Multiscale, multiphysics modeling of turbulent transport and heating in collisionless, magnetized plasmas

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Overview

• Collisionless plasma dynamics are hard
• Let’s make life simpler: a mean field approach for turbulence and transport/heating in tokamak plasmas
• Numerical modeling approach: multiscale, hybrid kinetic/fluid code Trinity
• Issues and opportunities
Hot, magnetized plasmas
What do we want?

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \Gamma = \ldots \]

\[ \rho \frac{\partial u}{\partial t} + \nabla \cdot P = \ldots \]

\[ \frac{df}{dt} = C[f] \]
A tempting thought

“Think? Why think?! We have computers to do that for us.”

-- Jean Rostand
Range of scales

Time scale (seconds)

- $\Omega_e^{-1}$
- $\Omega_i^{-1}$
- $L/v_{te}$
- $L/v_{ti}$
- $\tau_c$

Space scale (meters)

- $\rho_e$
- $\rho_i$
- $L$

Gyromotion
Turbulence
Mean profiles
Collisions
Expense (brute force)

Time scale (seconds)

- Temporal grid: $\sim 10^{13}$ time steps

Space scale (meters)

- Spatial grid: $\sim 10^6$ grid points x 3-D = $10^{18}$ grid points
- Velocity grid: $\sim 10$ grid points x 3-D = $10^3$ grid points

Total: $\sim 10^{34}$ total grid points
Scale separation

Energy content vs. $k, \omega, \rho$

- Macroscale
- Microscale
Multiscale, multiphysics

Fast camera image of MAST plasma
Equilibrium macroscale spatial profile
Microscale fluctuations

GYRO simulation
J. Candy and R. Waltz
Equilibrium macroscale speed distribution

\[ f = f(\mathbf{r}, \mathbf{v}, t) \]
Microscale fluctuations

\( \delta f \)

GS2 simulation
Scale separation

\[ f(r, v, t) = F + \delta f \]
Macro drives micro

\[ f(r, v, t) = F + \delta f \]
Micro feeds back into macro

\[ f(r, \mathbf{v}, t) = F + \delta f \]
Coarse-grain average

In space...

...and in time...

...and moment approach in velocities
Multiscale model

Turbulent fluctuations calculated in small regions of fine space-time grid embedded in coarse grid for mean quantities (implemented in TRINITY code)
Gyrokinetic description of dynamics

\[
\frac{\partial f_s}{\partial t} + \frac{d\mathbf{r}}{dt} \cdot \frac{\partial f_s}{\partial \mathbf{r}} + \frac{d\mathbf{v}}{dt} \cdot \frac{\partial f_s}{\partial \mathbf{v}} = C[f_s]
\]

- Average over fast gyro-motion and follow ‘guiding center’ position
- Eliminates fast time scale and gyro-angle variable (6-D $\rightarrow$ 5-D)
Multiscale gyrokinetics

Decompose $f$ into mean and fluctuating components:

$$f = F + \delta f$$

Mean varies perpendicular to mean field on system size while fluctuations vary on scale of gyro-radius:

$$\nabla_\perp \ln F \sim L^{-1} \quad \nabla_\perp \ln \delta f \sim \rho^{-1}$$

Fluctuations are anisotropic with respect to the mean field:

$$\nabla_\parallel \ln \delta f \sim L^{-1}$$
Mixing length estimates

\[ \frac{\Delta n}{n} \sim \frac{\rho}{L} \]

Eddy size \( \sim \rho \)

Mixing length \( \sim (\text{step size}) \times (\text{# steps})^{1/2} \)

Macro time scale \( \sim (\text{step time}) \times (\text{# steps to mix over length } L) \)
\( \sim \left( \frac{L}{\rho} \right)^2 \times (\text{step time}) \)
Multiscale gyrokinetics

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Fluctuations are anisotropic with respect to the mean field:

$$\nabla_\parallel \ln \delta f \sim L^{-1}$$

$\Rightarrow$ Turbulent fluctuations are low amplitude: $\delta f \sim \epsilon f$

$\Rightarrow$ Mean profile evolution slow compared to turbulence:

$$\epsilon \equiv \frac{\rho}{L} \ll 1 \quad \frac{\partial \ln F}{\partial t} \sim \epsilon^2 \omega \sim \epsilon^3 \Omega$$
Gyrokinetic equation for fluctuation dynamics:

\[
\frac{\partial \langle \delta f \rangle}{\partial t} + \left( \frac{d\mathbf{R}}{dt} \right) \cdot \frac{\partial}{\partial \mathbf{R}} \left( \langle \delta f \rangle - q \langle \delta \Phi \rangle \frac{\partial F}{\partial \varepsilon} \right) + \left( \langle \frac{d\mathbf{R}}{dt} \rangle - \langle \frac{d\mathbf{R}}{dt} \rangle \right) \cdot \frac{\partial F}{\partial \mathbf{R}} = \langle C[\delta f] \rangle
\]

Fluid conservation equations for mean dynamics:

\[
\frac{\partial \bar{n}}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} \left( V' \bar{\Gamma} \right) = \bar{S}_n
\]

\[
\frac{\partial \bar{L}}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} \left( V' \bar{\Pi} \right) = \bar{S}_L
\]

\[
\frac{3}{2} \frac{\partial \bar{p}}{\partial t} + \frac{1}{V'} \frac{\partial}{\partial r} \left( V' \bar{Q} \right) = \bar{S}_p
\]

Fluxes are functions of fluctuating quantities
Expense (multiscale gyrokinetics)

Time scale (seconds)

Space scale (meters)

Temporal grid: \( \sim 10^5 \) time steps

mean-fluctuation separation

Perpendicular spatial grid: \( \sim 10^5 \) grid points \( \times \) 2-D = \( 10^{10} \) grid points

Parallel spatial grid: \( \sim 10 \) grid points \( \times \) 1-D = 10 grid points

Velocity grid: \( \sim 10 \) grid points \( \times \) 2-D v-space = \( 10^2 \) grid points

Total: \( \sim 10^{18} \) total grid points (\( 10^6 \) savings)
TRINITY schematic

Steady-state turbulent fluxes and heating

Macro profiles

Transport solver

Flux tube 1 → GS2/GENE
Flux tube 2 → GS2/GENE
Flux tube 3 → GS2/GENE
Flux tube N → GS2/GENE
Transport equations are stiff, nonlinear PDEs:

$$\frac{3}{2} \frac{\partial p_s}{\partial t} = -\frac{1}{V'} \frac{\partial}{\partial \psi} \left( V' \langle Q_s \cdot \nabla \psi \rangle \right) + ...$$

$$Q_s = Q_s [n(\psi, t), T(\psi, t); \psi, t]$$

Implicit treatment needed for stiffness
Newton solve

- Challenge: requires computation of quantities like

$$\Gamma_{j}^{m+1} \approx \Gamma_{j}^{m} + (y_{m+1} - y_{m}) \frac{\partial \Gamma_{j}}{\partial y} \bigg|_{y_{m}}$$

$$y = [\{n_{k}\}, \{p_{s_{k}}\}, \{L_{k}\}]^{T}$$

- Local approximation:

$$\frac{\partial \Gamma_{j}}{\partial n_{k}} = \frac{\partial \Gamma_{j}}{\partial n_{j}} + \frac{\partial \Gamma_{j}}{\partial (R/L_{n})_{j}} \frac{\partial (R/L_{n})_{j}}{\partial n_{k}}$$

- Simplifying assumption: normalized fluxes depend primarily on gradient scale lengths

- Implicit treatment allows for time steps $\sim 0.1$ seconds (vs. turbulence sim time $\sim 0.001$ seconds)
Parallelization

Calculating flux derivative approximations:

• at every radial grid point, simultaneously calculate
  \[ \Gamma_j \left[ \left( \frac{R}{L_n} \right)_j^m \right] \text{ and } \Gamma_j \left[ \left( \frac{R}{L_n} \right)_j^m + \delta \right] \]
  using 2 different flux tubes

• Possible because flux tubes independent (do not communicate during turbulence calculation)

• Perfect parallelization

• use 2-point finite differences for derivative:
  \[
  \frac{\partial \Gamma_j}{\partial \left( \frac{R}{L_n} \right)_j} \approx \frac{\Gamma_j \left[ \left( \frac{R}{L_n} \right)_j^m \right] - \Gamma_j \left[ \left( \frac{R}{L_n} \right)_j^m + \delta \right]}{\delta}
  \]
Example calculation with 10 radial grid points:

• Evolve electron density, toroidal angular momentum, and ion/electron pressure profiles

• Simultaneously calculate fluxes for equilibrium profile and for perturbed profiles (one for each time-varying gradient scale length, i.e. 4)

• Total of 50 flux tube simulations running in parallel
Flux tube scaling

- **GS2 strong scaling**
  - Speedup: 14.2 / 16

- **GENE strong scaling**

- **GENE weak scaling**
  - Larger (global) problems are expected to scale up to many million cores

**Charts:**
- BG/L at Rochester, Minnesota: 2 – 2k procs
- BG/L at Watson Research C., NY: 2k – 32k procs

**GS2 strong scaling**
- Seaborg, RS/6000 SP
- IBM Blue Gene/L
- Dawson
- Bassi
- Franklin

**GENE weak scaling**
- Ideal
- Time per step

Authors: H. Lederer et al.
Example calculation with 10 radial grid points:

- Evolve electron density, toroidal angular momentum, and ion/electron pressure profiles
- Simultaneously calculate fluxes for equilibrium profile and for perturbed profiles (one for each time-varying gradient scale length, i.e. 4)
- Total of 50 flux tube simulations running in parallel
- ~2-4k cores or more per flux tube => scaling to over 100k’s processors with very high efficiency
Example: JET H-mode

- 10 radial grid points
- Costs ~120k CPU hrs (<10 clock hrs)
- Dens and temp profiles agree within ~15% across device
- Energy off by 5%
- Incremental energy off by 15%
Issues and opportunities
Issue: Scale separation?

- Energy content
- Macroscale
- Microscale

$k, \omega, p$
Issue: Scale separation?
From T. S. Eliot’s *Little Gidding*,

“We shall not cease from exploration
And the end of all our exploring
Will be to arrive where we started
And know the place for the first time.”
Issue: Computational expense

- Could reduce computational expense considerably by using a reduced model for the microscale physics
  - fluid model
  - proper orthogonal decomposition
  - LES for kinetics

- These approaches share weakness that they are not universal

- This weakness can be ameliorated by the multiscale approach
Equilibrium macroscale spatial profile