Low-Frequency δf PIC Models with Fully Kinetic Ions

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Outline:

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Motivation for Fully Kinetic Ions

Gyrokinetic Ion Models

Modern research on low-frequency, ion-Larmor-radius scale fluctuations in magnetized plasmas is based on GK ion models.

- Analytically eliminate timescale of gyromotion while retaining important effects due to finite gyro-orbit width.

  Finite Larmor Radius (FLR) effects

- GK formalism is based on a number of ordering assumptions:

$$\frac{\rho_i}{L_{eq}} \sim \frac{\omega}{\Omega_i} \sim \frac{e\phi}{T_e} \sim \frac{\delta B}{B_{ext}} \sim k_{\parallel}\rho_i \sim O(\epsilon), \qquad k_{\perp}\rho_i \sim O(1)$$

$$\Downarrow$$

- GK Vlasov equation + modifications to Maxwell's equations
- Enormous sucess in treating idealized core turbulence.

Motivation for Fully Kinetic Ions

Fully Kinetic Ion Models

Low-frequency fully kinetic (FK) ion models, based on resolving the gyromotion, are feasible and have important applications.

- Advanced numerical algorithms and computing architectures, e.g. GPUs, hold promise for handling the more expensive particle integration.
- GK simulation is treating tougher problems.
  - W. Wan, et al. *Phys. Plasmas* **20**, 055902 (2013)
    H-mode edge pedestal: $\Omega_i \Delta t = 1.0$
  - J. Chowdhury, et al. *Phys. Plasmas* **23**, 012513 (2016)
    Microtearing in NSTX edge (top of pedestal): $\Omega_i \Delta t = 0.25$
- Verification of GK models where ordering parameters are not so small, e.g. how small does ρ_i / L_{eq} need to be?

Outline:

Basic Fully Kinetic Ion Model

Governing equations

- Vlasov equation for ions:

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i + \frac{q_i}{m_i} \left(\mathbf{E} + \mathbf{v} \times \mathbf{B} \right) \cdot \nabla_{\mathbf{v}} f_i = 0$$

- Testbed model

$$\mathbf{E} = -\nabla_{\mathbf{x}} \phi, \qquad n_e = n_{e0} \left(1 + \frac{e\phi}{T_e} \right), \qquad n_e = n_i = \int_{\mathbb{R}^3} f_i d^3 v$$

- Full model includes electromagnetic effects and drift kinetic electrons

"PIC simulation with Vlasov ions and drift kinetic electrons",
Y. Chen and S.E. Parker, *Phys. Plasmas* **16**, 052305 (2009).

Ion Temperature Gradient Instability Model

Equilibrium

- Vlasov Equilibrium Equation:

$$\underbrace{\mathbf{v}\cdot\nabla_{\mathbf{x}} f_{i0}}_{O(1)} + \underbrace{\frac{q_i}{m_i}\left(\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{v}} f_{i0}}_{O(\epsilon^{-1})} = 0, \qquad \epsilon = \frac{\rho_i}{L_{eq}} \ll 1$$

- Equilibrium solution constructed from "constants" of motion: $f_{i0}(K, R_x)$

$$K = \frac{m_i}{2}\mathbf{v}\cdot\mathbf{v}, \qquad R_x = x + \frac{\mathbf{v}\times\hat{\mathbf{b}}}{\Omega_i}\cdot\nabla x + O(\epsilon^2), \qquad \nabla x\cdot\mathbf{B} = 0$$

- Solve for perturbations from equilibrium $\Rightarrow f_i = f_{i0} + \delta f$:

$$\frac{\partial}{\partial t}\delta f + \mathbf{v}\cdot\nabla\delta f + \frac{q_i}{m_i}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{v}}\delta f = -q_i\mathbf{v}\cdot\mathbf{E}\frac{\partial f_0}{\partial K} - \underbrace{\frac{\mathbf{E}\times\hat{\mathbf{b}}}{B}\cdot\nabla x\frac{\partial f_0}{\partial R_x}}_{\text{Gradient Drive}}$$

"Low Frequency Fully Kinetic Simulation of the Toroidal ITG Instability",
B. Sturdevant et al., to appear in *Phys. Plasmas*

Ion Temperature Gradient Instability Model

Linear Studies for Shearless Slab

- Linear dispersion relations derived for the FK model and equivalent GK model:

$$\varepsilon_{FK}(\mathbf{k},\omega) = 0; \qquad \varepsilon_{GK}(\mathbf{k},\omega) = 0$$

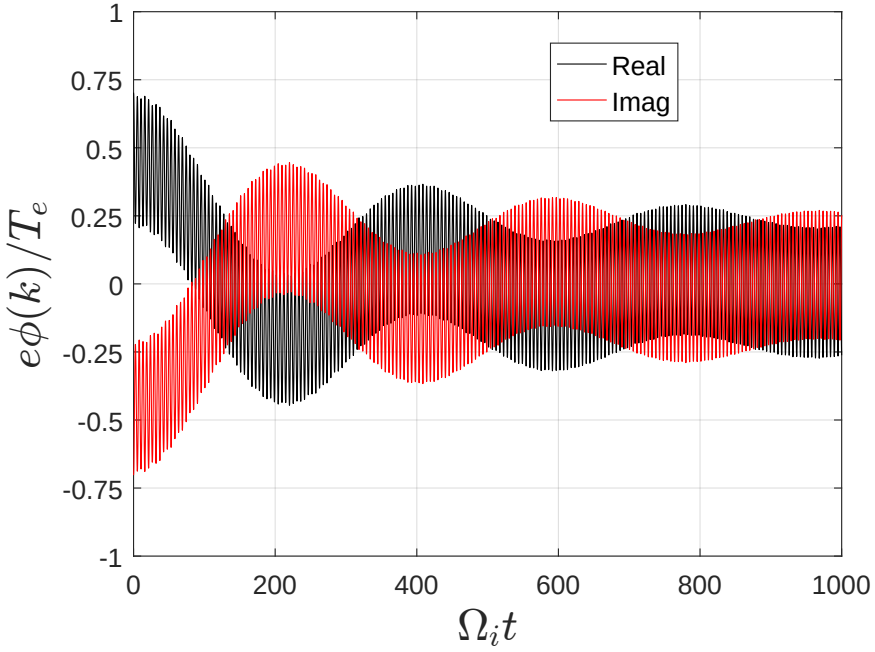
- Expansion of ε_{FK} in GK ordering parameters:

$$\boxed{\varepsilon_{FK}(\mathbf{k},\omega) = \varepsilon_{GK}(\mathbf{k},\omega) + O(\epsilon^2)}$$

- FK model correctly captures low-frequency normal modes of GK.
- Additional high-frequency modes in FK
  - Ion Bernstein Modes: $\omega_{IBW} \approx \pm n\Omega_i$
  - Compressional Alfven Wave (EM): high frequency for $k_\perp \rho_i \sim 1$

Simulation Results

Ion Acoustic Wave in Slab Geometry



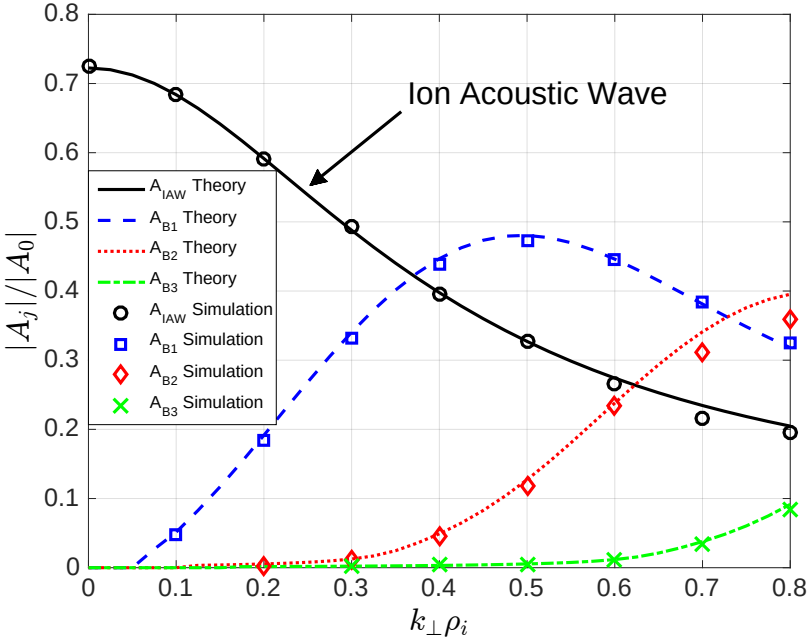


Figure: $k_\perp \rho_i = 0.3$ (left); $k_{||} \rho_i = 6.28 \times 10^{-3}$; $\frac{q_i T_e}{e T_i} = 5.0$; $\kappa_N = \kappa_T = 0.0$

- Ion Bernstein modes can have significant amplitudes for $k_\perp \rho_i \sim 1$.
- Theory from Laplace transform analysis is derived to give relative amplitudes of normal modes from initial condition:

$$\delta f(\mathbf{x}, \mathbf{v}, t = 0) = A_0 e^{i\mathbf{k}\cdot\mathbf{x}} f_0(\mathbf{v})$$

Outline:

Implicit Orbit Averaging and Sub-Cycling

Algorithm

Reformulation of field equation:

$$\frac{e\phi}{T_e} = \frac{\delta n_i}{n_0} \quad \rightarrow \quad \frac{\partial}{\partial t}\left(\frac{e\phi}{T_e}\right) = -\nabla \cdot \left(\frac{\delta(n_i \mathbf{u}_i)}{n_0}\right), \qquad \delta(n_i \mathbf{u}_i) = \int_{\mathbb{R}^3} \mathbf{v} \delta f_i d^3 v$$

- Micro time step Δt resolves fast cyclotron motion. Macro time step ΔT to resolves the low-frequency fields. $\Delta T / \Delta t = M$
- Time interpolated fields used in particle advance (sub-cycling):

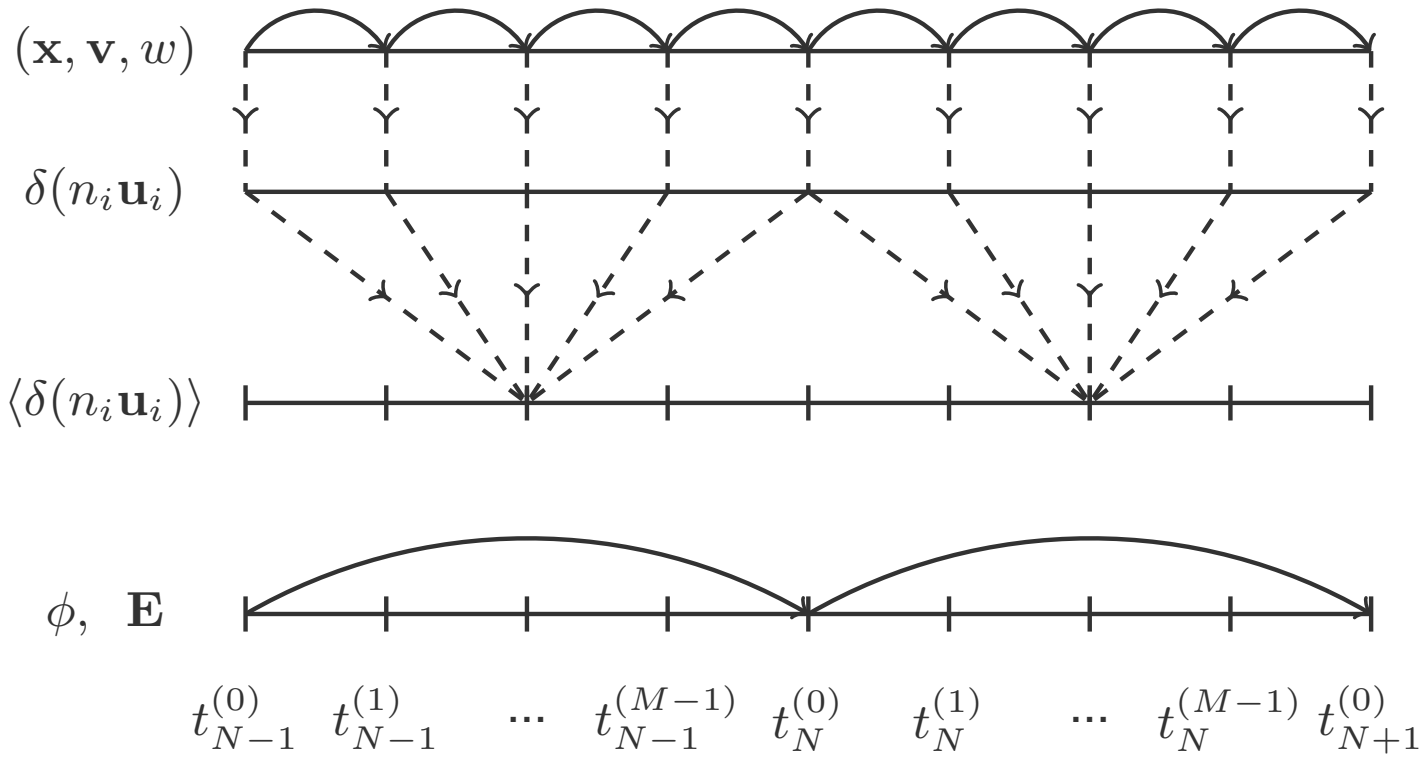
$$\mathbf{E}_\nu = (1 - \frac{\nu}{M})\mathbf{E}_N + \frac{\nu}{M}\mathbf{E}_{N+1}.$$

- Time averaged current density used in field solve (orbit averaging):

$$\langle \delta(n_i \mathbf{u}_i) \rangle_{N+1/2} = \frac{\Delta T}{M+1} \sum_{\nu=0}^{M} \delta \left(n_i \mathbf{u}_i\right)_\nu .$$

Implicit Orbit Averaging and Sub-Cycling

Algorithm



"An implicit δf PIC method with sub-cycling and orbit averaging for Lorentz ions", B. Sturdevant et al., *J. Comput. Phys.* **316**, p.519-533 (2016).

Outline:

Implicit Orbit Averaging and Sub-Cycling

Simulation Results

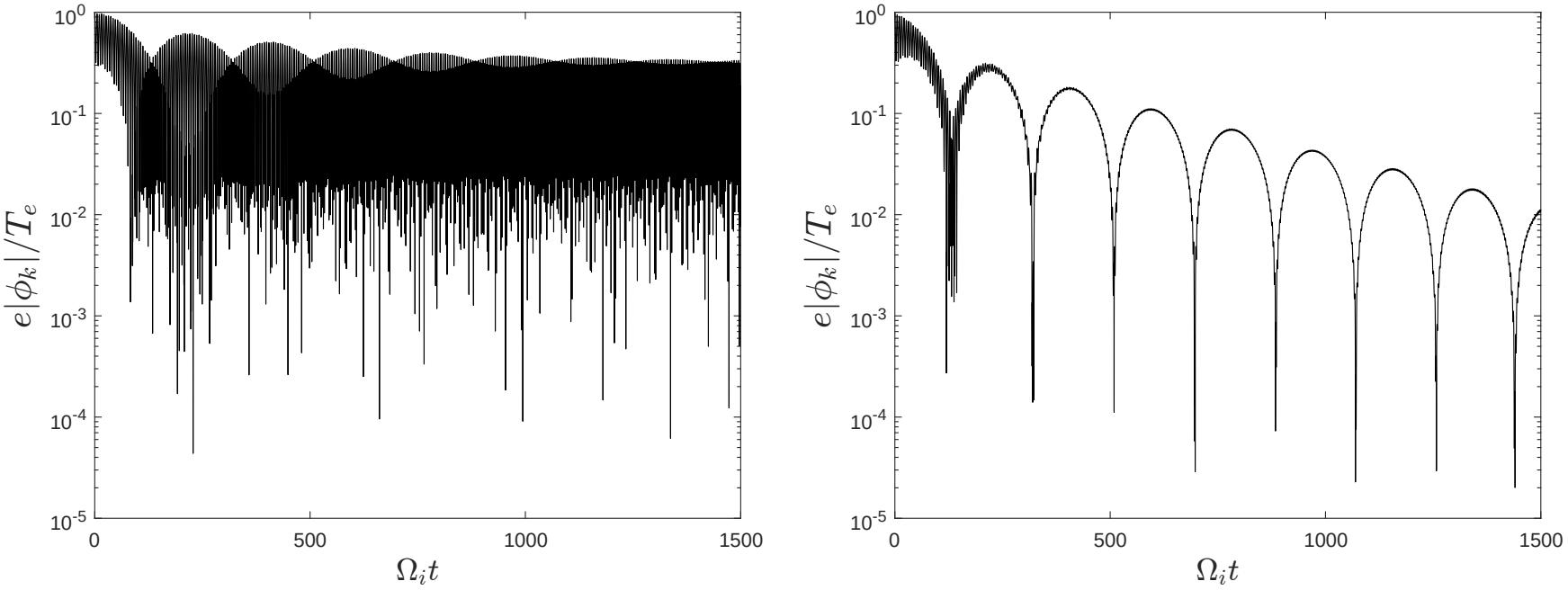


Figure: Original field equation (left). Reformulated field equation (right)

- Numerical analysis was performed explaining effect of velocity moments on implicit schemes:

"Finite Time Step and Spatial Grid Effects in δf Simulation of Warm Plasmas", B. Sturdevant and S.E. Parker, *J. Comput. Phys.* **305**, p.647-663 (2016).

Implicit Orbit Averaging and Sub-Cycling

Simulation Results

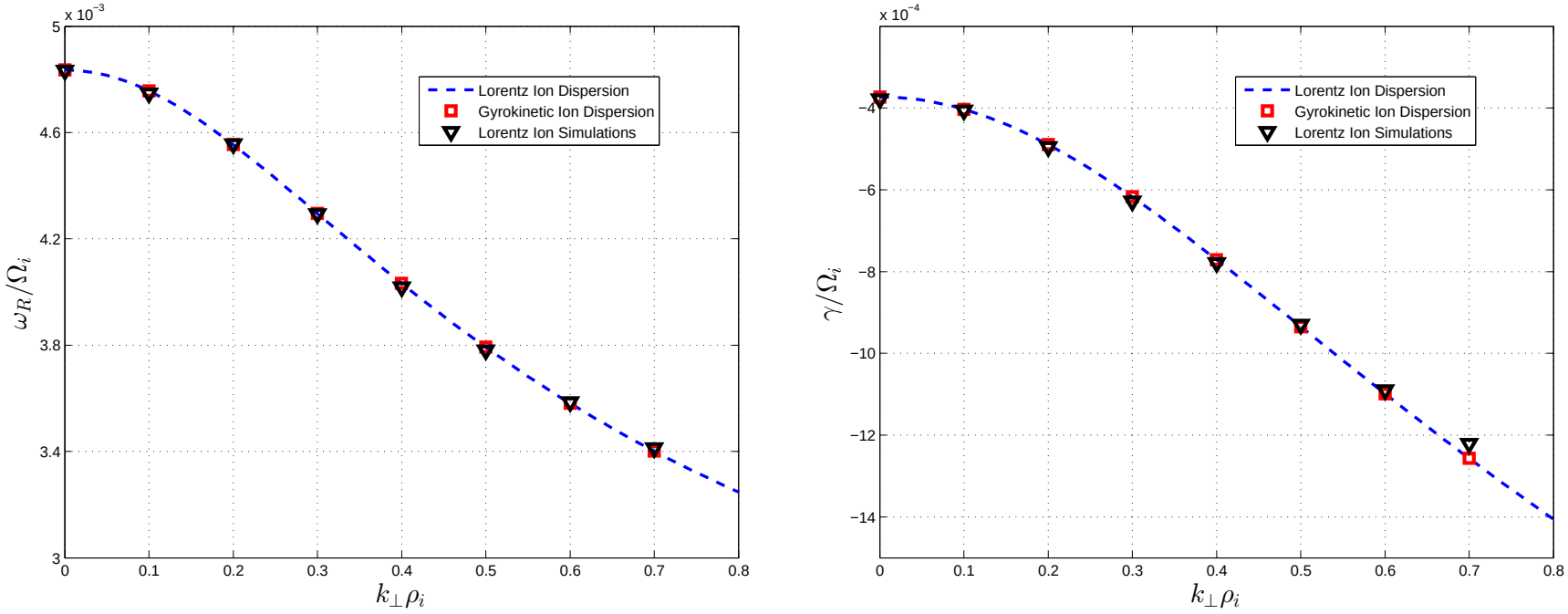


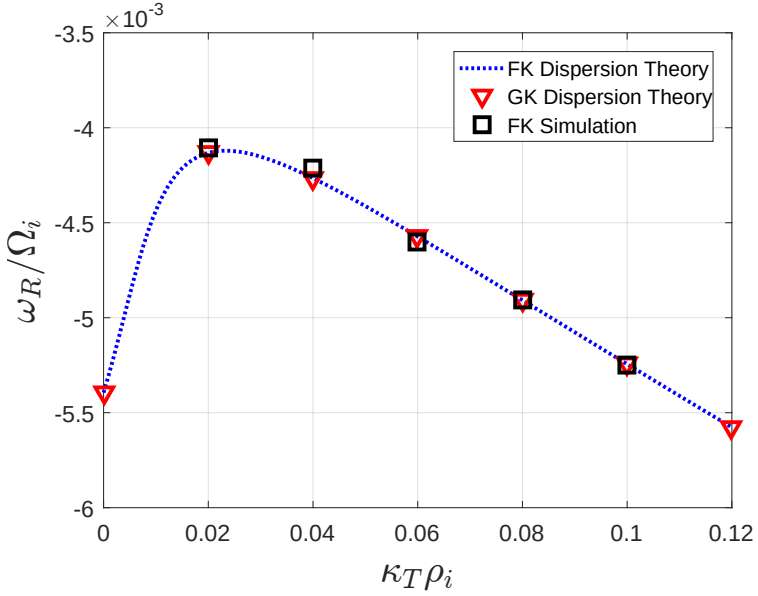
Figure: Dispersion results showing FLR effects on the ion acoustic wave.

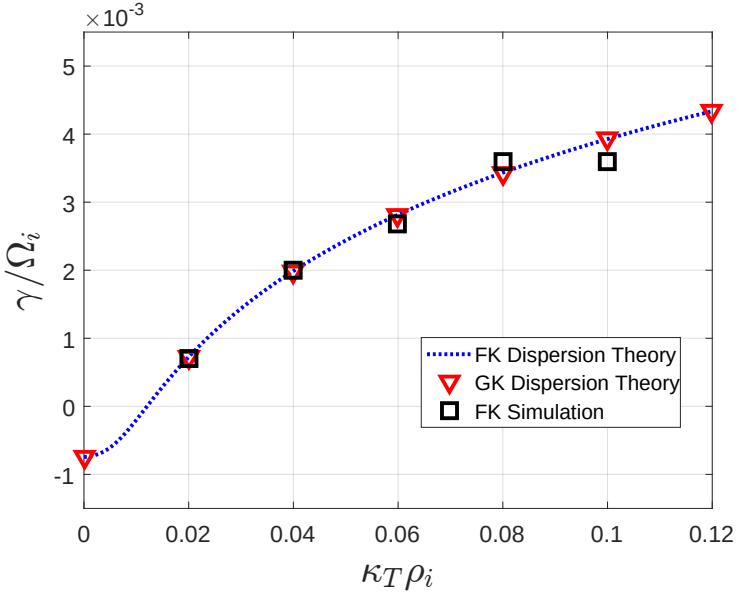
Parameters:

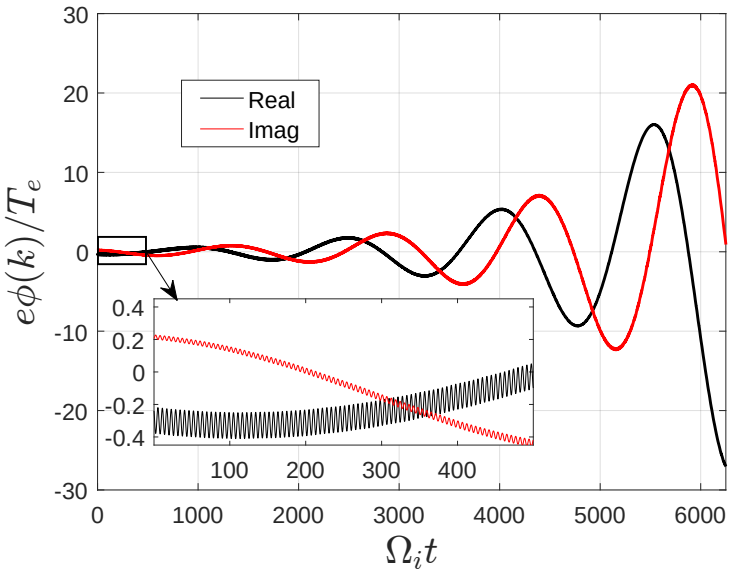
$$\frac{q_i T_e}{e T_i} = 5.0, \quad k_{\|}\rho_i = 1.61 \times 10^{-3}, \quad \Omega_i \Delta T = 0.75, \quad M = 18$$

ITG Instability in Slab Geometry

Simulation Results







$$\frac{q_i T_e}{e T_i} = 4.0$$

$$k_{\parallel}\rho_i = 2.0 \times 10^{-3}$$

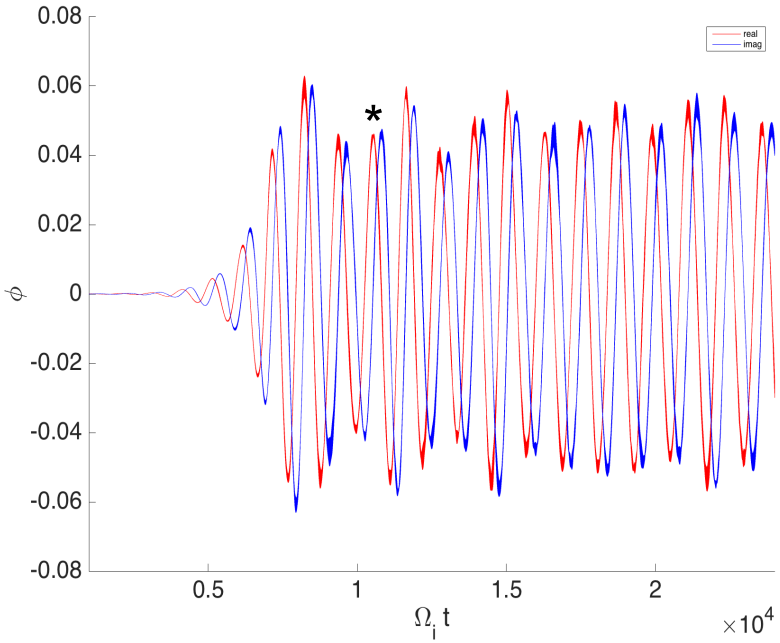
$$k_{\perp}\rho_i = 0.2$$

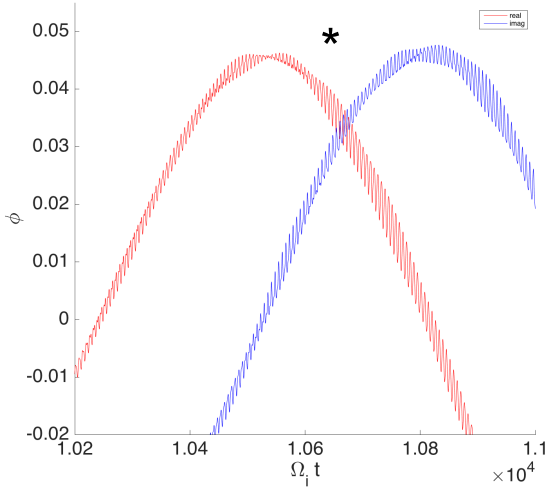
$$\kappa_T \rho_i = 0.02$$

$$\kappa_N \rho_i = 0.0$$

Nonlinear ITG Simulation

Simulation Results





M. Miecnikowski, Univ. of Colorado

- 2D slab (x,y), $\phi(1,1)$ mode (no zonal flow)
- Full kinetic nonlinear saturation due to $\mathbf{E} \times \mathbf{B}$ wave particle trapping
- Old GK results, e.g.

  Lee and Tang PoP 1988, Parker et al. PoP 1994

Outline:

Toroidal ITG Mode

Field Line Following Coordinates and Domain

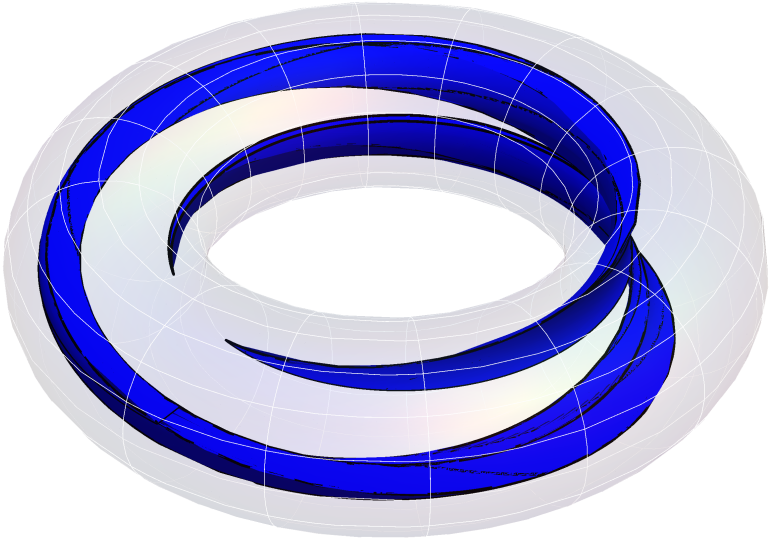


Figure: Flux Tube Domain

Field Line Following Coordinates: (x, y, z)

$$x = r - r_0$$

$$y = \frac{r_0}{q_0}\left(\int_0^\theta \frac{\mathbf{B}\cdot\nabla\zeta}{\mathbf{B}\cdot\nabla\theta}d\theta' - \zeta\right)$$

$$z = q_0 R_0 \theta$$

Reference Minor Radius: r_0

Safety Factor: $q_0 = q(r_0)$

$$\frac{\partial \mathbf{x}}{\partial z} \propto \mathbf{B} \quad \rightarrow \quad \mathbf{B}\cdot\nabla x = \mathbf{B}\cdot\nabla y = 0$$

$$D = \left\{(x, y, z)\middle| -\frac{l_x}{2} \leq x \leq \frac{l_x}{2}, -\frac{l_y}{2} \leq y \leq \frac{l_y}{2}, -q_0 R_0 \pi \leq z \leq q_0 R_0 \pi\right\}$$

Toroidal ITG Mode

Particle Integration Scheme

- Particle push is performed in cylindrical (R, Z, ζ) coordinates: yields simpler equations of motion than in (x, y, z).
- Need to capture particle motion accurately on long time scales.

$$\boxed{\text{An integrator is derived based on variational principles.}}$$

- Such integrators exhibit excellent conservation properties: energy, Lagrangian symmetries, symplectic, ...
- Starting point: formulate equations of motion as the vanishing variation of a functional.

$$\mathcal{S}\left[\mathbf{q}\right] = \int_0^{t_{\text{end}}} \mathcal{L}(\mathbf{q}(t), \dot{\mathbf{q}}(t))dt, \qquad \frac{\delta \mathcal{S}}{\delta \mathbf{q}(t)} = 0$$

Toroidal ITG Mode

Particle Integration Scheme

Discrete Lagrangian:

$$\mathcal{L}_d(\mathbf{q}^\nu, \mathbf{q}^{\nu+1}) \approx \int_{t^\nu}^{t^{\nu+1}} \mathcal{L}(\mathbf{q}(t), \dot{\mathbf{q}}(t))dt$$

E.g. trapezoidal rule:

$$\mathcal{L}_d(\mathbf{q}^\nu, \mathbf{q}^{\nu+1}) = \frac{\Delta t}{2}\mathcal{L}\left(\mathbf{q}^\nu, \frac{\mathbf{q}^{\nu+1} - \mathbf{q}^\nu}{\Delta t}\right) + \frac{\Delta t}{2}\mathcal{L}\left(\mathbf{q}^{\nu+1}, \frac{\mathbf{q}^{\nu+1} - \mathbf{q}^\nu}{\Delta t}\right)$$

Discrete action:

$$\mathcal{S}_d\left[\mathbf{q}\right] = \sum_{\nu=0}^{N-1} \mathcal{L}_d\left(\mathbf{q}^\nu, \mathbf{q}^{\nu+1}\right)$$

Variational principle:

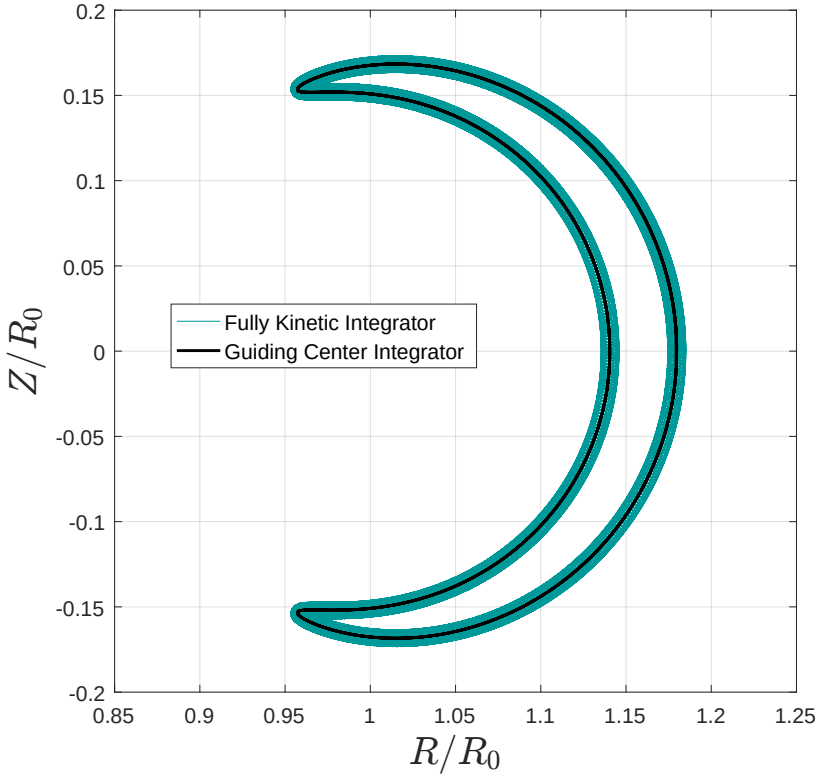
$$\frac{\delta \mathcal{S}_d}{\delta \left\{\mathbf{q}^\nu\right\}_{\nu=0}^N} = 0$$

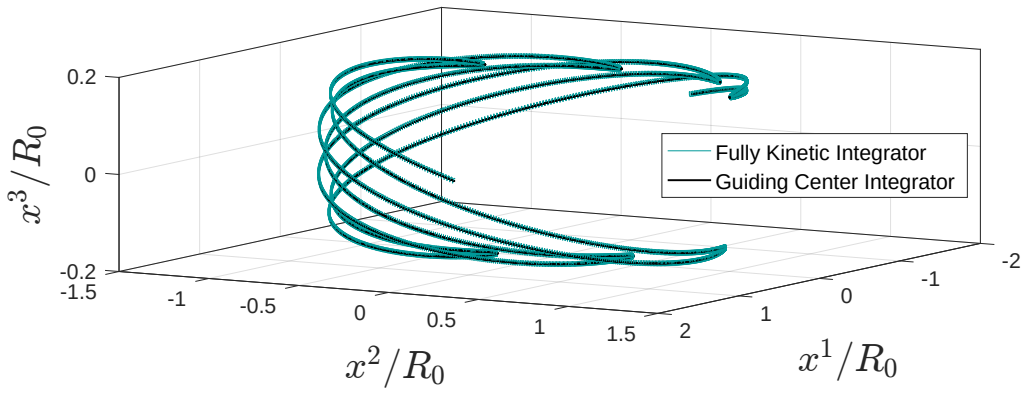
Toroidal ITG Mode

Particle Integration Scheme

Charged particle Lagrangian:

$$\mathcal{L} = \frac{m}{2}v^2 + q\mathbf{v}\cdot\mathbf{A} - q\phi$$

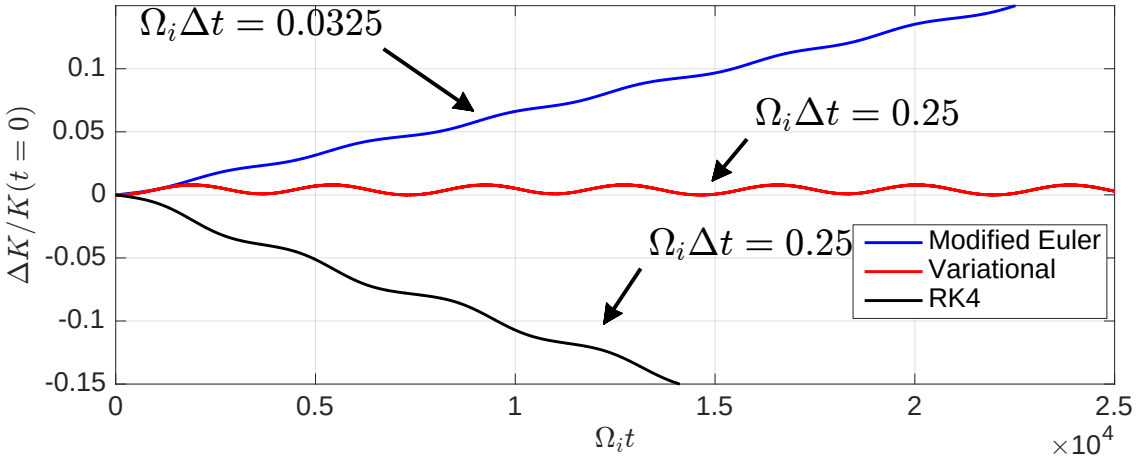


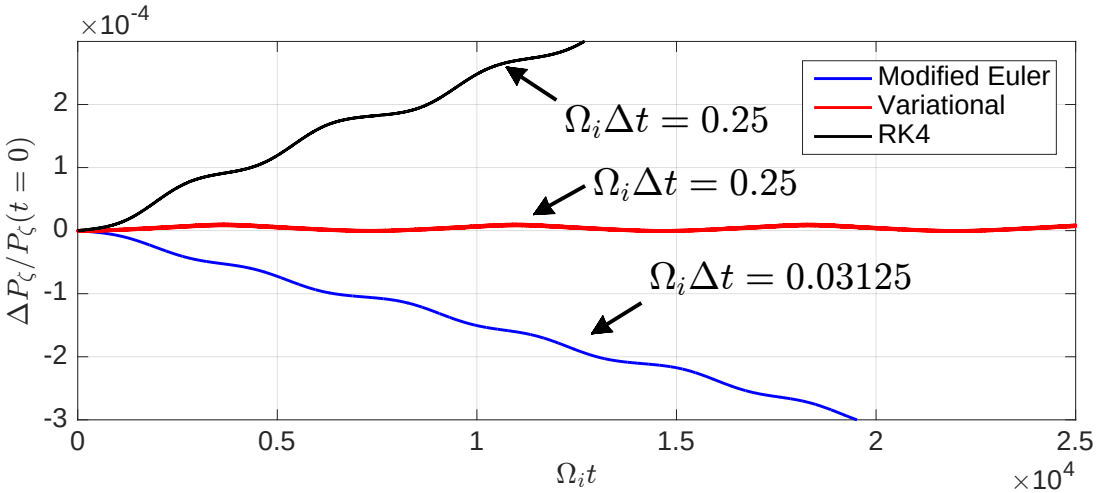


Toroidal ITG Mode

Particle Integration Scheme

Conservation of kinetic energy K and toroidal angular momentum p_ζ



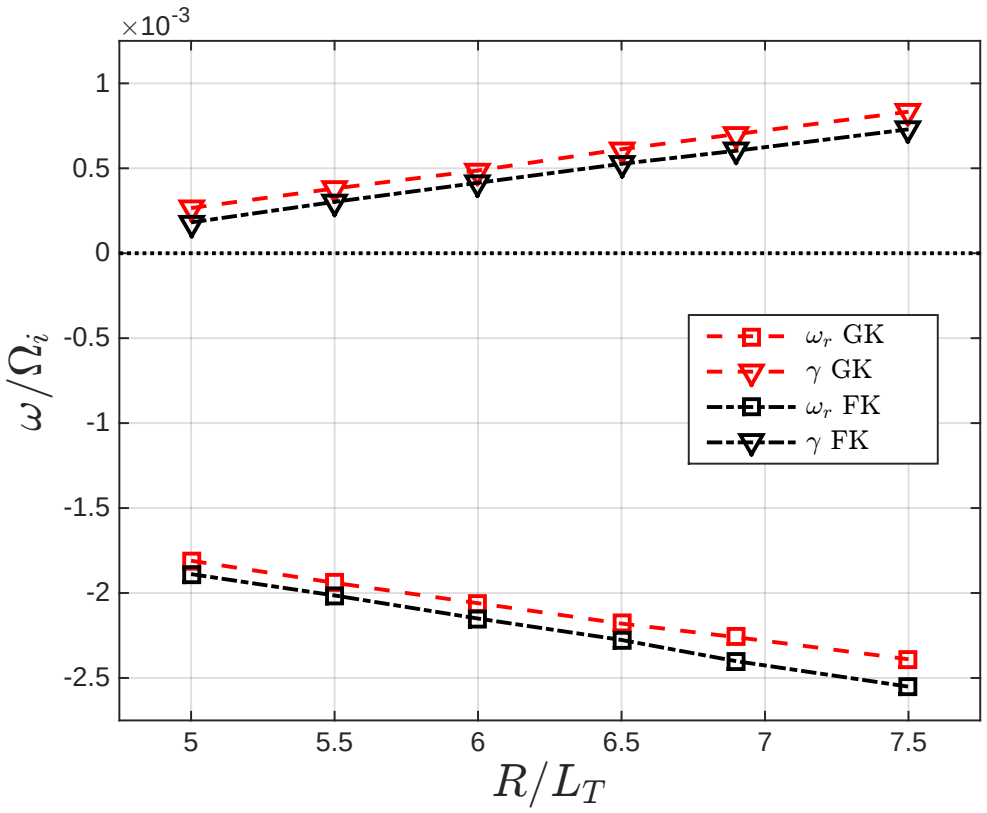


Toroidal ITG Mode

Simultaion Results

R_0/ρ_i	r_0/R_0	q_0	$\hat{s}$	R_0/L_T	R_0/L_N	q_iT_e/eT_i
445.0	0.18	1.4	0.78	6.9	2.2	1.0

Table: Cyclone DIII-D base case parameter set



Outline:

Summary

Summary

- A fully kinetic implicit multiscale model would be useful
  - Verification of GK when ordering parameters are not so small
  - Study strengths and limitations of GK
- Timesteps are not so small for many topical GK problems

$$\Omega_i \Delta t = 0.2 - 1$$

- Fully kinetic multiscale 3D toroidal code is operational
- Successful linear cyclone base case benchmark
- Beginning nonlinear GK comparisons

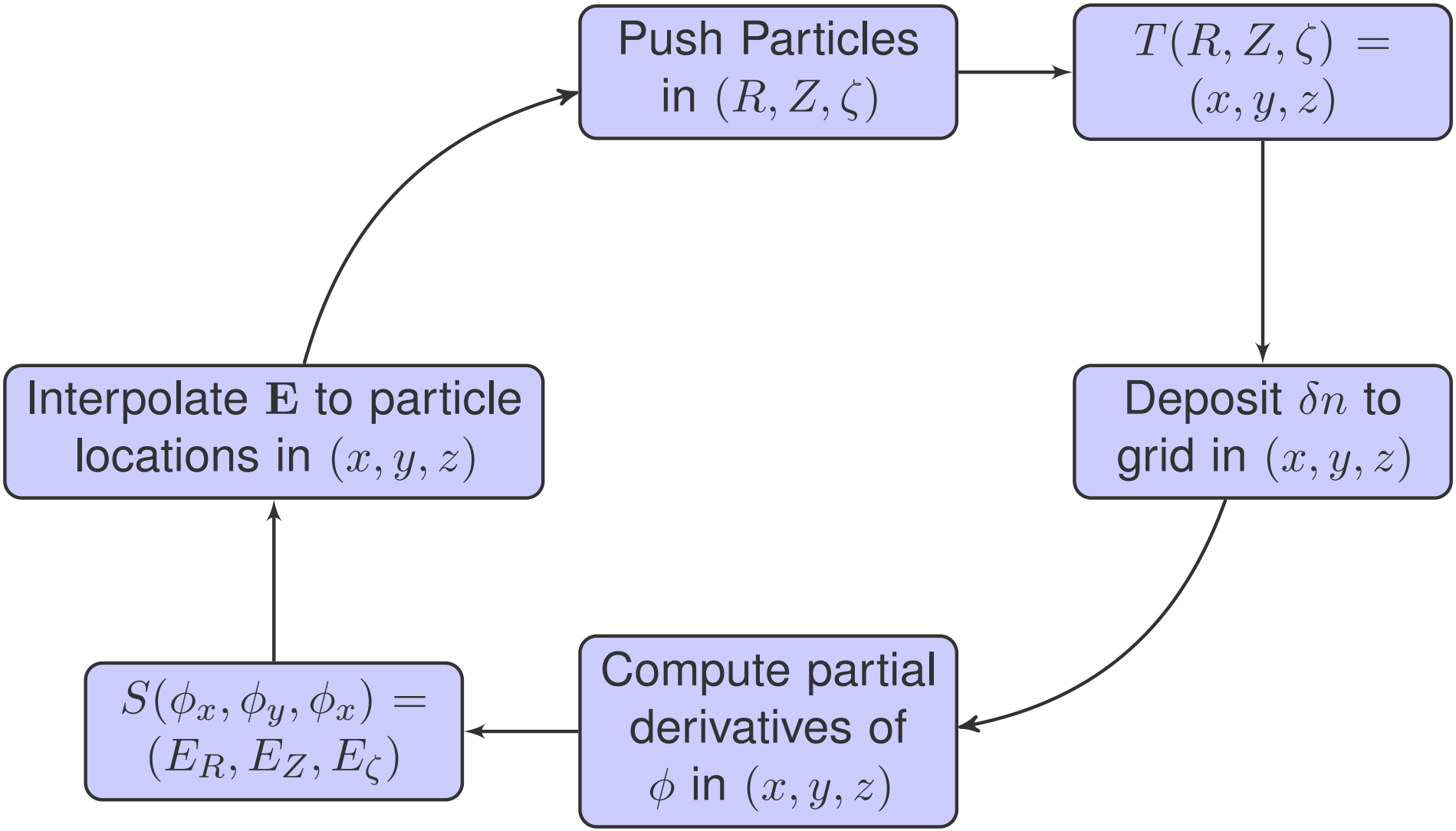
Questions?

Please ask!

Questions?

Toroidal ITG Mode

Algorithm Overview



Particle-In-Cell Method

Iteration Cycle for Implicit PIC