Third Year Status
on
SciDAC Center for Gyrokinetic Particle Simulation of Turbulence Transport in Burning Plasmas

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Outline

• Center Activities
  -- Fall Meeting
  -- Invited talks and Publications

• Code Development

• Code Validation

• Physics Investigations

• The noise and growing weight issues

• Conclusions
FALL MEETING
SciDAC Center for Gyrokinetic Particle Simulation
of Turbulent Transport in Burning Plasmas

Room 407-408
Philadelphia Marriott Hotel, Philadelphia, PA

November 2, 2006

7:00P  Lee - Opening remarks
7:10P  Wang - Shaped plasma simulations and future plans
7:25P  Ethier - GTC performance and optimization issues
7:40P  Lin - Status and plan in global GTC turbulence simulation
7:55P  Nishimura - Shear Alfvén wave studies in electromagnetic global gyrokinetic
simulator of tokamak plasmas
8:10P  Parker - ETG Convergence Studies, GEM Team status
8:25P  Y. Chen - The growing weight problem
8:40P  Rewoldt -- Application of GEM code for experimentally-realistic tokamak cases
8:55P  Hahm - Theory team status and plan
9:10P  Coffee break
9:25P  Holod - Particle noise-driven flux in GTC simulations
9:35P  Xiao - Theory of zonal flow residual level with arbitrary wavelength and collisionality
9:45P  Jenkins – Particle noise issues
9:55P  Diamond – Concluding remarks
10:05P Klasky - Data Management, Visualization and MPP issues
10:15P Plans for re-competition
11:15P Recess
Invited Talks and Review Papers


Publications

Review of Modern Physics: 1
Physics of Plasmas: 11 published, 2 submitted
Journal of Computational Physics: 2 published
IAEA: 4 published
Other Journals: 3 published
Conference Proceedings: 11 published
Code Development

• GTS
  -- A global code for turbulence transport simulations
  -- Shaped plasma in general geometry interface with TRANSP, JSOLVER and ESC
  -- Electron dynamics based on the split-weight scheme:
    \[\delta h, \text{non-adiabatic part of } \delta f\]
  -- GK Poisson’s equation is solved simultaneously for zonal flows and perturbed potentials

• GTC
  -- Adiabatic electron version for high performance computing
  -- Electrostatic electron dynamics based on the hybrid scheme
  -- Electromagnetic electron dynamics based on the hybrid scheme:
    \[|\omega/k_\parallel|v_\parallel| \ll 1\]
• GTC-neo -- For neoclassical transport simulations in
  -- General toroidal geometry
  -- Fully operational collision operators

• GEM
  -- A wedge code with multi-ion species for turbulence and gyrokinetic MHD simulations
  -- Shaped plasma in general geometry with interface with TRANSP and JSOLVER
• Object Oriented GTC framework -- Based on Fortran-90 to facilitate team coding
GTC is very portable, scalable and efficient on both cache-based and vector-parallel MPPs.

20 TeraFlops/sec performance has been achieved with 74 billion particles on Jaguar (ORNL) with 22,976 cores and 2.8 times faster than with 32,786 BG/L cores.

S. Ethier, PPPL, Apr. 2007
Numerical Considerations for Gyrokinetic Simulation Codes

• Flux Tube codes are valid for large \((m, n)\) modes

• Wedge codes include radial variations and some are valid only for large \((m, n)\) modes

• Global codes are valid for any \((m, n)\) modes and are truly five dimensional

• Physics of turbulence transport alone dictates the usefulness of these codes, i.e.,

  -- are radial modes local or global?

  -- does energy cascade to lower or higher \((m, n)\) modes?

  -- how about enstrophy, to higher \((m, n)\) modes?

  -- perpendicular spatial resolution: ion gyroradius, electron skin depth or electron gyroradius?

  -- parallel spatial resolution: field line following coordinates?

  -- velocity space resolution?
    √ trapped particle dynamics
    √ wave-particle interactions
    √ artificial dissipation
    √ discrete particle noise

  -- collisions: can neoclassical transport be simulated?
• Global Turbulence Dynamics in Shaped Plasmas

• Interfaced with TRANSP and JSOLVER and ESC

• Re-Write of GTC

ITG Turbulence Spreading

ITG Energy Cascade to longer wavelength modes

Turbulent transport is a global phenomena
$E \times B$ Shear Layer Blocks Turbulence Spreading

- $\omega_{E \times B}^{\text{max}} = 0$: turbulence widely spreads to fill up big area in both directions
- $\omega_{E \times B}^{\text{max}} = 0.13 \frac{c_s}{a}$: inward spreading partially blocked
- $\omega_{E \times B}^{\text{max}} = 0.26 \frac{c_s}{a}$: almost completely blocked
- Shear layer not only reduces turbulence spreading extension but also slows down the spreading
- Turbulence level not increased in source region as spreading blocked
- Outward spreading is not affected

W. X. Wang - GTS
Recent Development of GTC-S and NSTX-physics-oriented Algorithm

- Generalized Poisson Solver to solve integral equation for total potential \( \Phi = \delta \Phi + \langle \Phi \rangle \) using superLU/PETSc.
  
  Previous solver solves \( \delta \Phi \) and \( \langle \Phi \rangle \) separately using approximations:
  
  i) Pade approximation \( \Gamma_0(b) = I_0(b)e^{-b} \approx 1/(1 + b) \) and
  
  ii) \( \langle \tilde{\Phi} \rangle \approx \langle \Phi \rangle \) – not justified for NSTX geometry!
General Geometry GTC-neo

W. X. Wang [PoP, ‘06]
Comparisons of GEM with NSTX: Energy Flux Measurements

- First results - does not include parallel ion equilibrium flows! (which are transonic or supersonic)
- 128 particles / species / grid cell, 3 ion species, experimental $\beta$
ITG simulations with for adiabatic electrons based on Cyclone-based parameters using GTC

Peak $\chi_i$ (bin 3) - $a/\rho_i=125$
(part/cell=10, mzetamax=32, cyclone case profile, parallel non-linearity study)

- Steady state fluxes remain essentially the same with or without zonal flows and with or without parallel velocity space nonlinearity for a small simulation volume.

- But, these nonlinearities become progressively important for larger systems

Lee, Ethier and Kolesnikov
• For example, zonal flows are essential for maintaining steady state flux for a larger simulation volume.

Lee, Ethier and Kolesnikov
Both zonal flows and velocity-space nonlinearity are essential for maintaining steady state flux for an even larger system ($a/\rho = 500$).

• There is no steady state without these nonlinearities in large scale global simulations.

Lee, Ethier and Kolesnikov
Conservation properties of ITG simulation (20 particles/cell)

\[ \int \left( \frac{1}{2} m v^2 \right) j \, d^3 v \]

Time evolution of particle energy
(Cyclone base case -- a/p = 125 -- 20 particles/cell)

\[ \int |\nabla \Phi|^2 j \, dx^3 \]

Time evolution of turbulence energy
(Cyclone base case -- a/p = 125 -- 20 particles/cell)

\[ \int |\delta \Phi|^2 j \, dx^3 \]

Time evolution of adiabatic electron energy
(Cyclone base case -- a/p = 125 -- 20 particles/cell)

\[ \int |V_E \times B|^2 j \, dx^3 \]

Time evolution of zonal flow energy
(Cyclone base case -- a/p = 125 -- 20 particles/cell)

Lee, Ethier and Kolesnikov
\( \chi^i \) is enhanced above the adiabatic electron level (with NLV)

- ITG simulation with kinetic electrons using GTC with the split-weight scheme [Lewandowski et al]
- TEM simulation with collisionless electrons using GEM with the split-weight scheme [Lang, Parker and Chen]

**Enhanced electron particle flux**

Zonal flows develop finer structures
GTC-EM: fluid electron model

Mode structures for (a) the electrostatic potential and (b) the vector potential

Growth rates and real frequencies for finite-beta modified ITG modes

Nishimura, Lin and Wang
Momentum Pinch from Magnetic Curvature

Two different mechanisms for non-diffusive momentum flux

\[ m_i B^* \frac{d\nu}{dt} = -(eB + m_i c v_{\|} \nabla \times \hat{b}) \cdot \nabla \delta \phi \]

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<tbody>
<tr>
<td>Symmetry-breaking:</td>
<td>(-e_i B \nabla_{|} \delta \phi)</td>
<td>(-m_i c v_{|} \nabla \times \hat{b} \cdot \nabla \delta \phi)</td>
</tr>
<tr>
<td>Symmetry-breaking:</td>
<td>(k_{|}) over the spectral width</td>
<td>curvature drift (~\hat{b} \times (\hat{b} \cdot \nabla)\hat{b}) over the flux surface</td>
</tr>
<tr>
<td>Provided by:</td>
<td>mean ExB shear shifting fluctuations radially</td>
<td>ballooning mode structure causing finite net parallel acceleration over the flux surface</td>
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<td>Main consequence:</td>
<td>residual stress driven by ExB shear (or (\nabla P / n_i) and velocity shear via radial force balance)</td>
<td>convective pinch-like term (the TEP-like piece is insensitive to mode details)</td>
</tr>
<tr>
<td>Most likely to be relevant for:</td>
<td>plasmas with strong ExB shear, incl. H-mode, ITB’s</td>
<td>pinch is likely to be inward for OH and electron-heated plasmas</td>
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Hahm et al.
Discrete particle noise in particle-in-cell simulations of plasma microturbulence

[Nevins, Hammett, Dimits, Dorland, and Shumaker, PoP 12, 122305 (2005)]

\[
\begin{align*}
\{1 + [1 - \Gamma_0(k^2 \rho_e^2)]\} \frac{e \phi_k}{T} & = \frac{S_G(k)}{N_p} \sum_p S(k_p) \sum_i w_i J_o(k \rho_i) \\
& \times \exp(-i k_p \cdot x_i),
\end{align*}
\]

(1)

\[
\left\langle \left| \frac{e \phi}{T} \right|^2 \right\rangle = \sum_k \left\langle \left| \frac{e \phi_k}{T} \right|^2 \right\rangle = \frac{\langle w^2 \rangle}{n_p V_{\text{shield}}},
\]

(8)

\[
V_{\text{shield}}^{(N)} \equiv \left\{ \frac{1}{(2 \pi)^3} \int d^3k \frac{S_G^2 \Gamma_0(k^2 \rho_e^2)}{[2 - \Gamma_0(k^2 \rho_e^2)]^2} \right\}^{-1},
\]

(9)

\[
V_{\text{shield}}^{(H)} \equiv \left\{ \frac{1}{(2 \pi)^3} \int d^3k \frac{S_G^2 \Gamma_0(k^2 \rho_e^2)}{(2 - \Gamma_0)[2 - (1 - S_G d||) \Gamma_0]} \right\}^{-1}.
\]

(10)

- Since dynamic plasma response is not included in the calculation, it is difficult to assess the effect of the shielding volume noise on long wavelength modes.
Discrete Particle Noise for Equilibrium Plasmas

- Fluctuation-Dissipation Theorem

\[ L|E(k, \omega)|^2 / 8\pi = -(T/\omega)Im(1/\epsilon) \]

- Fluctuations per \( k \)-mode

\[ L|E(k)|^2 / 8\pi = \int (d\omega/2\pi) L|E(k, \omega)|^2 / 8\pi = (T/2)[1/\epsilon(k, \omega = \infty) - 1/\epsilon(k, \omega = 0)]. \]

\[ L|E(k)|^2 / 8\pi = (T/2)(\lambda_D^2 / \rho_s^2) \]

Figure 4.1: Contour integration

(John Reynders, PhD thesis, Princeton University, 1992)
Fluctuation Dissipation Theorem applied to a nonlinearly saturated driven system

\[ 1 + k_{\perp}^2 - i \sqrt{\frac{\pi}{2} \frac{\omega_* - \omega}{k_{\parallel} v_{te}}} \left[ 1 - \frac{k_{\perp}^4}{\gamma_l^2} |\phi|^2 \right] - \frac{\omega_*}{\omega} = 0 \]

- Noise level for high frequency modes
  \[
  \frac{|e\Phi|^2}{T_e}_{HF-noise} = \frac{<w^2>}{N k_{\perp}^2 \rho_s^2},
  \]

- Noise level for low frequency modes
  \[
  \frac{|e\Phi|^2}{T_e}_{LF-noise} = \frac{<w^2>}{N (1 + k_{\perp}^2 \rho_s^2)}
  \]

- Nonlinear saturation amplitude
  \[
  \frac{|e\Phi|^2}{T_e}_{NL} = \frac{\gamma_L/\Omega_i}{2k_x k_y \rho_s^2}
  \]

[Jenkins and Lee, PoP ‘07]
Discrete Particle Noise in Nonlinearly Saturated Plasmas

2D drift wave simulations with $N = 32K, 500K, 1M$

- high frequency noise decreases with particle number,
- saturation level is independent of particle number,
- background change is small.

[Jenkins and Lee, PoP ‘07]
Electron transport in ETG simulation: total (solid line), noise driven contribution estimated by scramble test (dashed line) and estimated from $\delta f$ weight (dotted line).

[Holod and Lin, PoP ‘07]
Entropy conservation in ITG turbulence: velocity-space nonlinearity, collisions and numerical noise & dissipation in steady state

\[ \frac{\partial}{\partial t} \langle \int \frac{\delta f_i^2}{F_0i} dv_\parallel + \tau \phi^2 + \tau |\nabla_\perp \phi|^2 \rangle + \langle \tau \frac{\partial \phi}{\partial x_\parallel} \int v_\parallel \frac{\delta f_i^2}{F_0i} dv_\parallel + 2\tau v_\parallel \int \mathcal{F}_0i \left( \frac{\partial \delta f_i}{\partial v_\parallel / v_{ti}} + \frac{v_\parallel}{v_{ti}} \delta f_i \right)^2 \rangle = \kappa T_i \langle Q_{ix} \rangle \]

Monotonic increase in time
Vanishes in steady state
Velocity Space Nonlinearity
Collisional and/or numerical dissipation
Entropy production

\[ \tau \equiv \frac{T_e}{T_i} \quad \kappa T_i \equiv -\frac{d \ln T_{0i}}{dx} \]

\[ \langle \cdots \rangle \equiv \int dx/V \]

• Coarse graining in velocity space has to be taken with great care [Parker and Chen ’06, Watanabe and Sugama ‘06]
The Growing Weight Problem? and The Particle-Continuum Method

Resetting particle weights on a phase space grid periodically solves the so-called growing weight problem: no re-setting (black) vs. resetting (green and red)

[Chen and Parker]
• It is important for simulating ITER-size devices
• Scaling inefficiencies point to large numbers of Translation Lookaside Buffer (TLB) misses on some processes on XT4/3 with larger grids.

Two dimensional grid domain decomposition on GTC
[Adams, Ethier, Wichmann]
Visualization

[Klasky, ORNL; Ethier, Wang, PPPL]

[Ma, UC-Davis]

UCDAVIS
Conclusions

• It has been an exciting three years

• Too bad that we can’t keep the same team together for the next three years

• The PPPL team’s work on
  -- GTC performance on MPP
  -- GTS and GTC-Neo and their V&V work
  -- PNL and noise
  -- Theory

• The UCI team’s work on
  -- ETG, TEM and noise using GTC
  -- EM capability for GTC

• The Colorado team’s work on
  -- GEM for TEM
  -- Particle continuum method
  -- EM capability in GEM and the V&V work

• The SAPP team on
  -- Solvers
  -- Visualization
  -- Data management
Future Directions

• Verification and Validation

• Electromagnetic physics in GTS

• ITER simulation capabilities

• Integrated simulation: Heating, Turbulence, MHD, Transport