A Framework for First-Principles Simulations of Coupled Turbulent Transport

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Challenges

• Turbulent transport in ITER and other fusion plasmas involves interaction of phenomena spanning a wide range of time and space scales:

<table>
<thead>
<tr>
<th>Physics</th>
<th>Perpendicular spatial scale</th>
<th>Temporal scale</th>
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</thead>
<tbody>
<tr>
<td>Electron energy transport from ETG modes</td>
<td>$k_\perp^{-1} \sim 0.001 - 0.1$ cm</td>
<td>$\omega_* \sim 0.5 - 5.0$ MHz</td>
</tr>
<tr>
<td>Ion energy transport from ITG modes</td>
<td>$k_\perp^{-1} \sim 0.1 - 8.0$ cm</td>
<td>$\omega_* \sim 10 - 100$ kHz</td>
</tr>
<tr>
<td>Transport barriers</td>
<td>Measurements suggest width $\sim 1 - 10$ cm</td>
<td>100 s or more in core?</td>
</tr>
<tr>
<td>Discharge evolution</td>
<td>Profile scales $\sim 100$ cm</td>
<td>Energy confinement time</td>
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<td>$\sim 2 - 4$ s</td>
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</table>
• Turbulence driving transport is kinetic (requires 5D description):

Electrostatic potential from GS2 spherical tokamak simulation (courtesy W. Dorland)

Velocity space structure in gyroaveraged distribution function (courtesy T. Tatsuno)
Resolving kinetic turbulence

• Fine scales possible in velocity space:

\[ \frac{\partial h}{\partial t} + (v_\parallel + \bar{v}\chi + v_d) \cdot \nabla h = -\bar{v}\chi \cdot \nabla F_0 + \frac{q}{T_0} \frac{\partial \bar{\chi}}{\partial t} F_0 + \bar{C}[h] \]

\[ \frac{\partial h_s}{\partial t} \sim \bar{C}[h_s] \sim \nu_s v_{th}^2 \frac{\partial^2 h_s}{\partial v^2} \Rightarrow \left( \frac{\delta v}{v_{th}} \right)_s \sim \sqrt{\frac{\nu_s}{\omega}} \]

For ITER:

\[ \omega \sim \omega_* \sim 10^4 \ Hz, \ \nu_i \sim 10^2 \ Hz \]

\[ \Rightarrow \frac{\delta v}{v_{th}} \sim 0.1 \]
Can monitor v-space resolution by estimating error in numerical evaluation of field integrals:

- Only nontrivial v-space operation in collisionless GK eqn. is integration to get fields
- Estimate error in field integrals by comparing with integrals performed after dropping grid points in v-space

Drop all points with same pitch-angle (red points on right) to get error estimate for pitch-angle integration and repeat for each pitch-angle
- Same process for energy (blue points on right)
• Can also monitor v-space resolution by calculating relative amplitude of coefficients in distribution function expansion:

\[ h(x) \approx \sum_{i=1}^{N} c_i P_i(x) \Rightarrow c_i \sim \int dx \ P_i(x) h(x) \]

\[ \text{Error estimate} \equiv \max_{i=N-2} \frac{c_i}{\max_{i=1} c_i} \]

• Error estimate for each scheme is conservative
  – for integral scheme, this is due to use of Gaussian quadrature rules (dropping grid point changes order of accuracy from 2N-1 to N-2)
  – for spectral scheme, this is due to fact that we can only accurately calculate \( c_i \) for \( i < N \) (because it’s a numerical integral over the product of two polynomials)
Linear, toroidal ITG mode

Error estimates conservative, require empirical scaling
Collisionless damping of kinetic Alfven wave

- Unable to resolve damping indefinitely with finite grid spacing in absence of dissipation
Model collision operator for gyrokinetics

- Implemented new collision operator in GS2

\[
C_{\text{GK}}[h_k] = L[h_k] + D[h_k] + U_L[h_k] + U_D[h_k] + E[h_k]
\]

\[
L[h_k] = \frac{\nu_D}{2} \frac{\partial}{\partial \xi} \left(1 - \xi^2\right) \frac{\partial h_k}{\partial \xi} - \frac{k_\perp^2 v^2}{4 \Omega_0^2} \nu_D \left(1 + \xi^2\right) h_k
\]

\[
D[h_k] = \frac{1}{2v^2} \frac{\partial}{\partial v} \left(\nu_\parallel v^4 F_0 \frac{\partial h_k}{\partial v} F_0\right) - \frac{k_\perp^2 v^2}{4 \Omega_0^2} \nu_\parallel \left(1 - \xi^2\right) h_k
\]

\[
U_L[h_k] = \nu_D F_0 \left( J_0 \nu_\parallel \frac{\int d^3v \nu_D v_\parallel J_0 h_k}{\int d^3v \nu_D v_\parallel^2 F_0} + J_1 \nu_\perp \frac{\int d^3v \nu_D v_\perp J_1 h_k}{\int d^3v \nu_D v_\perp^2 F_0} \right)
\]

\[
U_D[h_k] = -\Delta \nu F_0 \left( J_0 \nu_\parallel \frac{\int d^3v \Delta \nu v_\parallel J_0 h_k}{\int d^3v \Delta \nu v_\parallel^2 F_0} + J_1 \nu_\perp \frac{\int d^3v \Delta \nu v_\perp J_1 h_k}{\int d^3v \Delta \nu v_\perp^2 F_0} \right)
\]

\[
E[h_k] = \nu_E v^2 J_0 F_0 \frac{\int d^3v \nu_E v^2 J_0 h_k}{\int d^3v \nu_E v^4 F_0}
\]
Numerical properties

• Fully implicit
  – Pitch-angle scattering and energy diffusion treated separately through Godunov splitting
  – Finite difference scheme first order accurate and satisfies discrete versions of Fundamental Theorem of Calculus and integration by parts (upon double application). Leads to tridiagonal matrices
  – Conserving terms incorporated at little additional cost using repeated application of Sherman-Morrison formula:

\[
\text{If } Mx = b \text{ and } M = A + u \otimes v, \text{ then } x = y - \frac{v \cdot y}{1 + v \cdot z} z,
\]

where: \( y = A^{-1}b \) and \( z = A^{-1}u \)
Exact local conservation of particle number, momentum, and energy

Solid lines: conservative discretization used in GS2
Short dashed lines: non-conservative discretization
Long dashed lines: model operator without conserving terms.
Satisfies H-Theorem

\[ \frac{dS}{dt} \geq 0 \]

Correct viscous, collisional, and collisionless damping

homogeneous slab initialized with noise in \( v \)-space

high-\( \beta \) slow mode
Correctly captures resistivity

For electrons:

\[
C_{eK}^{e} [h_e] = C_{eK}^{ee} [h_e] + \frac{\nu_D^{ei}}{2} \frac{\partial}{\partial \xi} \left( 1 - \xi^2 \right) \frac{\partial h_e}{\partial \xi} - \frac{k^2 v^2}{4 \Omega_0^2} \nu_D^{ei} (1 + \xi^2) h_e + \nu_D^{ei} \frac{2 v_i}{v_{th,e}^2} J_0 F_0
\]
Efficient small-scale cutoff in phase space

- Weakly collisional, electrostatic turbulence in Z-pinch. No artificial dissipation necessary to obtain steady-state fluxes
Weakly collisional damping of kinetic Alfven wave

- Small collisionality leads to well-resolved long-time simulation and recovery of collisionless damping rate
Adaptive collisionality

- Specify v-space error tolerance and calculate v-space error estimate
- Adaptively change collisionality to ensure error not too large
- Provides approximate minimal collisionality necessary for resolution
Coupling turbulence and transport

Steady-state turbulent fluxes

Flux tube 1

Flux tube 2

Flux tube 3

Transport solver

Updated profiles

Flux tube N

Initial profiles

GS2
Minimizes simulation volume

- Flux tube simulations take advantage of statistical periodicity along field lines, giving factor of $n_\phi$ savings in volume compared to global simulations ($n_\phi \equiv$ toroidal mode #)
Optimizes grid resolution

- Standard global simulations use fixed $k_\perp$ range across minor radius
- Each flux tube calculation is independent, allowing for different $k_\perp$ ranges at each radial position

\[ \alpha < k_\perp < \beta \text{ vs. } \tilde{\alpha} < k_\perp \rho(\psi) < \tilde{\beta} \]

- Results in factor of $\sqrt{T_C/T_E}$ savings in required $k_\perp$ range ($T_C \equiv$ core temp, $T_E \equiv$ edge temp)
Minimizes number of time steps

- Transport and turbulence time scales separated in gyrokinetic ordering:
  \[ t \sim \epsilon^2 \tau, \quad \tau \equiv \text{transport time scale} \]
  \[ \epsilon \sim \rho_*, \quad t \equiv \text{turbulence time scale} \]

- Multiscale scheme exploits intrinsic scale separation by:
  - taking small turbulence time steps to get steady-state fluxes (with stationary background profiles)
  - taking large transport time steps to evolve background profiles (factor of \( \epsilon^{-2} \) bigger than turbulent time steps)
Example: ITER simulation savings

• Relevant $n_\phi \sim 100$ --> factor of $\sim 100$ savings in simulation volume

• $T_C/T_E \sim 7$ --> factor of $\sim 3$ savings in $k_\perp$ resolution

• $\rho_* \sim 10^{-5}$ --> factor of $\sim 10^6$ savings in number of time steps

• Overall factor of $\sim 10^8$ savings over standard global simulation!

• Translates to hours of gigaflop computations instead of weeks of petaflop computations
Transport model

\[
\frac{\partial n_s}{\partial t} = -\frac{\partial \psi}{\partial V} \frac{\partial}{\partial \psi} \left[ \frac{\partial V}{\partial \psi} \langle \mathbf{T}_s \cdot \nabla \psi \rangle \right] \quad \text{particle transport}
\]

\[
\frac{3}{2} \frac{\partial (n_s T_s)}{\partial t} = -\frac{\partial \psi}{\partial V} \frac{\partial}{\partial \psi} \left[ \frac{\partial V}{\partial \psi} \langle \mathbf{Q}_s \cdot \nabla \psi \rangle \right] \quad \text{energy transport}
\]

\[
+ \quad T_s \left( \frac{\partial \ln n_s}{\partial \psi} - \frac{3}{2} \frac{\partial \ln T_s}{\partial \psi} \right) \langle \mathbf{T}_s \cdot \nabla \psi \rangle + \frac{\partial \ln T_s}{\partial \psi} \langle \mathbf{Q}_s \cdot \nabla \psi \rangle
\]

\[
- \quad \left\langle \int d^3 \mathbf{v} \frac{h_s T_s}{F_{0,s}} \langle C(h_s) \rangle_{\mathbf{R}} \right\rangle + n_s \nu^s_{\mathcal{E}} (T_u - T_s)
\]
Comments on multiscale scheme

• Turbulent flux calculations are orders of magnitude more expensive than advancing transport equations

• Calculation of turbulent fluxes in each flux tube is completely independent of other flux tubes

• Consequently, coupling of multiple flux tubes is almost perfectly parallelizable

• Critical for computational feasibility:
  – optimized nonlinear flux calculations in GS2
  – minimized number of sets of nonlinear flux calculations required for background profiles to reach steady-state
Transport solver algorithm

• Currently using 4th-order compact differencing in space with optional artificial dissipation for smoothing
• Time advanced at present with explicit predictor-corrector for fluxes and implicit Crank-Nicholson for all other terms
• Full nonlinearly implicit scheme (Newton solver) being implemented
  – based on algorithm developed by Jardin et. al*
  – algorithm implemented in existing production tokamak transport codes and shown to improve stability of standard Crank-Nicholson scheme

Preliminary results

- Collisionless, adiabatic electrons, single transport channel, quasilinear estimate for heat flux, Cyclone geometry
- Qualitatively correct behavior for and fluxes and profiles:

Future work

- Finish implementation of Newton solver
- Implement more sophisticated quasilinear model as preconditioner for nonlinear simulations
- Include neoclassical transport and evolving background magnetic field (via Grad-Shafronov)
- Include sheared radial electric field profile
- Include equations for parallel and toroidal angular momentum transport
- Apply algorithm to nonlinear simulations of multiple species, electromagnetic turbulent transport
Validity of local approximation

- lines represent global simulations from GYRO
- dots represent local simulations from GS2
- good agreement for $\rho_* \ll 1$

Transport model (2)

- Definitions:

\[ \langle \mathcal{F} \rangle \equiv \text{flux surface average of } \mathcal{F} \]

\[ V \equiv \text{infinitesimal volume between flux surfaces} \]

\[ \Gamma_s = \int d^3v \, v \chi h_s, \quad Q_s = \int d^3v \frac{m_s v^2}{2} v \chi h_s \]

\[ v \chi = \frac{c}{B_0^2} \left( \hat{b} \times \nabla \chi \right), \quad \chi = \Phi - \frac{v}{c} \cdot A \quad h_s = \delta f_s + \frac{q_s \Phi}{T_s} \]

- Derivation of equations describing momentum transport is work in progress.

- However, recent studies suggest that inclusion of momentum transport is negligible effect.
Efficiency of GS2 flux calculations

• Simulation length at new transport time step decreased by initializing with parameters from end of previous transport time step (bypasses linear phase of flux evolution)

Change in $R/L_T$

Time averaged flux