GTC Framework Development and Application

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GPS-TTBP Workshop on GTC Framework Development

- UC Irvine, January 24, 2008
- 20 attendees from UCSD, UCI, UCLA, UCD, USC, U. Texas, PPPL, & ORNL
- Talks and discussions on project overview, GTC status & application, GTC framework development plan
- Near term action items
  - GTC CVS version for ORNL pioneer application (*Xiao*, done)
  - Version integration (*Decyk*)
  - I/O and Daskboard (*Klasky*)
  - Particle-field interaction & front tracking in CTEM (*Ma*)
  - Optimization for Jaguar (*Hall & Ethier*)
  - Parallelization for 100,000+ cores ?

GPS-TTBP Computing Resources

- Joint INCITE proposal by GPS-TTBP, GSEP & CPES awarded 8M hours of Jaguar @ORNL
- ORNL Jaguar CPU hours: 3.7M (INCITE + Director's)+4.5M (250TF pioneer application)
- NERSC Franklin MPP hours: 9.5M (~1.5M ORNL hours)
- TACC at U. Texas Lonestar & Ranger ?

GTC Physics Modules

UCI

- Fluid-kinetic hybrid electron model for electrons
  - Collisionless trapped electron mode (CTEM) turbulence *[Xiao & Lin, TTF08]*
  - Electromagnetic turbulence with kinetic electrons *[Nishimura et al, TTF08]*
  - Shear Alfven wave excited by energetic particle *[Nishimura et al, TTF08]*
- Perturbative (δf) method for ions
  - Pinch-like & gradient-driven momentum fluxes *[Holod & Lin, APS07 & TTF08]*
- Multi-species via OO Fortran
  - Energetic particle diffusion by microturbulence *[Zhang et al, TTF08]*
- Guiding center Hamiltonian in magnetic coordinates
- Global field-aligned mesh: truly global geometry
- General geometry MHD equilibrium using spline fit
- Fokker-Planck collision operators via Monte-Carlo method

GTC Computational Methods

UCI

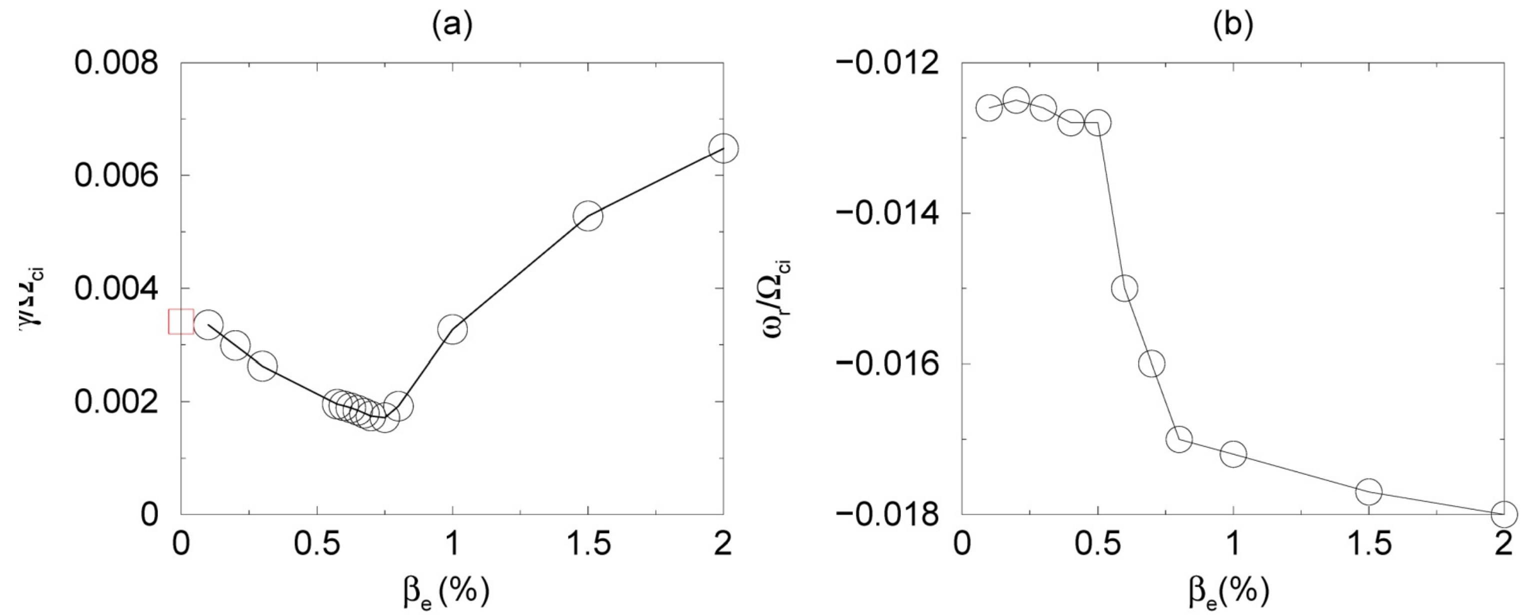
- Finite difference & finite element elliptic solvers
  - Iterative method for electrostatic simulation
  - Sparse matrix solver (PETSc) for direct solver
  - Pade approximation & integral gyrokinetic Poisson equation
- Multi-level parallelism
  - Particle-field domain-decomposition: uni-directional MPI
  - MPI-based particle decomposition
  - Loop-level parallelization using OpenMP: multi-core
- PIC optimization: electron sub-cycling, vectorization
- Statistical analysis of fluctuations/particles, and noise control
  [Lin TTF08; Lin et al, PRL2007; Holod & Lin, PoP2007]
- Visualization of 3D fluid and 5D particle data

Fluid-kinetic Hybrid Electron Model in GTC

UCI

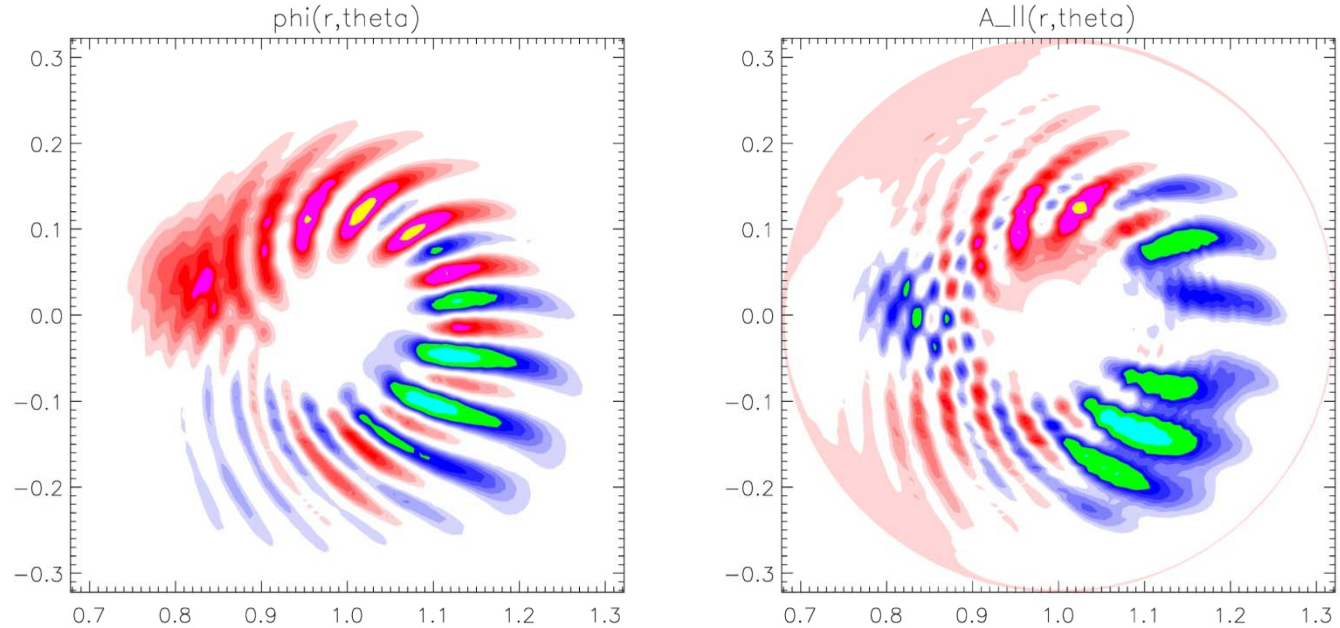
- Electron response expanded using $\delta=(m_e/m_i)^{1/2}$ [*Lin & Chen, PoP2001*]
- Lowest order response adiabatic: massless fluid electron
  - Remove collisionless tearing mode and its well-known numerical difficulties
  - Recover MHD equations when all kinetic effects suppressed; allow $\delta E_{||}$
- Higher order response treats kinetic effects
  - Retain wave-electron resonance & magnetically trapped electrons
  - Reduce electron noise and relax Courant condition
- Penalty: no inductive $\delta E_{||}$ ($k_{||}=0$), i.e., no collisionless tearing mode
- Model treats rigorously all other $k_{||}=0$ modes: electrostatic $\delta\mathbf{E}$, magnetic $\delta\mathbf{B}$, zonal flows/fields, all ideal & resistive MHD modes
- Model optimal for drift & Alfvenic turbulence on ρ_i scales
  - Electrostatic ITG/CTEM simulation: linear [*Rewoldt, Lin & Idomura, CPC2007*], nonlinear [*Lin et al, PPCF2007*]
  - Toroidal electromagnetic formulation & simulation of drift & Alfven waves [*Nishimura, Lin & Wang, PoP2007*]

Effect of finite beta on the ITG linear growth rate is demonstrated



$\eta_i = 7.0$, γ and ω_r for $n = 10$ mode shown. Finite beta stabilization and unstable branch (KBM onset).

Higher order kinetic electron effect is incorporated into EMGK simulations



Enhancement of linear growth rate observed with KE.[a]

[a]Nonlinear electrostatic simulation with kinetic electrons : Lin *et al.* PPCF 2007 (in press).

GTC Plan

UCI

- Version integration & control (with *Decyk*)
- Physics modules
  - Full-f ion & profile evolution
  - GTC-XGC core-edge coupling (with CPES), turbulence-Alfven wave coupling (with GSEP), & turbulence-neoclassical coupling
- Particle noise analysis and control
  - Characterization of particle noise in full-f
  - Deterministic collision operator (with *Hinton*)
- Particle-field domain-decomposition for 100,000+ cores
- PIC optimization for multi-core (with *Hall* of PERI & *Wichmann* of Cray, *Either*)
- Visualization of particle-field interaction (with *Ma* of IUSV)
- Parallel I/O, data streaming, workflow, & dashboard (with *Klasky* of SDM)
- Synthetic diagnostics (with *Holland* & *Tynan*)

Main physical and numerical features

- Gyrokinetic Tokamak Simulation (GTS) code: generalized gyrokinetic particle simulation model
- Shaped cross-section; experimental profiles; consistent rotation and equilibrium $\mathbf{E} \times \mathbf{B}$ flow; linear Coulomb collisions; $\cdots$
- Interfaced with MHD equilibrium codes and TRANSP data base
- Kinetic(electrostatic) electrons via split-weight scheme

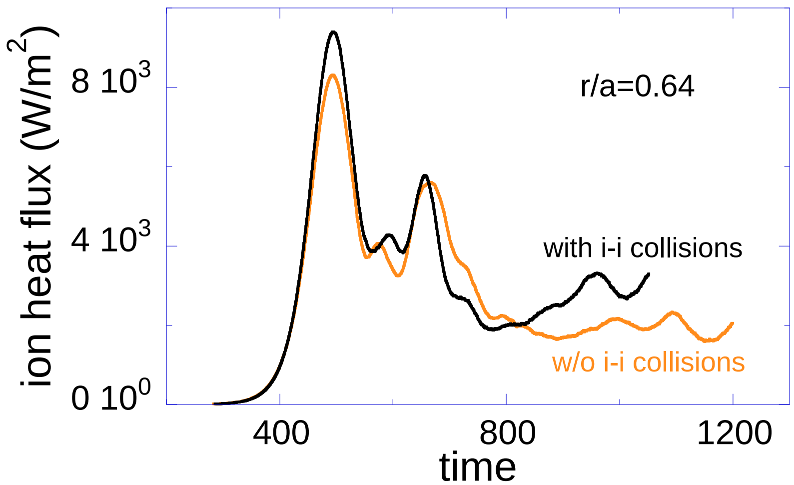
Linear Coulomb collision models

- Linear like-particle collisions (i-i, e-e):

$$C^l_{aa}(\delta f) = \underbrace{C(\delta f, f_0)}_{\text{(drag \& diffusion)}} + \underbrace{C(f_0, \delta f)}_{\text{(effect of perturbed field particles)}}$$

- Lorentz model for e-i collisions

$$C_{RI}(\delta f_e) = \frac{\nu_e}{2} \frac{\partial}{\partial \lambda} (1 - \lambda^2) \frac{\partial}{\partial \lambda} \delta f_e$$

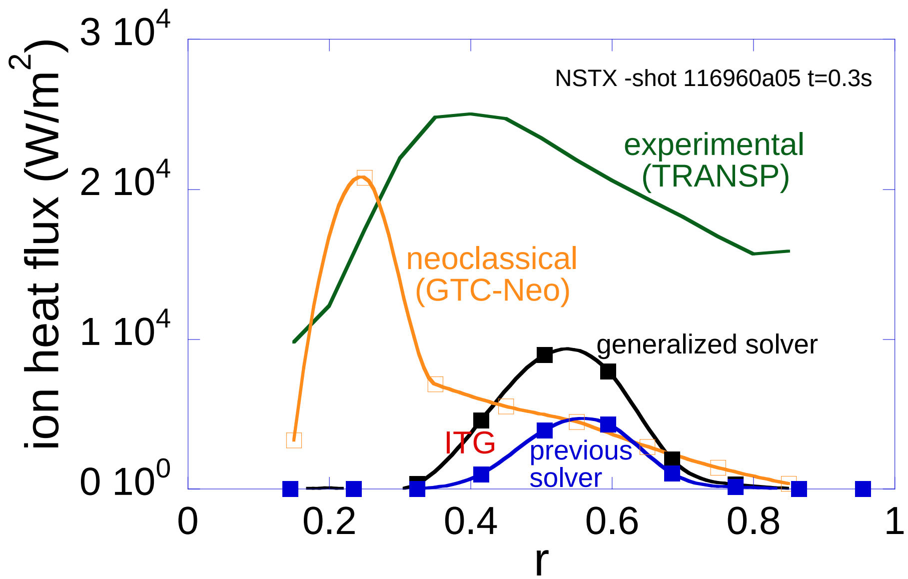


PPPL PRINCETON PLASMA PHYSICS LABORATORY

Physics-oriented Algorithm – Generalized Poisson Solver

- Poisson Solver for total potential $\Phi = \delta\Phi + \langle\Phi\rangle$ in general geometry

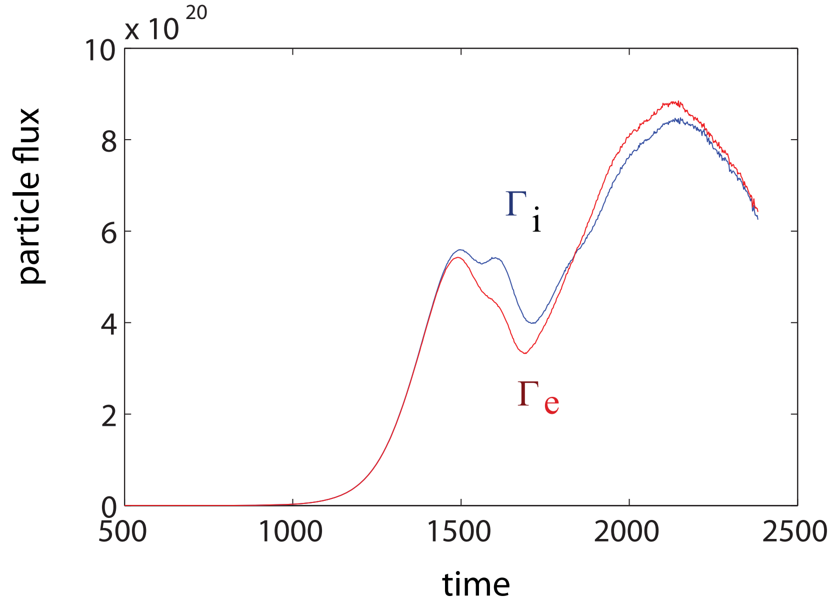
$$\left(1+\frac{T_i}{T_e}\right)\frac{e\Phi}{T_i} - \frac{e\widetilde{\Phi}}{T_i} - \frac{e\langle\Phi\rangle}{T_e} = \frac{\delta\bar{n}_i}{n_0} - \frac{\delta n_e^{(1)}}{n_0}$$



Kinetic electron model

- Electron physics via split-weight scheme (Manuilskiy & Lee)

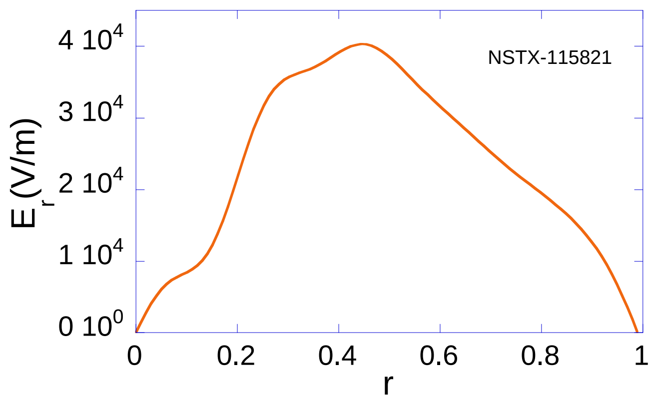
if electron= 1 $\Longrightarrow$



Coupling with other simulations

– Linear coupling between turbulent and neoclassical simulations

- Equilibrium $\mathbf{E} \times \mathbf{B}$ shear flow calculated by GTC-NEO simulation (or simply by radila force balance) is imported to the GTS turbulence simulation
- On the other hand, the GTS simulation can serve to provide a steady state turbulence background for the neoclassical simulation to investigate turbulence impact on neoclassical physics such as bootstrap current.



– Coupling to reflectometry simulation, providing spatio-temporal fluctuation background

Future plan

- web-based user interface
- full-f capability
- multi-ion species
- EM