Continuum kinetic code for edge plasmas and the ESL project*

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What is the ESL?

- **ESL = Edge Simulation Laboratory**
  - Develop an edge gyrokinetic code using continuum [evolving \( f(x,v) \) on a 5-D mesh] methods
  - OFES base-program activity
  - Collaboration: LLNL, GA, UCSD, LBNL, CompX, Lodestar, PPPL. Others welcome
  - Outgrowth of LLNL LDRD project which has developed TEMPEST, presently a 4-D edge kinetic code

- **Why a kinetic code?**
  - Ion drift orbit width \( \Delta \sim \) pedestal width \( L_p \)
  - Collisional mean free path \( \sim \) connec. length
  - ITER pedestal deeply in kinetic regime; divertor strongly collisional

- **Gyrokinetic, because still \( \omega \ll \omega_c \)**
  - But extensions required because \( \Delta \sim L_p \)
Kinetic equations for F include drifts, acceleration, and Fokker-Planck collision

\[
\frac{\partial F_\alpha}{\partial t} + \vec{v}_d \cdot \nabla_\perp F_\alpha + (\vec{v}_{||\alpha} + v_{Banos}) \nabla_|| \partial F_\alpha \\
+ \left[ q \frac{\partial \langle \Phi_0 \rangle}{\partial t} + \bar{\mu} \frac{\partial B}{\partial t} - \frac{qB}{B^*} \vec{v}_|| \nabla_|| \langle \delta \phi \rangle - qv_0^0 \cdot \nabla \langle \delta \phi \rangle \right] \frac{\partial F_\alpha}{\partial E_0} \\
= C(F_\alpha, F_\alpha),
\]
Why we chose the continuum approach

• Noise in PIC simulations, especially a concern for edge because
  – Inapplicability of $\delta f$ (can have large fluctuations; a priori unknown background $f$; growing weights problem following L-H transition)
  – Still need accuracy in regions and times with small fluctuations
  – Large density variation across region

• Expense of fully nonlinear gyrokinetic PIC collision operators in strongly collisional limit (and hardly any examples)

• Advanced fluid numerical techniques available to continuum GK
  – High-order discretizations
  – AMR in $v$ and $x$ -- can have high res in $v$ space only where needed
  – Implicit timestepping

• Successful examples of core continuum GK codes (GS2, GYRO, GENE) -- substantial physics, extensively applied
Main code features (current/planned)

- Continuum solution to GK equations
- Full-f, and δf option available
- Extension of GK equations for improved applicability to edge problems
- Electrostatic initially; will be electromagnetic
- Full divertor geometry; full 2D equilibrium potential structure
- Runnable as
  - 4-D for transport with $F(\Psi, \theta, \epsilon, \mu)$, or
  - 5-D for turbulence with $F(\Psi, \theta, \phi, \epsilon, \mu)$
- Adaptivity
  - Built in AMR framework
  - Funding permitting: dynamic grid alignment (to follow large δB)
- Optional fluid equations in same framework
Some recent history: LLNL LDRD funding has been used to initiate an edge continuum code (FY04-06)

We were successful in convincing LLNL management to utilize assets of three LLNL groups

1. **Fusion Energy Program**
   - Underlying edge gyrokinetic equations (with PPPL)
   - Edge physics and (core) gyrokinetic simulations
   - V&V

2. **Center for Advanced Scientific Computing**
   - Code framework
   - Numerical methods

3. **Chemistry and Material Sciences**
   - Impurity production via material sputtering
   - Near-surface plasma chemistry (with UCB)
LLNL LDRD code development strategy: systematic progression of increasing complexity

- **Prototype**
  - 1D Space / 2D Velocity
  - Collisions and Advection

- **FY05**
  - 2D Space / 2D Velocity
  - A Kinetic Analogue to UEDGE

- **FY06**
  - 3D Space / 2D Velocity
  - A Kinetic Analogue to BOUT

ESL →
Current technical status for LDRD work

- **TEMPEST code operational in 4D**
  - Physics content: parallel streaming, drifts, Fokker-Planck collisions (linear, nonlinear), toroidal annulus or full divertor geometry, electrostatic field solve (gyrokinetic Poisson)
  - V&V in progress: endloss physics, neoclassical transport, field solve
  - Generalized GK formulation for steep gradients (LDRD support for PPPL); next step is distillation of dominant terms

- **5D extension formulated; coding beginning**
  - Will enable electrostatic edge turbulence simulation
  - Expect to complete this summer
  - Will be “0th generation” ESL Code -- lessons learned will feed into first formal ESL design
We have designed and implemented a 4D edge simulation framework; added physics “born parallel”
We have implemented a gyrokinetic Poisson equation field solver

\[
\left( \sum_{\alpha} \frac{\rho_\alpha^2}{2\lambda_{D\alpha}^2} \right) \nabla^2 \Phi + \left( \sum_{\alpha} \frac{\rho_\alpha^2}{2\lambda_{D\alpha}^2} \nabla \cdot \ln N_\alpha \right) \cdot \nabla \Phi + \nabla^2 \Phi = -4\pi e \left( \sum_{\alpha} Z_\alpha N_\alpha - n_e \right) - \sum_{\alpha} \frac{\rho_\alpha^2}{2\lambda_{D\alpha}^2} \frac{1}{N_\alpha Z_\alpha e} \nabla^2 P_{\perp \alpha}
\]

- Discretized in y-q coordinates using standard finite differencing
- Uses Hypre library of parallel linear algebra solvers and preconditioners
  - Solvers:
    - Conjugate Gradient (CG)
    - Generalized Minimum Residual (GMRES)
    - Stabilized BiConjugate Gradient (BiCGSTAB)
  - Preconditioners
    - Diagonal scaling
    - Block Gauss-Seidel with PFMG or SMG in each block
    - BoomerAMG
- Currently implemented with adiabatic electron model
It is important to have physical conservation properties in the collision and moment packages.
We have verified aspects of the 3D & 4D TEMPEST on known physics problems (see A. Xiong talk, Thurs.)

Examples of key physics aspects tested

1. Fokker-Planck collisions for scattering into velocity-space loss cones; important because:
   • electrons are potentially confined by divertor/wall sheath potentials - non-Maxwellian, high-energy tails can develop
   • magnetically trapped ions scattering into loss-cones near magnetic separatrix

2. Neoclassical flow and transport for core ions
   • high temperature and low turbulence for H-mode can result in neoclassical ion transport being important

3. Electrostatic field generation and geodesic acoustic modes
   • shear-flow and zonal flows key to turbulence suppression
Test 1: TEMPEST recovers collisional confinement for combined B, $\Phi$ well using modest v-space resolution

\[ B, \Phi \]

\[ S_\parallel \]

Empty loss-cone (Pastukhov); $\sim \tau_p$

Filled loss-cone (collisional); $\sim \tau_c$

Confinement time versus density

Particle confinement time (sec)

Density (cm$^{-3}$)

\[ \tau = \tau_p + \tau_c \]

Theory

Simulation
Test 2: Neoclassical parallel flow on closed flux surfaces is reproduced

\[ <U_{||}> = \frac{E_r}{B_p} - \frac{T_i}{eB_p} (\frac{\partial}{\partial r})(\ln P_i - k \ln T_i) \]

and \( k \) depends on collisionality regime

Simplest test for \( E_r = 0 \) and \( \frac{\partial T_i}{\partial r} = 0 \)

Neoclassical energy transport is also simulated
Test 3: Generation electrostatic potential and Landau damping of geodesic acoustic modes is observed

- Frequency and residual of $\Phi$ appear close to Rosenbluth-Hinton theory
Plans
FY06 continuing LDRD code development projects

- **Infrastructure**
  - Improve I/O capabilities (input, viz, etc.)
  - Complete velocity-space finite volume transition
  - Implement 5D data communication routines

- **Physics Algorithms**
  - Generalize gyrokinetic field solve
  - Implement parallel gyroaveraging algorithm
  - For 5D, implement field-aligned ballooning coordinates and physics modules

\[ x = \psi - \psi_s, \]
\[ y = \theta, \]
\[ z = \zeta - \int_{\theta_0}^{\theta} \nu(x, y) dy. \]
FY06-09 ESL plan is based on 4/1/06 start and current budget level

Phase 1
- Design
  - Chombo mods
  - 5D linear EM GK capability; 5D nonlinear ES; transition to Chombo
  - Zero-viscosity e⁻ fluid capability
  - Simple fluid neutrals capability
- Code development:
  - LLNL LDRD (4D, 5D electrostatic GK capability)
- V&V:
  - 4D Design
  - 4D Testing
  - 5D ES Design
  - 5D ES testing

Phase 2
- Design
  - Phase 2 Implementation
    - Fully GK collisions; Nonlinear EM
    - Adaptive grid
- Implementation:
  - 1/1/08
  - 8/1/08
  - 2/1/09
  - 6/1/09

Phase 1 Testing
- Start up long-range activities (multiscale, advanced neutrals) if increased funding allows
Some common areas for possible collaboration with CPES

• Testing math algorithms for solving field equations (electrostatic and electromagnetic)
  – preconditioners; iterative solvers; boundary conditions

• Formulation of complete GK edge equations and useful reductions

• Compare orbit loss (i.e., across separatrix) for steep gradients and self-consistent potential; compare GAM frequency and damping

• Compare parallel kinetic electron heat flux for SOL varying from short (divertor) to long(er) at midplane

• 5D turbulence benchmark, first Cyclone, and then edge-specific

• Common high-level data representation to facilitate comparisons; visualization tools?
Summary

- Continuum gyrokinetic edge code TEMPEST with Fokker-Planck is now working in 4D and passed various verification tests

- The continuum code work has been “nationalized” with the start of the ESL project

- An electrostatic 5D code is the goal by this fall

- There are various areas for collaboration between ESL and CPES