Low-Frequency $\delta f$ PIC Models with Fully Kinetic Ions

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Outline:

1 Motivation for Fully Kinetic Ions

2 A Fully Kinetic ITG Model

3 Implicit Orbit Averaging and Sub-Cycling

4 Simulation Results

5 Toroidal ITG Mode

6 Summary
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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:
  \[
  \frac{\rho_i}{L_{eq}} \sim \frac{\omega}{\Omega_i} \sim \frac{e\phi}{T_e} \sim \frac{\delta B}{B_{ext}} \sim k_\parallel \rho_i \sim O(\epsilon), \quad k_\perp \rho_i \sim O(1)
  \]

- GK Vlasov equation + modifications to Maxwell’s equations

- Enormous success in treating idealized core turbulence.
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.
    H-mode edge pedestal: \( \Omega_i \Delta t = 1.0 \)
    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 \( \rho_i/L_{eq} \) need to be?
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Basic Fully Kinetic Ion Model

Governing equations

- Vlasov equation for ions:

\[
\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_x f_i + \frac{q_i}{m_i} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_v f_i = 0
\]

- Testbed model

\[
\mathbf{E} = -\nabla_x \phi, \quad n_e = n_{e0} \left(1 + \frac{e\phi}{T_e}\right), \quad n_e = n_i = \int_{\mathbb{R}^3} f_i d^3v
\]

- Full model includes electromagnetic effects and drift kinetic electrons

Ion Temperature Gradient Instability Model

Equilibrium

• Vlasov Equilibrium Equation:

\[
\mathbf{v} \cdot \nabla_x f_{i0} + \frac{q_i}{m_i} (\mathbf{v} \times \mathbf{B}) \cdot \nabla \mathbf{v} f_{i0} = 0, \quad \epsilon = \frac{\rho_i}{L_{eq}} \ll 1
\]

\[O(1) \quad O(\epsilon^{-1})\]

• Equilibrium solution constructed from “constants” of motion: \(f_{i0}(K, R_x)\)

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

• Solve for perturbations from equilibrium \(\Rightarrow f_i = f_{i0} + \delta f:\)

\[
\frac{\partial}{\partial t} \delta f + \mathbf{v} \cdot \nabla \delta f + \frac{q_i}{m_i} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla \mathbf{v} \delta f = -q_i \mathbf{v} \cdot \mathbf{E} \frac{\partial f_0}{\partial K} - \frac{\mathbf{E} \times \hat{\mathbf{b}}}{B} \cdot \nabla x \frac{\partial f_0}{\partial R_x}
\]

“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:
  \[ \varepsilon_{FK}(k, \omega) = 0; \quad \varepsilon_{GK}(k, \omega) = 0 \]

- Expansion of \( \varepsilon_{FK} \) in GK ordering parameters:
  \[ \varepsilon_{FK}(k, \omega) = \varepsilon_{GK}(k, \omega) + O(\epsilon^2) \]

- 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 Alfvén Wave (EM): high frequency for \( k_\perp \rho_i \sim 1 \)
Figure: \( k_\perp \rho_i = 0.3 \) (left); \( k_\parallel \rho_i = 6.28 \times 10^{-3} \); \( \frac{q_i T_e}{e T_i} = 5.0 \); \( \kappa_N = \kappa_T = 0.0 \)

- 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:

\[
\delta f(x, v, t = 0) = A_0 e^{i \mathbf{k} \cdot \mathbf{x}} f_0(v)
\]
Reformulation of field equation:

\[
\frac{e\phi}{T_e} = \frac{\delta n_i}{n_0} \rightarrow \frac{\partial}{\partial t} \left( \frac{e\phi}{T_e} \right) = -\nabla \cdot \left( \frac{\delta (n_i u_i)}{n_0} \right), \quad \delta (n_i u_i) = \int_{\mathbb{R}^3} v \delta f_i d^3 v
\]

- Micro time step \( \Delta t \) resolves fast cyclotron motion. Macro time step \( \Delta T \) to resolves the low-frequency fields. \( \Delta T / \Delta t = M \)

- Time interpolated fields used in particle advance (sub-cycling):

\[
E_{\nu} = (1 - \frac{\nu}{M})E_N + \frac{\nu}{M}E_{N+1}.
\]

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

\[
\langle \delta (n_i u_i) \rangle_{N+1/2} = \frac{\Delta T}{M + 1} \sum_{\nu=0}^{M} \delta (n_i u_i)_{\nu}.
\]
Implicit Orbit Averaging and Sub-Cycling Algorithm

\[(x, v, w)\]
\[\delta(n_i u_i)\]
\[\langle \delta(n_i u_i) \rangle\]
\[\phi, E\]
\[t^{(0)}_{N-1} \quad t^{(1)}_{N-1} \quad \cdots \quad t^{(M-1)}_{N-1} \quad t^{(0)}_N \quad t^{(1)}_N \quad \cdots \quad t^{(M-1)}_N \quad t^{(0)}_{N+1}\]

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 $\delta f$ Simulation of Warm Plasmas”,
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

\[ \frac{q_i T_e}{e T_i} = 4.0 \]
\[ k_{\parallel} \rho_i = 2.0 \times 10^{-3} \]
\[ k_{\perp} \rho_i = 0.2 \]
\[ \kappa_T \rho_i = 0.02 \]
\[ \kappa_N \rho_i = 0.0 \]
M. Miecnikowski, Univ. of Colorado

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

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Toroidal ITG Mode
Field Line Following Coordinates and 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: \(q_0 = q(r_0)\)

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

\[
D = \left\{ (x, y, z) \bigg| -\frac{l_x}{2} \leq x \leq \frac{l_x}{2}, -\frac{l_y}{2} \leq y \leq \frac{l_y}{2}, -q_0 R_0 \pi \leq z \leq q_0 R_0 \pi \right\}
\]
Toroidal ITG Mode
Particle Integration Scheme

- Particle push is performed in cylindrical \((R, Z, \zeta)\) coordinates: yields simpler equations of motion than in \((x, y, z)\).

- Need to capture particle motion accurately on long time scales.

  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.

\[
S[q] = \int_0^{t_{\text{end}}} \mathcal{L}(q(t), \dot{q}(t)) \, dt, \quad \frac{\delta S}{\delta q(t)} = 0
\]
Discrete Lagrangian:

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

E.g. trapezoidal rule:

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

Discrete action:

\[ S_d[q] = \sum_{\nu=0}^{N-1} \mathcal{L}_d(q^\nu, q^{\nu+1}) \]

Variational principle:

\[ \frac{\delta S_d}{\delta \{q^\nu\}_{\nu=0}^N} = 0 \]
Charged particle Lagrangian:

\[ \mathcal{L} = \frac{m}{2} v^2 + qv \cdot A - q\phi \]
Conservation of kinetic energy $K$ and toroidal angular momentum $p_\zeta$
Table: Cyclone DIII-D base case parameter set

<table>
<thead>
<tr>
<th>$R_0/\rho_i$</th>
<th>$r_0/R_0$</th>
<th>$q_0$</th>
<th>$\hat{s}$</th>
<th>$R_0/L_T$</th>
<th>$R_0/L_N$</th>
<th>$q_iT_e/eT_i$</th>
</tr>
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<tr>
<td>445.0</td>
<td>0.18</td>
<td>1.4</td>
<td>0.78</td>
<td>6.9</td>
<td>2.2</td>
<td>1.0</td>
</tr>
</tbody>
</table>
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!
Push Particles in \((R, Z, \zeta)\)

\[ T(R, Z, \zeta) = (x, y, z) \]

Deposit \(\delta n\) to grid in \((x, y, z)\)

Interpolate \(E\) to particle locations in \((x, y, z)\)

Compute partial derivatives of \(\phi\) in \((x, y, z)\)

\[ S(\phi_x, \phi_y, \phi_z) = (E_R, E_Z, E_\zeta) \]
Particle-In-Cell Method

Iteration Cycle for Implicit PIC

Initial Guess
\( \mathbf{E}^{(i=0)}_{\nu+1} \)

Next Iteration
\( i \rightarrow i + 1 \)

Update Particles
\( \mathbf{E}^{(i)}_{\nu+1}, \mathbf{v}^{(i)}_{\nu+1} \)

Update Fields
\( \mathbf{E}^{(i)}_{\nu+1} \)

Deposit Particles
\( n^{(i)}_{\nu+1} \)