Progress of Gyrokinetic Particle Simulations of Energetic Particle Instability

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Outline

- Introduction
- Hybrid electron model in toroidal geometry
- GTC development status
- TAE benchmarks

GTC: gyrokinetic toroidal particle-in-cell code [Z. Lin, *et al.*, Science **281**, 1835 (1998)]

- 3D global toroidal geometry with field-aligned mesh;
- delta-f method to reduce noise;

Electromagnetic capabilities are required to describe TAE and EPM

Time step restrictions associated with the electron Courant condition $k_{\parallel} v_e \Delta t < 1$ and existence of high-frequency modes $\omega_H \Delta t < 1$;

The Gyro-Kinetic Equation (GKE) for ions

$$\frac{dw_i}{dt} = (1 - w_i)\left[-\frac{1}{B_0}\mathbf{b}_0 \times \nabla\left(\phi - v_\parallel \lambda B_0\right) \cdot \left.\frac{\nabla f_0}{f_0}\right|_{v_\perp} + \frac{Z_i}{T_i} v_\parallel E_\parallel - \frac{Z_i}{T_i}\mathbf{v}_d \cdot \nabla\phi\right]$$

Hamiltonian equations of motion

$$\dot{\zeta} = \frac{v_\parallel B_0\left(q + \rho_c I' + I\partial_{\psi_p}\lambda\right)}{D} - \frac{I}{D}\left[\frac{1}{Z_\alpha}\frac{\partial\varepsilon}{\partial B_0}\frac{\partial B_0}{\partial\psi_p} + \frac{\partial\phi}{\partial\psi_p}\right]$$

$$\dot{\theta} = \frac{v_\parallel B_0\left(1 - \rho_c g' - g\partial_{\psi_p}\lambda\right)}{D} + \frac{g}{D}\left[\frac{1}{Z_\alpha}\frac{\partial\varepsilon}{\partial B_0}\frac{\partial B_0}{\partial\psi_p} + \frac{\partial\phi}{\partial\psi_p}\right]$$

$$\dot{\psi}_p = \frac{1}{Z_\alpha}\frac{\partial\varepsilon}{\partial B_0}\left(\frac{I}{D}\frac{\partial B_0}{\partial\zeta} - \frac{g}{D}\frac{\partial B_0}{\partial\theta}\right) + \frac{I}{D}\frac{\partial\phi}{\partial\zeta} - \frac{g}{D}\frac{\partial\phi}{\partial\theta} + v_\parallel B_0\left(\frac{g}{D}\frac{\partial\lambda}{\partial\theta} - \frac{I}{D}\frac{\partial\lambda}{\partial\zeta}\right)$$

$$\begin{aligned}\dot{\rho}_\parallel = &-\frac{\left(1 - \rho_c g' - g\partial_{\psi_p}\lambda\right)}{D}\left[\frac{1}{Z_\alpha}\frac{\partial\varepsilon}{\partial B_0}\frac{\partial B_0}{\partial\theta} + \frac{\partial\phi}{\partial\theta}\right] \\ &- \frac{\left(q + \rho_c I' + I\partial_{\psi_p}\lambda\right)}{D}\left[\frac{1}{Z_\alpha}\frac{\partial\varepsilon}{\partial B_0}\frac{\partial B_0}{\partial\zeta} + \frac{\partial\phi}{\partial\zeta}\right] \\ &+ \frac{(I\partial_\zeta\lambda - g\partial_\theta\lambda)}{D}\left[\frac{1}{Z_\alpha}\frac{\partial\varepsilon}{\partial B_0}\frac{\partial B_0}{\partial\psi_p} + \frac{\partial\phi}{\partial\psi_p}\right] - \frac{\partial\lambda}{\partial t}\end{aligned}$$

Electrons are described as massless fluid in the lowest order of $\mathcal{O}\left(m_e/m_i\right)$

Dimensionless continuity equation

$$\frac{\partial \delta n_e}{\partial t} + B_0 \mathbf{b}_0 \cdot \nabla \left(\frac{n_0 \delta u_{\parallel e}}{B_0} \right) + B_0 \mathbf{v}_E \cdot \nabla \left(\frac{n_0}{B_0} \right) - n_0 \left(\mathbf{v}_* + \mathbf{v}_E \right) \cdot \frac{\nabla B_0}{B_0} = 0$$

where

$$\mathbf{v}_* = -\frac{1}{n_0 B_0} \mathbf{b}_0 \times \nabla \left(\delta P_\parallel + \delta P_\perp \right)$$

$$\delta P_\perp^{(0)} = n_0 \phi_{\text{eff}}^{(0)} + \frac{\partial (n_0 T_e)}{\partial \psi_p} \delta \psi + \frac{\partial (n_0 T_e)}{\partial \alpha_0} \delta \alpha$$

$$\delta P_\parallel^{(0)} = n_0 \phi_{\text{eff}}^{(0)} + \frac{\partial (n_0 T_e)}{\partial \psi_p} \delta \psi + \frac{\partial (n_0 T_e)}{\partial \alpha_0} \delta \alpha$$

Inverse Ampére's law

$$\delta u_{\parallel e} = \frac{T_e}{B_0^2} \frac{1}{\beta_e} \nabla_\perp^2 A_\parallel + Z_i \delta u_{\parallel i}$$

Kinetic electrons are implemented in the higher order of $\mathcal{O}\left(m_e/m_i\right)$

High-order electron drift-kinetic equation

$$\frac{dw_e}{dt} = \left(1 - \frac{\delta f_e^{(0)}}{f_{0e}} - w_e\right)\left[-\mathbf{v}_E \cdot \left.\frac{\nabla f_{0e}}{f_{0e}}\right|_{v_\perp} - \frac{\partial}{\partial t}\frac{\delta f_e^{(0)}}{f_{0e}} - \right.$$
$$\left. \mathbf{v}_d \cdot \nabla\left(\frac{1}{T_e}\phi_{\text{ind}}^{(0)} + \frac{1}{f_{0e}}\left.\frac{\partial f_{0e}}{\partial \psi_0}\right|_{v_\perp}\delta\psi\right) + \left(\frac{1}{T_e}\mathbf{v}_d + \frac{1}{B_0}\mathbf{b}_0 \times \nabla\frac{\delta f_e^{(0)}}{f_{0e}}\right)\cdot\nabla\langle\phi\rangle\right]$$

with

$$\frac{\delta f_e^{(0)}}{f_{0e}} = \frac{1}{T_e}\phi_{\text{eff}}^{(0)} + \frac{1}{f_{0e}}\left.\frac{\partial f_{0e}}{\partial \psi_0}\right|_{v_\perp}\delta\psi$$

Lowest order parallel electric field from adiabatic electron response

$$\frac{\phi_{\mathrm{eff}}^{(0)}}{T_e} = \frac{\delta n_e}{n_0} - \frac{\delta\psi}{n_0}\frac{\partial n_0}{\partial\psi_0} - \frac{\delta\alpha}{n_0}\frac{\partial n_0}{\partial\alpha_0}$$

Electrostatic potential from gyrokinetic Poisson's equation

$$\phi - \tilde{\phi} = \frac{T_i}{n_0}\left(Z_i \delta n_i - \delta n_e\right)$$

Inductive potential

$$\phi_{\mathrm{ind}} = \phi_{\mathrm{eff}} - \phi$$

Evolution equation for the vector potential

$$\frac{\partial A_\parallel}{\partial t} = \mathbf{b}_0 \cdot \nabla\phi_{\mathrm{ind}}$$

Perturbed magnetic field label evolution

$$\frac{\partial\delta\psi}{\partial t} = -\frac{\partial\phi_{\mathrm{ind}}}{\partial\alpha_0}$$
$$\frac{\partial\delta\alpha}{\partial t} = \frac{\partial\phi_{\mathrm{ind}}}{\partial\psi_0}$$

Zonal flows and zonal fields

Poisson equation for zonal potential

$$\frac{\rho_s^2}{\lambda_D^2}\langle\nabla_\perp^2\phi\rangle = 4\pi\left(\langle\delta n_e\rangle - Z_i\langle\delta n_i\rangle\right)$$

Ampére's law for zonal field

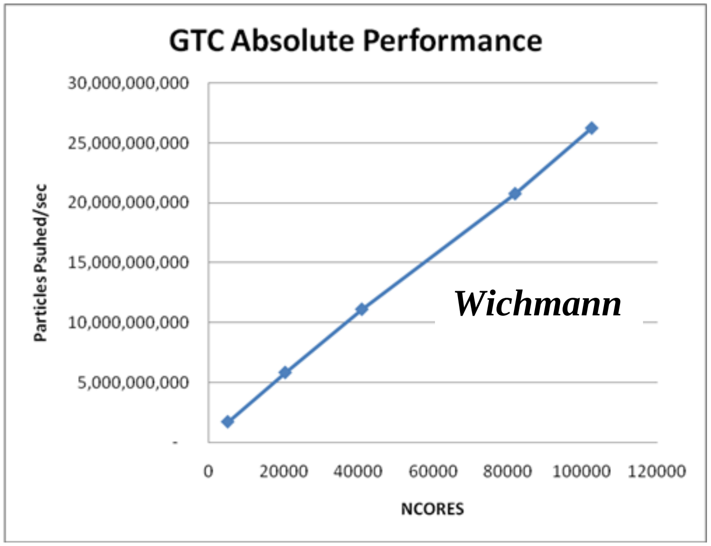
$$\langle\nabla_\perp^2 A_\parallel\rangle - \frac{1}{\delta_e^2}\langle A_\parallel\rangle = \frac{4\pi n_0}{c}\left(e\langle\delta u_{\parallel e}\rangle - Z_i\langle\delta u_{\parallel i}\rangle\right)$$

the solution on scale length larger than δ_e: zonal fields are heavily screened

$$\langle A_\parallel\rangle = \frac{4\pi n_0 c}{\omega_{pe}^2}\left(Z_i\langle\delta u_{\parallel i}\rangle - e\langle\delta u_{\parallel e}\rangle\right)$$

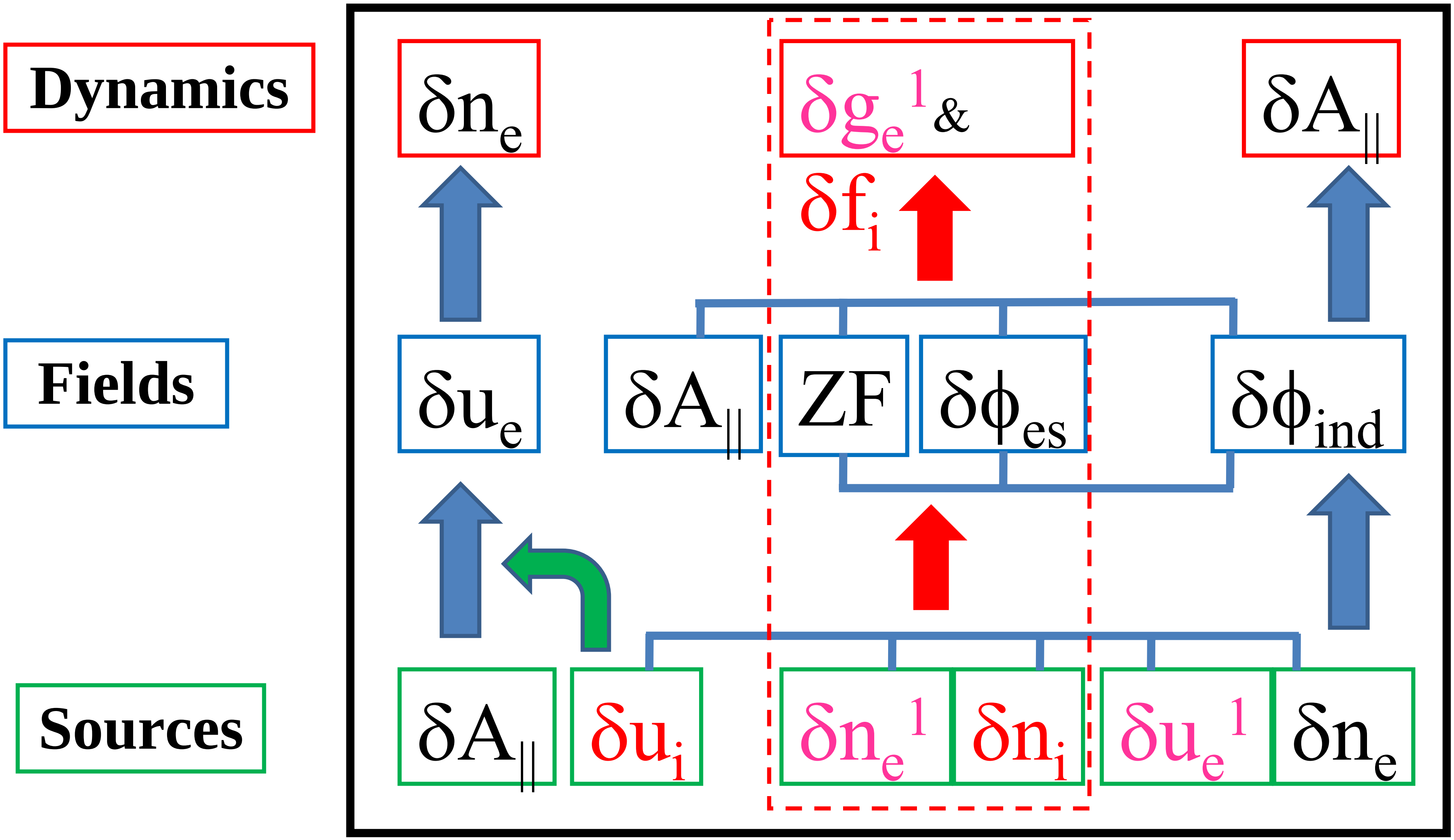
Gyrokinetic Troidal Code (GTC) Status

- Integration of key capabilities in a single GTC version
  - Kinetic electrons using fluid-kinetic hybrid electron model
  - Electromagnetic solver using PETSc
  - General geometry using spline fit of EFIT MHD equilibrium and profiles data
  - Fokker-Planck collision operators conserving momentum and energy
  - Global field-aligned mesh using magnetic coordinates
  - Multi-level parallelism using mixed mode of MPI/OpenMP
  - Advanced I/O using ADIOS
- GTC: part of benchmark suites for DOE OASCR, NERSC, and Cray; early applications of ORNL 1.6PF jaguarpf; SciDAC GPS, GSEP, & CPES
- GTC simulation of electron turbulence selected as "*Top Breakthroughs in Computational Science*", SciDAC Review, 2009

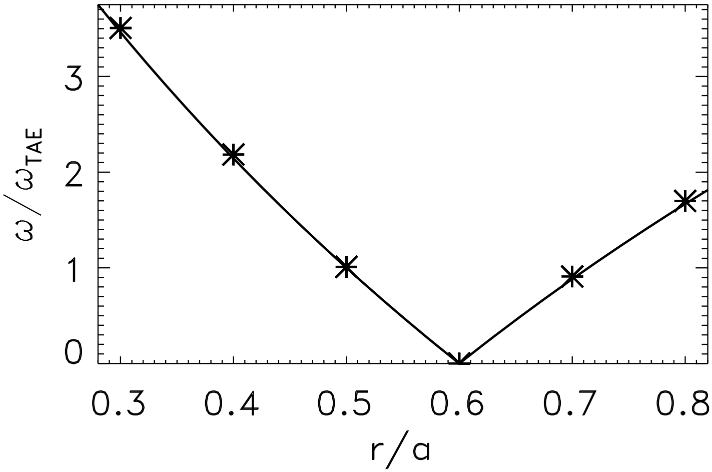


[Lin et al, Science98]; http://gk.ps.uci.edu/GTC

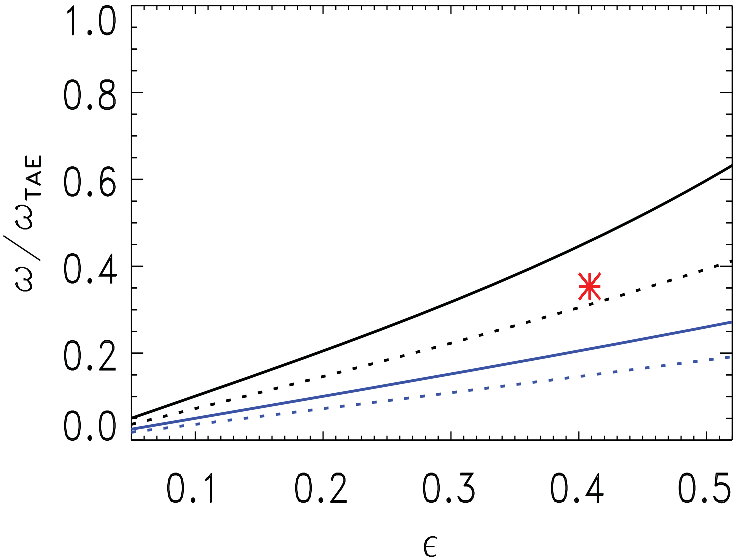
Electromagnetic GTC via Fluid-Kinetic Electron



Verification of New GTC Version with General Geometry for Simulations of TAE and EPM

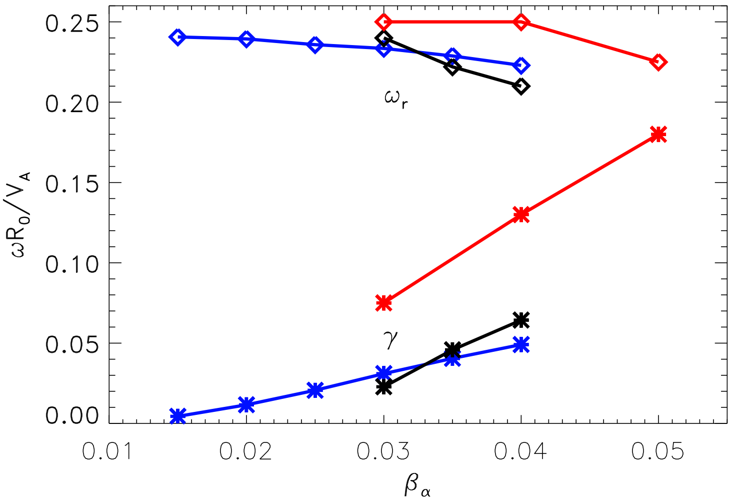


Alfven Continue Spectrum in Cylindrical Geometry:
Simulation points agrees with theoretical prediction.



TAE Gap Width in Toroidal Geometry:
Red points from the GTC simulation. solid line are theoretical width without finite magnetic shear correction, dash lines are those with shear correction; black line are result proportional to 2ϵ, whileas blue ϵ.

TAE Excitation by Energetic Particles

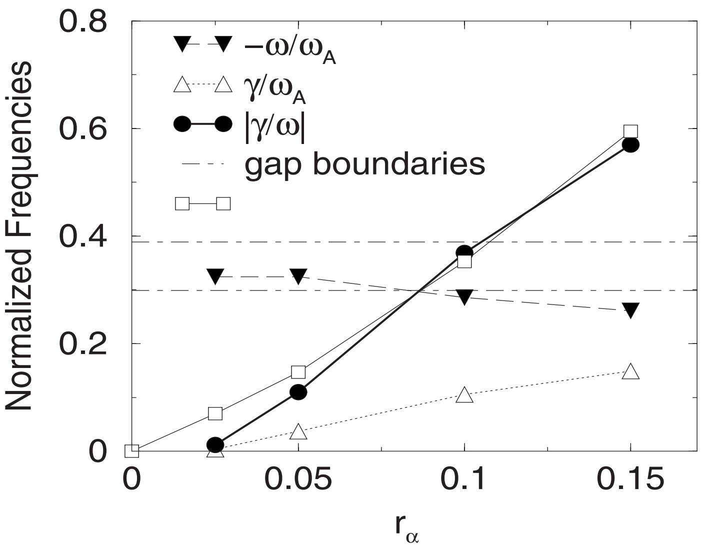


Benchmarking with TAEFL/HMGC

$n = 3$ mode Parameters:

$v_\alpha/V_A = 1,\quad \beta_e = 2\%,$
$R_0/a = 3.0,\quad a/\rho_s = 400.0,$
$T_\alpha/T_e = 50.0,\quad R_0/L_{n\alpha} = 27.0$

where blue from TAEFL, red HMGC (different $R_0/L_{n\alpha}$), and Black GTC.



Benchmarking with Fu'89

$n = 1$ Parameters:

$v_\alpha/V_A = 1,\quad \beta_e = 1\%,$
$a/R_0 = 0.375,\quad a/\rho_s = 400.0,$
$T_\alpha/T_e = 100.0,\quad R_0/L_{n\alpha} = 8.0$

where square points from Fu'89, solid dot GTC. *[Y. Nishmura, POP'09]*