A Fully Implicit Kinetic Electromagnetic Model for Magnetically Confined Fusion Plasma Simulations

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PPPL PRINCETON PLASMA PHYSICS LABORATORY

HBPS High-fidelity Boundary Plasma Simulation

Outline:

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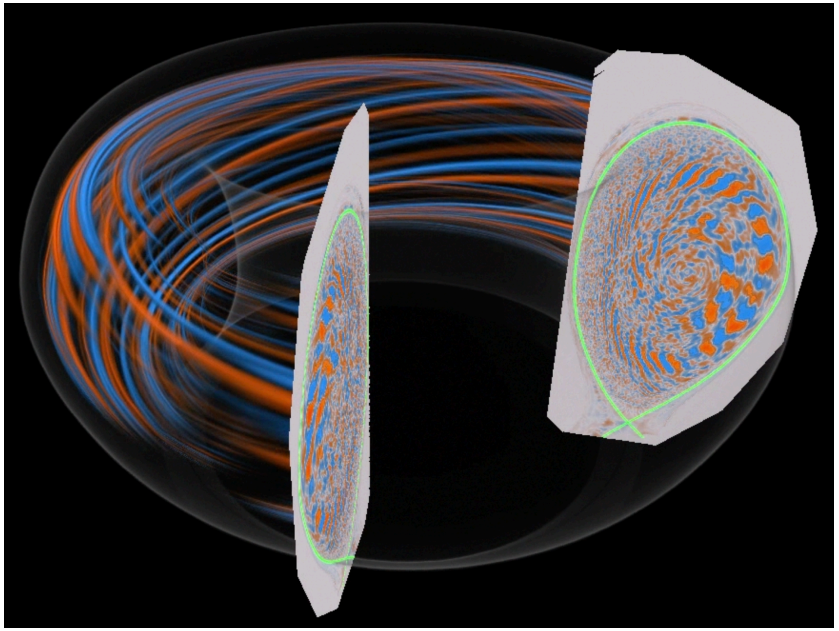
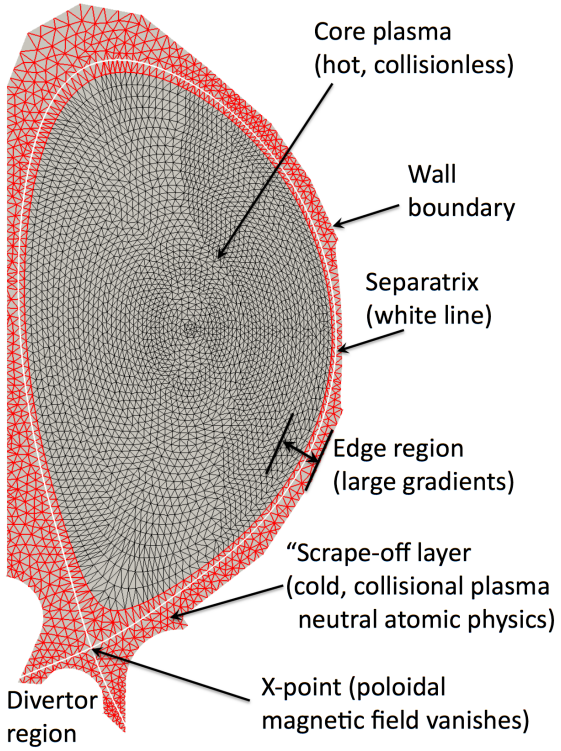
Background

XGC and Magnetic Confinement Fusion

- Approach to fusion energy in which a hot (100 million + degree) fuel, in form of plasma, is confined by strong magnetic fields
- Tokamak uses twisted magnetic fields wrapped around toroidal surfaces
- XGC is a comprehensive gyrokinetic particle-in-cell code for simulating fusion relevant plamsas confined in toroidal magnetic fields





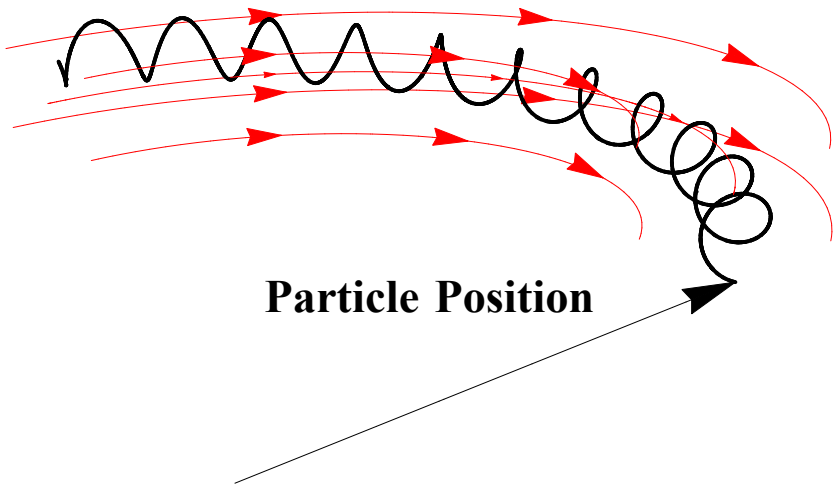
Background

Electromagnetic Gyrokinetics

- MHD/fluid type electromagnetic modes are important in magnetically confined fusion devices (e.g. edge localized modes, sawtooth oscillations, Alfvén eigenmodes, etc.)
- Important effects may be missing from fluid models (e.g. trapped particle effects, wave-particle interactions, finite Larmor radius effects, etc.)
- Characteristic frequencies of modes of interest are smaller than the gyrofrequency $\rightarrow$ gyrokinetic ions, drift kinetic electrons
- There are known numerical difficulties, however, associated with electromagnetic gyrokinetic PIC (cancellation problem for $p_{\|}$, inductive component of electric field for $v_{\|}$)
- A fully implicit PIC method can mitigate these issues, however, we need an efficient way to invert the resulting system of nonlinear equations at each time step to make this practical.

Gyrokinetics

Particle Motion in a Magnetic Field



- Gyration perpendicular to $\mathbf{B}$
- Streaming parallel to $\mathbf{B}$
- Well defined "Guiding Center"

$$\mathbf{X} = \mathbf{x} - \frac{\hat{\mathbf{b}} \times \mathbf{v}}{\Omega_\alpha}$$

Parameters of Gyromotion

Gyrofrequency: $\Omega_\alpha = q_\alpha |\mathbf{B}| / m_\alpha$,

Gyroradius (Larmor): $\rho_\alpha = v_\perp / \Omega_\alpha$

Gyrokinetics (GK):

- Possible to reduce dynamics
- Treat gyrating particles as drifting charged rings

Gyrokinetics

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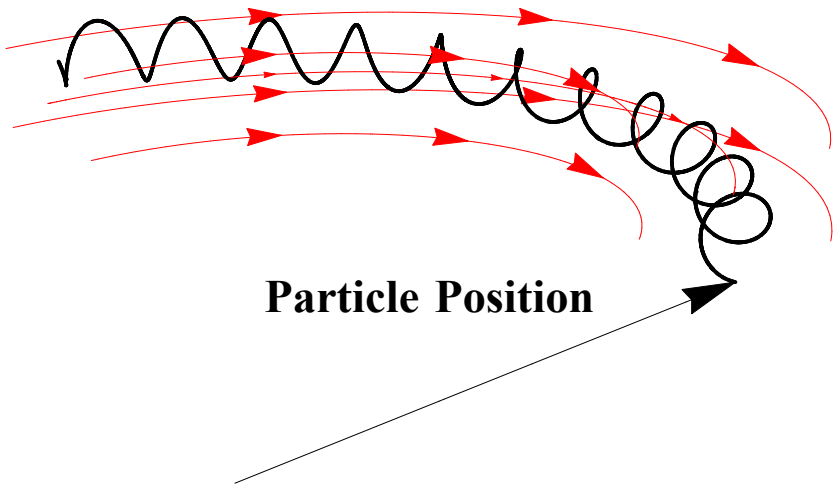

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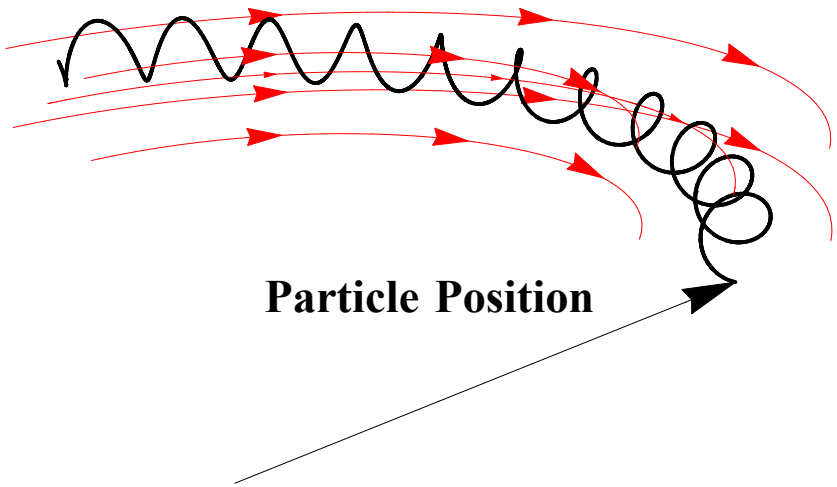

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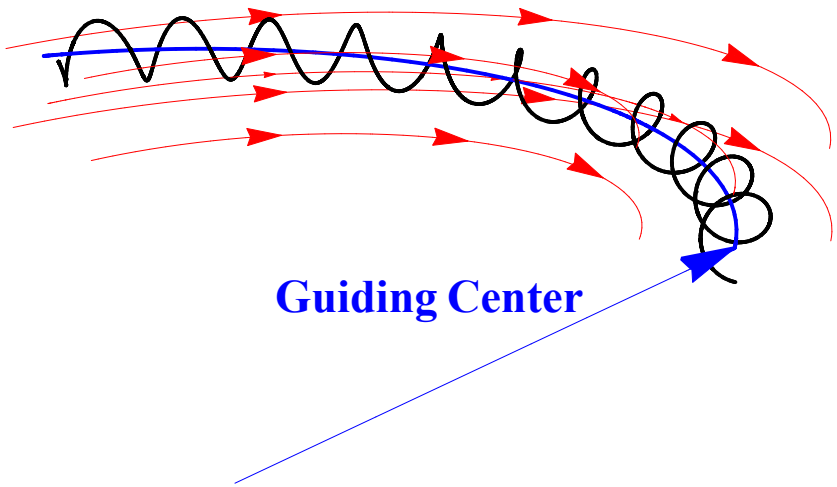

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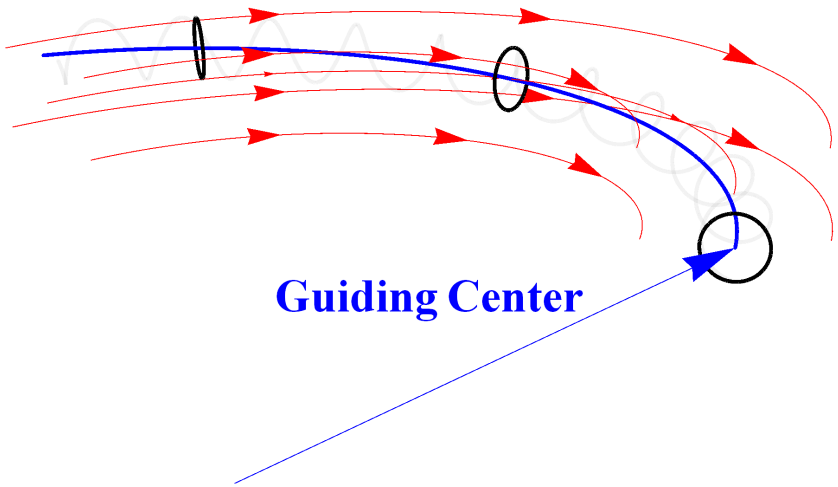

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Electromagnetic Gyrokinetics

Governing Equations

- Guiding center phase space distribution function for species $s = i, e$

$$f_s(\mathbf{X}, \mu, v_\parallel, t) : \mathbb{R}^5 \times \mathbb{R} \to \mathbb{R}^+$$

- Normalized with number of guiding centers for species s:

$$\int_{-\infty}^{\infty} \int_0^{\infty} \int_{\mathbb{R}^3} f_s(\mathbf{X}, \mu, v_\parallel) d^3X B d\mu dv_\parallel = N_s^{gc}$$

- GK Vlasov Equation:

$$\frac{\partial f_s}{\partial t} + \dot{\mathbf{X}} \cdot \frac{\partial f_s}{\partial \mathbf{X}} + \dot{v}_\parallel \frac{\partial f_s}{\partial v_\parallel} = 0$$

- Drift Motions:

$$\dot{\mathbf{X}} = \frac{1}{D}\left[v_\parallel\left(\hat{\mathbf{b}}_0 + \delta\hat{\mathbf{b}}\right) + \frac{m_s}{q_s B_0} v_\parallel^2 \nabla \times \hat{\mathbf{b}}_0 - \frac{m_s}{q_s B_0}\hat{\mathbf{b}}_0 \times \left(\frac{q_s}{m_s}\langle \mathbf{E}\rangle - \mu \nabla B_0\right)\right]$$

$$\dot{v}_\parallel = \frac{q_s}{m_s D}\left[\left(\hat{\mathbf{b}}_0 + \delta\hat{\mathbf{b}}\right) + \frac{m_s}{q_s B_0} v_\parallel \nabla \times \hat{\mathbf{b}}_0\right] \cdot \left(\langle \mathbf{E}\rangle - \frac{m_s}{q_s}\mu \nabla B_0\right)$$

$$D = 1 + \frac{m_s}{q_s B_0} v_\parallel \mathbf{b}_0 \cdot \nabla \times \mathbf{b}_0$$

Electromagnetic Gyrokinetics

Governing Equations

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Perturbed Fields:

$$\mathbf{E} = -\nabla\phi - \frac{\partial A_\parallel}{\partial t}\hat{\mathbf{b}}_0$$

$$\delta\mathbf{B} = \nabla \times \left(A_\parallel \hat{\mathbf{b}}_0\right)$$

Potential Equations:

$$-\frac{e n_0 m_i}{q_i B_0^2}\nabla_\perp^2 \phi = q_i \bar{n}_i - e n_e$$

$$-\frac{1}{\mu_0}\nabla_\perp^2 A_\parallel = j_{\parallel i} + j_{\parallel e}$$

Velocity Moments:

$$\bar{n}_i(\mathbf{x}) = \int_{-\infty}^{\infty}\int_0^{\infty} \left\langle f_i(\mathbf{X}, v_\parallel, \mu)\delta(\mathbf{X} - \mathbf{x} + \boldsymbol{\rho}_i)\right\rangle B d\mu dv_\parallel$$

$$n_e(\mathbf{x}) = \int_{-\infty}^{\infty}\int_0^{\infty} \left\langle f_e(\mathbf{X}, v_\parallel, \mu)\delta(\mathbf{X} - \mathbf{x})\right\rangle B d\mu dv_\parallel$$

$$j_{\parallel s}(\mathbf{x}) = q_s \int_{-\infty}^{\infty}\int_0^{\infty} v_\parallel \left\langle f_s(\mathbf{X}, v_\parallel, \mu)\delta(\mathbf{X} - \mathbf{x})\right\rangle B d\mu dv_\parallel$$

Gyrokinetic Vlasov:

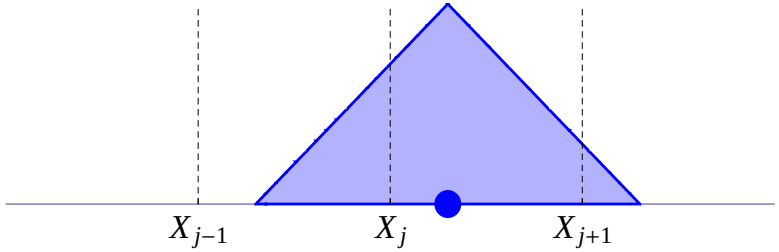
$$\frac{\partial f_s}{\partial t} + \dot{\mathbf{X}} \cdot \frac{\partial f_s}{\partial \mathbf{X}} + \dot{v}_\parallel \frac{\partial f_s}{\partial v_\parallel} = 0$$

Outline:

Particle-in-Cell Method

Elements of PIC

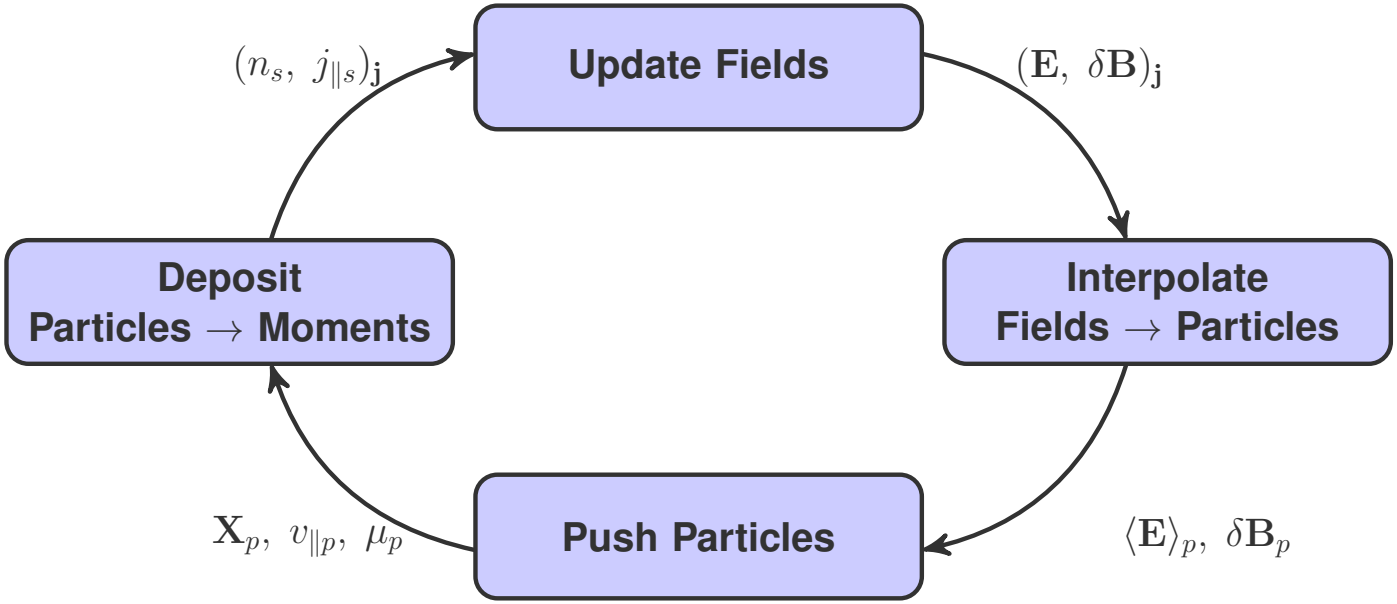
- Computational particles: $\mathbf{X}_p,\ v_{\|p},\ \mu_p$ for $p = 1, 2, ..., N_P$
- Computational mesh: $\mathbf{x}_j, \quad j = 1, 2, ..., N_M$
- Fields and moments defined on mesh: $(n_s,\ j_{\|s})_{\mathbf{j}}$ and $(\mathbf{E},\ \delta\mathbf{B})_{\mathbf{j}}$
- Shape function $S(\mathbf{x})$ communicates between mesh and particle quantities:



Particle-in-Cell Method

Computational Cycle

- Typically system is explicitly advanced in time:



- A fully implicit scheme advances particles and fields simultaneously each time step. (G. Chen, L. Chacón, D. Barnes, J. Comput. Phys., 2011)
- Requires solution of system of nonlinear equations at each time step.
- Made possible due to a low-dimensional residual formulation (Particles are coupled only through field quantities!)

Implicit Particle-in-Cell

Discrete Model

- Implicitly discretized fields:

$$\mathbf{E}^{n+1/2} = -\frac{1}{2}\left(\nabla\phi^{n+1} + \nabla\phi^{n}\right) - \frac{2}{\Delta t}\left(A_{\parallel}^{n+1/2} - A_{\parallel}^{n}\right)\hat{\mathbf{b}}_0$$

$$\delta\mathbf{B}^{n+1/2} = \nabla \times \left(A_{\parallel}^{n+1/2}\hat{\mathbf{b}}_0\right).$$

- Potential equations:

$$\mathcal{L}_1\phi^{n+1} = q_i\bar{n}_i^{n+1} - en_e^{n+1}, \qquad \mathcal{L}_1 \equiv -\frac{en_0m_i}{q_iB_0^2}\nabla_\perp^2$$

$$\mathcal{L}_2A_{\parallel}^{n+1/2} = j_{\parallel i}^{n+1/2} + j_{\parallel e}^{n+1/2}, \qquad \mathcal{L}_2 \equiv -\frac{1}{\mu_0}\nabla_\perp^2$$

- Nonlinear dependence on ϕ^{n+1} and $A_{\parallel}^{n+1/2}$ through particle system:

$$n_s^{n+1} = n_s(\phi^{n+1}, A_{\parallel}^{n+1/2})$$

$$j_{\parallel s}^{n+1/2} = j_{\parallel s}(\phi^{n+1}, A_{\parallel}^{n+1/2}).$$

Implicit Particle-in-Cell

Iteration Scheme

- Iteration Scheme:

$$\begin{pmatrix} \phi \\ A_\parallel \end{pmatrix}^{k+1} = \begin{pmatrix} \phi \\ A_\parallel \end{pmatrix}^{k} - \mathcal{P}^{-1} \begin{pmatrix} R_\phi \\ R_A \end{pmatrix}^{k}$$

Update Potentials:

$$\begin{pmatrix} \phi \\ A_\parallel \end{pmatrix}^{k+1} = \begin{pmatrix} \phi \\ A_\parallel \end{pmatrix}^{k} + \begin{pmatrix} \delta\phi \\ \delta A_\parallel \end{pmatrix}$$

XGC

Push and Deposit Particles:

$$n_s(\phi^k, A_\parallel^k), \qquad j_{\parallel s}(\phi^k, A_\parallel^k)$$

$$s = i, e$$

Construct Residuals:

$$\begin{pmatrix} R_\phi \\ R_A \end{pmatrix}^{k} = \begin{pmatrix} \mathcal{L}_1\phi^k - \sum_s q_s n_s(\phi^k, A_\parallel^k) \\ \mathcal{L}_2 A_\parallel^k - \sum_s j_{\parallel s}(\phi^k, A_\parallel^k) \end{pmatrix}$$

Fluid Preconditioner

Solve Linear System :

$$\mathcal{P}\begin{pmatrix} \delta\phi \\ \delta A_\parallel \end{pmatrix} = -\begin{pmatrix} R_\phi \\ R_A \end{pmatrix}^{k}$$

Outline:

Fluid Preconditioner Model

Basic Model

- If $\mathcal{P} = \mathcal{J}$, Newton's method, however, constructing $\mathcal{J}$ is infeasible.
- Use physics knowledge to postulate a model that captures the linear response of fastest timescales (physics-based preconditioning)

Note:

Approximations made in the preconditioner do NOT affect the converged solution

- Fastest timescales come from electron motions parallel to the background magnetic field:

$$\frac{\partial f_e}{\partial t} + \dot{\mathbf{X}} \cdot \frac{\partial f_e}{\partial \mathbf{X}} + \dot{v_\parallel} \frac{\partial f_e}{\partial v_\parallel} = 0$$

$$\dot{\mathbf{X}} \approx v_\parallel \mathbf{b}_0, \quad \dot{v_\parallel} \approx -\frac{e}{m_e} E_\parallel$$

- Captures shear Alfvén and Ω_H modes

Fluid Preconditioner Model

Basic Model

- Taking velocity moments of GK Vlasov and discretizing in time:

$$n_e^{n+1} - \Delta t \nabla_\parallel j_{\parallel e} = \mathrm{RHS}^n$$

$$\frac{m_e}{e^2 n_0} j_{\parallel e}^{n+1/2} + \frac{\Delta t}{4} \nabla_\parallel \phi^{n+1} + A_\parallel^{n+1/2} - \frac{\Delta t}{4} \frac{T_e}{e n_0} \nabla_\parallel n_e^{n+1} = \mathrm{RHS}^n$$

- Preconditioner matrix equation:

$$\begin{bmatrix} \mathcal{L}_1 & 0 & \mathcal{M} & 0 \\ 0 & \mathcal{L}_2/e & 0 & -\mathcal{M} \\ 0 & 0 & I & -\Delta t B \nabla_\parallel B^{-1} \\ \frac{\Delta t}{4}\nabla_\parallel & I & -\frac{\Delta t}{4n_0}\left(E_\parallel + \frac{T_e}{e}\nabla_\parallel\right) & \frac{m_e}{e n_0} \end{bmatrix} \begin{bmatrix} \delta\phi \\ \delta A_\parallel \\ \delta n \\ \delta j_\parallel / e \end{bmatrix} = - \begin{bmatrix} R_\phi \\ R_A \\ 0 \\ 0 \end{bmatrix}$$

- $R_\phi, \quad R_A$ come from particle system
- $\delta\phi, \quad \delta A_\parallel$ used to correct $\phi^k, \quad A_\parallel^k$.

Fluid Preconditioner Model

Anderson Acceleration

- Suppose we wish to solve $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, and we have a set of m iterates: $\mathbf{x}^l, \quad l = 1, 2, ..., m$.
- Select a linear combination in a way to reduce the residual as much as possible (if $\mathbf{f} = A\mathbf{x} - \mathbf{b}$).

$$\min_{\alpha \in \mathbb{R}^m} \left\| \sum_{j=0}^{m-1} \alpha_{j+1} \mathbf{f}^{k-j} \right\|^2, \qquad \text{where} \quad \sum_{j=1}^{m} \alpha_j = 1, \qquad \mathbf{f}^l \equiv \mathbf{f}(\mathbf{x}^l)$$

- The the new iterate is:

$$\mathbf{x}^{k+1} = \sum_{j=0}^{m-1} \alpha_{j+1} \mathbf{x}^{k-j}$$

- Related to GMRES
- D. G. Anderson, *J. Assoc. Comput. Mach.*, 12 (1965), pp. 547-560

Fluid Preconditioner Model

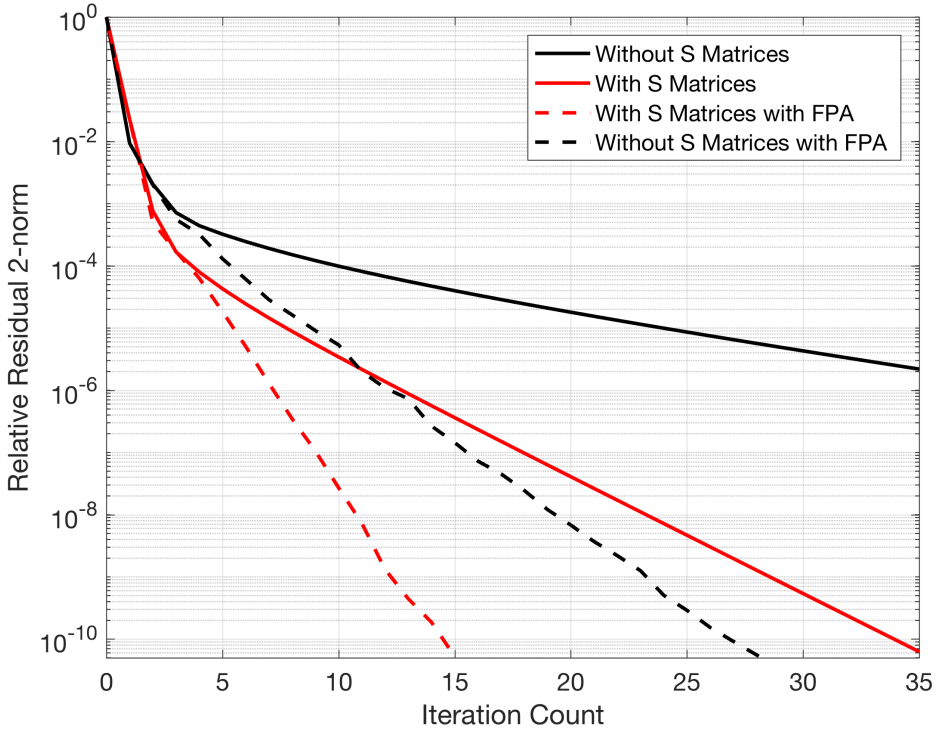
Particle-Mesh Interactions

- Fluid preconditioner converges too slowly to be practical. We need to understand what missing effects could influence fast timescale behaviors.
- Field data is interpolated to particles and particle data is deposited to mesh $\rightarrow$ fields are effectively smoothed in moment responses.
- In XGC, interpolation and deposition are done in field-line-following coordinates. A directional smoothing operator $\mathcal{S}$ to mimic this effect can be derived from PIC equations.

$$\begin{bmatrix} \mathcal{L}_1 & 0 & \mathcal{M} & 0 \\ 0 & \mathcal{L}_2/e & 0 & -\mathcal{M} \\ 0 & 0 & I & -\Delta t B \nabla_\parallel B^{-1} \\ \frac{\Delta t}{4}\mathcal{S}\nabla_\parallel & \mathcal{S} & -\frac{\Delta t}{4}\frac{T_e}{en_0}\nabla_\parallel & \frac{m_e}{en_0} \end{bmatrix} \begin{bmatrix} \delta\phi \\ \delta A_\parallel \\ \delta n \\ \delta j_\parallel/e \end{bmatrix} = - \begin{bmatrix} R_\phi \\ R_A \\ 0 \\ 0 \end{bmatrix}.$$

Fluid Preconditioner Model

Particle-Mesh Interactions



Δt	4.36×10^{-8} s
n_0	1.0×10^{19} m^{-3}
T_e	2.0 keV
m_e	9.11×10^{-30} kg
m_i	1.67×10^{-27} kg

$\frac{v_A \Delta t}{\Delta s}$	1.7
$\frac{v_{th} \Delta t}{\Delta s}$	0.8

Fluid Preconditioner Model

Three Field Model

- We are motivated to examine the term involving T_e:

$$\begin{bmatrix} \mathcal{L}_1 & 0 & \mathcal{M} & 0 \\ 0 & \mathcal{L}_2/e & 0 & -\mathcal{M} \\ 0 & 0 & I & -\Delta t B \nabla_{\parallel} B^{-1} \\ \frac{\Delta t}{4}\mathcal{S}\nabla_{\parallel} & \mathcal{S} & -\frac{\Delta t}{4}\frac{T_e}{en_0}\nabla_{\parallel} & \frac{m_e}{en_0} \end{bmatrix} \begin{bmatrix} \delta\phi \\ \delta A_{\parallel} \\ \delta n \\ \delta j_{\parallel}/e \end{bmatrix} = - \begin{bmatrix} R_\phi \\ R_A \\ 0 \\ 0 \end{bmatrix}.$$

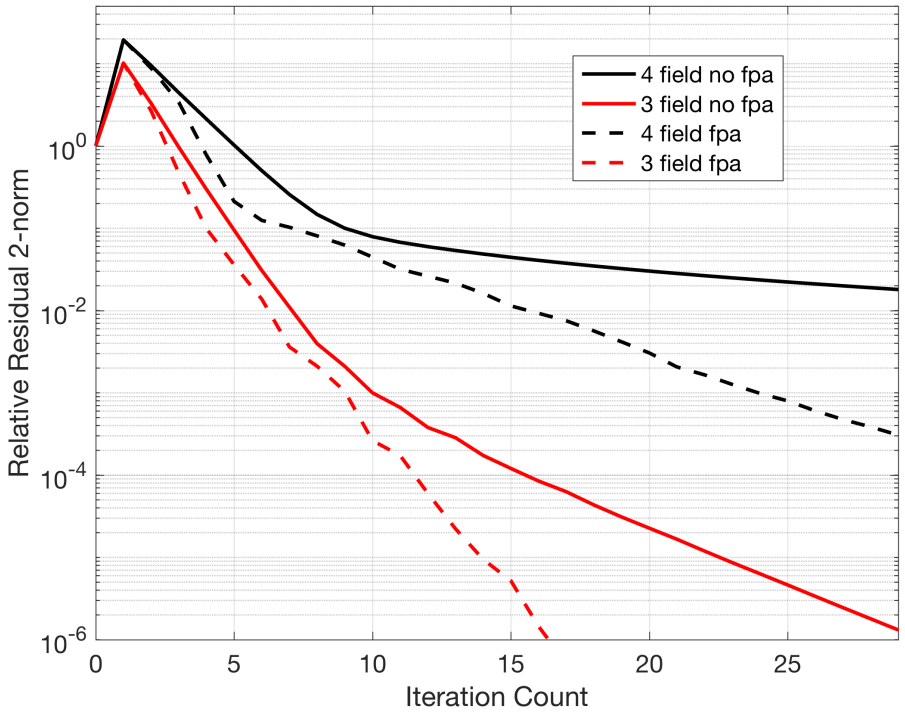
- The “red-black" mode is in the null space of a central differenced $\nabla_{\parallel}$ operator.
- Reformulate by eliminating third equation:

$$\begin{bmatrix} \mathcal{L}_1 & 0 & \Delta t \mathcal{M} B \nabla_{\parallel} B^{-1} \\ 0 & \mathcal{L}_2/e & -\mathcal{M} \\ \frac{\Delta t}{4}\mathcal{S}\nabla_{\parallel} & \mathcal{S} & \frac{m_e}{en_0} - \frac{\Delta t^2 T_e}{4en_0} B \nabla_{\parallel}^2 B^{-1} \end{bmatrix} \begin{bmatrix} \delta\phi \\ \delta A_{\parallel} \\ \delta j_{\parallel}/e \end{bmatrix} = - \begin{bmatrix} R_\phi \\ R_A \\ 0 \end{bmatrix},$$

- Standard three-point stencil for second order operator sees the “red-black" mode.

Fluid Preconditioner Model

Three Field Model



Δt	4.36×10^{-8} s
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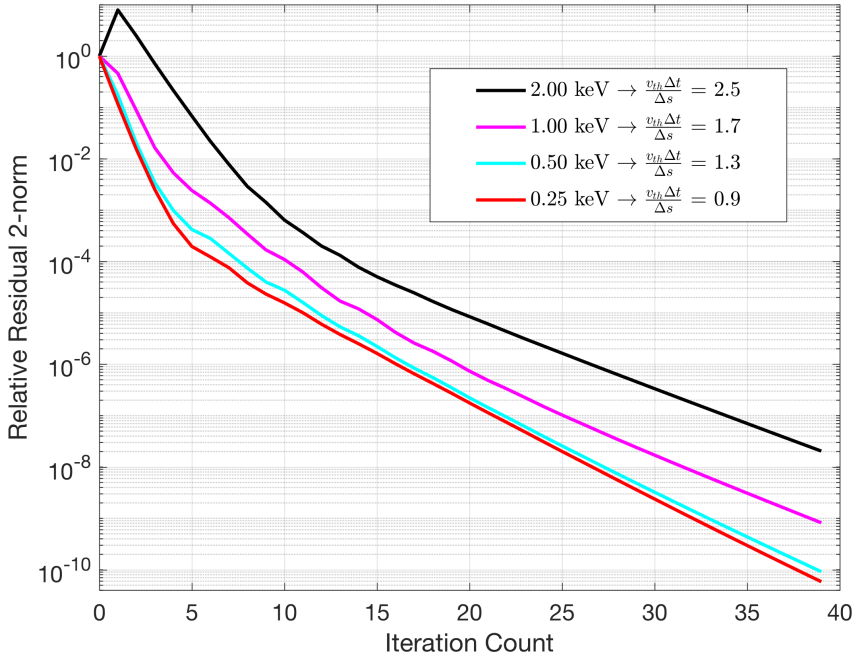
$\frac{v_A \Delta t}{\Delta s}$	1.7
$\frac{v_{th} \Delta t}{\Delta s}$	2.5

Fluid Preconditioner Model

Back to the Particle-in-cell model

- Convergence is still limited by “red-black" mode, but improves at lower temperatures.



- Spatial discretizations in the fluid equations have their origin in particle motions
- We are operating in a regime where electrons can cross a few poloidal planes over a time step (Moderate to large $v_{th}\Delta t/\Delta s$).

Fluid Preconditioner Model

Back to the Particle-in-cell model

- Sub-cycled electrons interpolate field data as they travel during a time step, carrying this information long distances
- It's possible to analyze these effects by returning to the PIC equations (Work in progress)
- We want to use this analysis to guide the choice of parallel gradient discretizations in the fluid model to include some nonlocality.

Outline:

Summary and Future Work

PPPL PRINCETON PLASMA PHYSICS LABORATORY

- Working to develop electromagnetic capability in XGC
- A fully implicit PIC method can overcome numerical difficulties associated with electromagnetic gyrokinetics (cancellation problem, inductive field component)
- Requires solution of nonlinear system of equations at each timestep $\rightarrow$ an effective precondition is essential!
- Several improvements have been made to reduce number of iterations needed for convergence
- Developing an understanding of the subtleties of our system and using this understanding to guide further improvements

Questions?

Please Ask!