \Phi \right\} = \rho,$$

using a prescribed density profile n_i and a magnetic field $\vec{\boldsymbol{B}} = B\vec{\boldsymbol{b}}$, from an analytically specified equilibrium model*.



Verification of 4^{th} order convergence

*Miller et al., "Noncircular, finite aspect ratio, local equilibrium model", Phys. Plasmas, Vol. 5, No. 4 (1998).



Potential computed from exact ρ

Convergence of *Hypre* CG solver preconditioned with multigrid solution of second-order operator

iter	Relative residual
1	6.62e-03
2	1.19e-03
3	2.24e-04
4	1.17e-04
5	4.59e-05
6	1.18e-05

We are laying the numerical foundation for a continuum edge code needed by the fusion community

- The Edge Simulation Laboratory (ESL) is a partnership between this ASCR/AMR project and a companion OFES-funded effort established to develop a continuum edge code.

  Physics collaborators:
  - LLNL: R. Cohen, B. Cohen A. Dimits, T. Rognlien, M. Umansky, X. Xu
  - General Atomics: P. Snyder, J. Candy, E. Belli
  - UCSD: S. Krasheninnikov, K. Bodi
- *Our algorithm research plan anticipates the needs of the ESL collaboration.*
- Intermediate ESL milestones:
  - 4D electrostatic (drift kinetic) in flux tube or simple core geometry
  - 4D electrostatic in divertor geometry
  - 4D electromagnetic with gyroaveraging
  - 5D
- Applied math milestones:
  - Coupled 4th-order Vlasov-Poisson on mapped grids
  - Renewal proposal:
    - Mapped multiblock
    - Arbitrary wavelength
    - Electromagnetic solver and implicit kinetic electrons
- The successful transfer of the algorithms in this project involves substantial software development (leveraged with SciDAC APDEC project).

Backup slides

Gyrokinetic edge simulation requires the solution of a special Vlasov-Poisson system

Evolution of plasma species distribution functions and potential:

$$\frac{\partial (B_\parallel^* f_i)}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{R}} \cdot \left(\dot{\boldsymbol{R}} B_\parallel^* f_i \right) + \frac{\partial}{\partial v_\parallel} \left(\dot{v}_\parallel B_\parallel^* f_i \right) = 0$$

Vlasov

$$\boldsymbol{\nabla} \cdot \left\{ \left[\epsilon_0 \boldsymbol{I} + \sum_i Z_i \bar{n}_i \frac{m_i c^2}{e B^2} \left(\boldsymbol{I} - \boldsymbol{b}\boldsymbol{b}^T \right) \right] \boldsymbol{\nabla} \Phi \right\} = e \left(n_e - \sum_i Z_i \bar{n}_i \right)$$

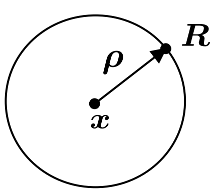
Poisson

$f_i \equiv f_i(\boldsymbol{R}, v_\parallel, \mu, t)$ Gyrocenter distribution functions

$\Phi \equiv \Phi(\boldsymbol{x}, t)$ Potential

$\boldsymbol{R}, v_\parallel, \mu$ Gyrocenter coordinates

$\boldsymbol{x}$ Lab coordinates



Gyroaveraging "push forward" / "pull back" between gyrocenter and lab coordinates

$$\bar{n}_i(\boldsymbol{x}, t) = \int f_i(\boldsymbol{R}, v_\parallel, \mu, t) \delta(\boldsymbol{R} - \boldsymbol{x} + \boldsymbol{\rho}) B_\parallel^\star d\boldsymbol{R} dv_\parallel d\mu d\theta$$

Special characteristics:

- Distribution functions are evolved in gyrocenter coordinates
- Poisson equation is posed in lab frame (gyroaveraged charge density yields additional polarization density terms)

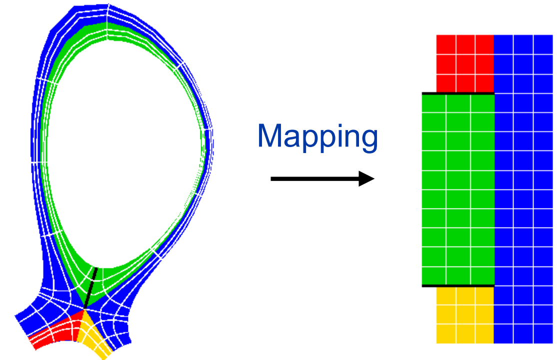
A mapped multiblock approach extends high-order discretizations to edge geometries

- Mapped multiblock will allow us to solve the Vlasov-Poisson system on edge geometries, where each logically distinct region (core, scrape-off, private flux) is treated as a block
- Approach:
  - Compute sufficiently accurate ghost cell values on smooth extensions of each block

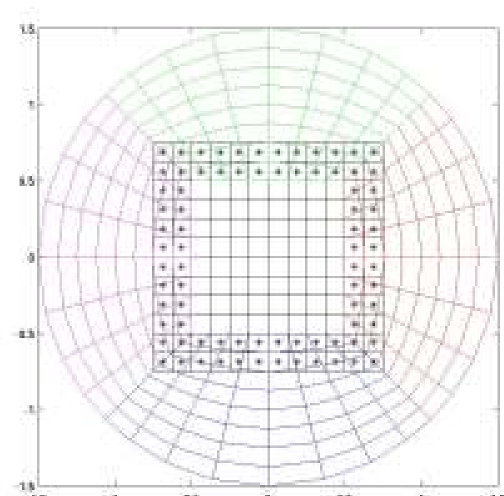
$$\varphi(\boldsymbol{x}) \approx \sum_{\boldsymbol{p}} a_{\boldsymbol{p}} \boldsymbol{x}^{\boldsymbol{p}} \ , \ \boldsymbol{x}^{\boldsymbol{p}} = \prod_{d=1}^{D} x_d^{p_d}$$

$$\int_{V_{\boldsymbol{v}}} \varphi(\boldsymbol{x}) d\boldsymbol{x} = \sum_{\boldsymbol{p}} a_{\boldsymbol{p}} \int_{V_{\boldsymbol{v}}} \boldsymbol{x}^{\boldsymbol{p}} d\boldsymbol{x} \ , \ \boldsymbol{v} \in \mathcal{V}$$

  - Use a set of control volumes such that the above system for the expansion coefficients is of maximal rank and can be solved using least squares. Then evaluate the polynomial or its moments to obtain the ghost values
  - Implement supporting infrastructure in Chombo
  - Use multiblock operator evaluations to perform Krylov matrix-vector products combined with a block preconditioner for the GK Poisson solve



Physical domain   Computational domain



Semi-implicit algorithms are needed for a fully electromagnetic edge model with kinetic electrons

An electromagnetic edge model requires the addition solution of Ampère's equation for the parallel magnetic potential:

$$\epsilon_0 \nabla^2 A_\| = e \int f_e v_\| dv$$

The inclusion a gyrokinetic electron model

$$\frac{\partial f_e}{\partial t} + \boldsymbol{\nabla}_{\boldsymbol{R}} \cdot \left(\dot{\boldsymbol{R}} f_e \right) + \frac{\partial}{\partial v_\|} \left(\dot{v}_\| f_e \right) = 0$$

introduces a fast time scale, since the phase space velocities $\dot{\boldsymbol{R}}$ and $\dot{\boldsymbol{v}}_\|$ are each given in terms of a Hamiltonian expression that is inversely proportional to the electron mass

We will pursue two options:

- Modified mass ratio in an explicit discretization
- Semi-implicit discretization