Limitations on a Kinetic Electron Closure for Extended Hybrid Electromagnetic Simulation of Drift Waves

Bruce I. Cohen, Andris M. Dimits, and W. M. Nevins
University of California Lawrence Livermore National Laboratory,
Livermore, California 94550

Yang Chen and Scott E. Parker
Department of Physics, University of Colorado at Boulder
Boulder, Colorado 80309

* This work was supported by the U.S. Department of Energy under Contract No. W-7405-ENG-48 at University of California Lawrence Livermore National Laboratory. This work is part of the SCIDAC Plasma Microturbulence Project sponsored by DOE OFES.

Kinetic Electron Closures for Electromagnetic Simulation -- Outline

1. A practical algorithm for particle simulation of electromagnetic drift-wave turbulence and transport with kinetic ions and electrons when electrons are nearly adiabatic.

2. Examples – Simulations of kinetic shear Alfvén waves, and collisionless drift wave and ion-temperature-gradient instabilities at finite β in a two-dimensional unsheared slab. This hybrid algorithm fails in a sheared slab.

3. Extension to toroidal flux-tube algorithm

4. Summary --

   -Successful particle simulations of shear-Alfvén waves and electromagnetic drift-wave and ITG instabilities with kinetic electrons for $\beta m_i / m_e > 1$ (hot core plasmas) in slab.

   -Sheared slab and toroidal implementations with mode rational surfaces fail because alogorithm does not give correct physics in electron resonance layers.

Related work within the SciDAC Plasma Microturbulence Project: continuum methods -- GS2 by W. Dorland, et al., and GYRO by Waltz and Candy; particle methods -- Z. Lin and L. Chen, W. Lee.

How to Accommodate $\beta m_i/m_e$>>1 ? -- Hybrid II Electromagnetic Algorithm

- Extend the "massless" electron hybrid model of Parker, *et al.* and P. Snyder (Ph.D. thesis, Princeton U., 1999) to include drift-kinetic electrons.
- Consider the modified electron momentum equation (Ohm's law) in slab geometry:

$$en_{0e}\vec{E}\cdot\hat{b}^{(0)} = -\nabla_{\|}P_{\|e} + \frac{\delta\vec{B}_{\perp}}{B}\cdot\nabla en_{0e}\phi - n_{0e}m_e(\partial/\partial t + \vec{v}_{ExB}\cdot\nabla)u_{\|e}$$

where $\nabla_{\|}P_{\|e} = \nabla_{\|}P_{\|e}^{(0)} + T_{\|e}^{(0)}\nabla_{\|}\delta n_e^{(0)} + n_{0e}\nabla_{\|}\delta T_{\|e}$ with $\nabla_{\|}(T_{\|e}^{eq} + \delta T_{\|e}) = 0$, $T_{\|e}^{(0)}$ is a constant, $\delta n_e^{(0)} = \delta n_e - \Delta n_e^K$ =electron fluid density, $\Delta n_e^K = \int d^3v h_e$ is the *split-weight* δf kinetic increment, and δn_e = total perturbed density consistent with moment of *split-weight* electron distribution function (like Lin and Chen, 2001):

$$f_e = f_M(\vec{x},\vec{v}) + \left(\delta n_e^{(0)}/n_{0e}\right) f_M(\vec{v}) + h_e(\vec{x},\vec{v})$$

- Use Ohm's law to advance $A_{\|}$, $\partial A_{\|}/c\partial t = (\vec{E} + \nabla\phi)\cdot\hat{b}^{(0)} = \ldots$

Hybrid II Electromagnetic Algorithm (cont'd)

- With updated $A_{\|}$ use Ampere's law to determine parallel electron current:

  $\Gamma_{\|e} = n_{0e} u_{\|e} = \frac{c^2}{4\pi e} \nabla_{\perp}^2 \frac{A_{\|}}{c} + \overline{\Gamma}_{\|i}$, where $\overline{\Gamma}_{\|i}$ is the gyrokinetic parallel ion current.

- Use the electron continuity equation to advance the total electron density:

$$\frac{\partial \delta n_e}{\partial t} + n_{0e}(\vec{B}^{(0)} + \delta\vec{B}_{\perp}) \cdot \nabla \frac{u_{\|e}}{B} + \vec{v}_{E\times B} \cdot \nabla(n_e^{eq} + \delta n_e) = 0$$

  (assumes no magnetic curvature)

- Determine the electric potential ϕ from the quasineutrality relation using the updated electron and gyrokinetic ion densities

- Advance the gyrokinetic ions and the drift-kinetic electrons with same Δt.

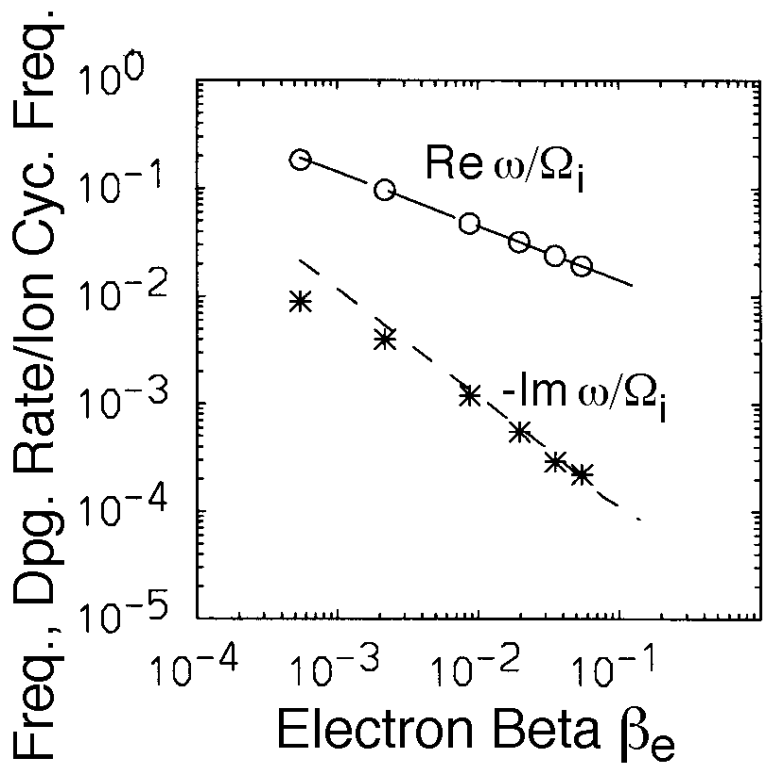
- From drift-kinetic equation for electrons with split-weights (after cancellations),

$$\frac{dw_j^e}{dt} = (\vec{\mathrm{v}}_{ExB} \cdot \hat{x} + \mathrm{v}_{\|} \frac{\delta B_x}{B_0}) \kappa_{Te} (\frac{\mathrm{v}^2}{\mathrm{v}_e^2} - \frac{3}{2}) + \nabla_{\|} u_{\|e}$$

  using $|\Delta n_e^K / \delta n_e^{(0)}| << 1$ as an expansion parameter.

Hybrid II δf Algorithm – Improved Shear Alfvén-Wave Simulations

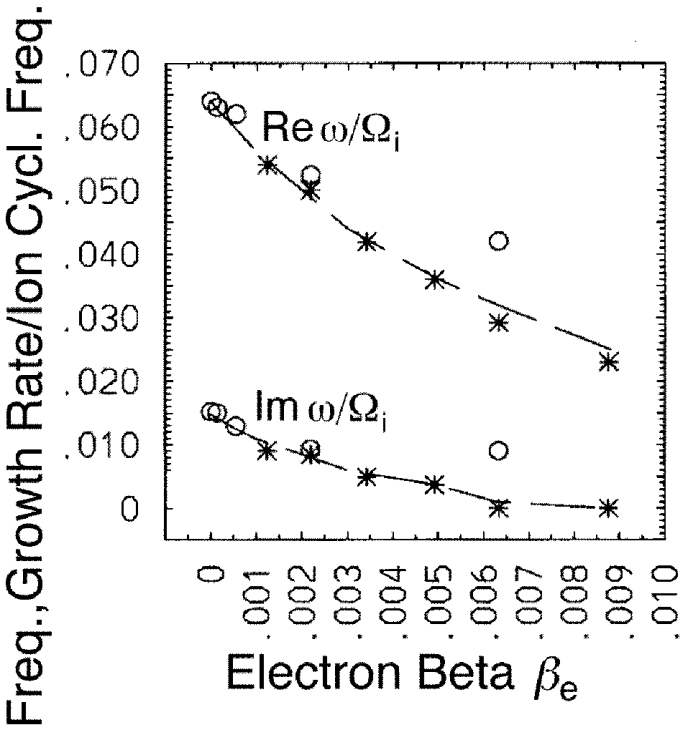
- Simulations of kinetic shear-Alfvén waves in slab.
  Parameters: $k_y\rho_s = \pi/8$, $T_e = T_i$, $B_y/B_0 = 0.01$, $\rho_s = 2\Delta y$, 32x32 grid, (0,1) mode
  theory - - - simulation results: o = $\mathrm{Re}\,\omega/\Omega_i$, $* = -\mathrm{Im}\,\omega/\Omega_i$ Landau dpg. rate

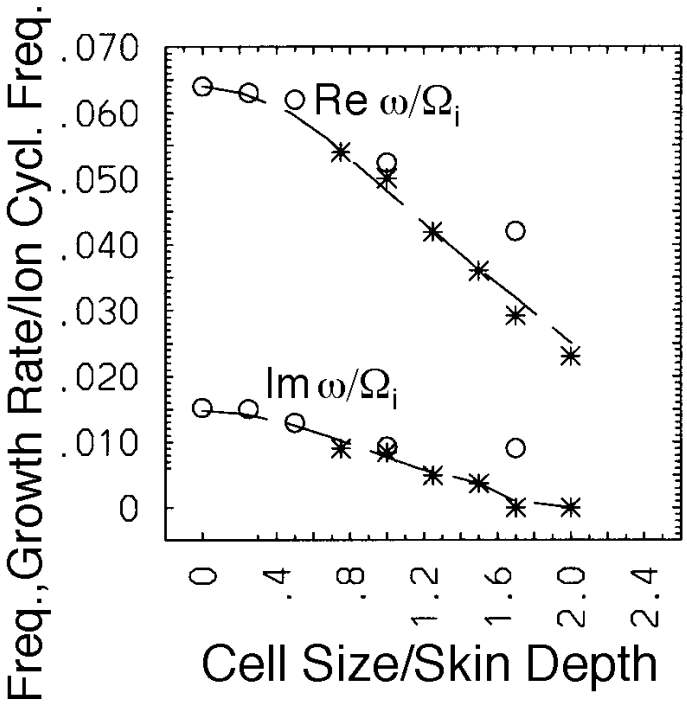


- No restriction on $\omega_{pe}\Delta y/c$ and results are similar to Z. Lin and L. Chen's 2001 reported results. (As $\beta_e m_i / m_e \to 0$ the algorithm fails and goes unstable.)

Extended Hybrid II δf Algorithm – Collisionless Drift-Wave Slab Simulations

- δf slab simulations of collisionless drift-wave instability with no magnetic shear. Parameters: $k_y\rho_s = \pi/4$, $\rho_s/L_n = 0.2$, $T_e = T_i$, $B_y/B_0 = 0.01$, $\rho_s = 2\Delta y$, 16x16 grid, and (0,1) mode, theory (J. Cummings Ph.D. thesis) - - -,
  o= standard δf simulation, $*$ = extended Hybrid II code with kinetic electrons.

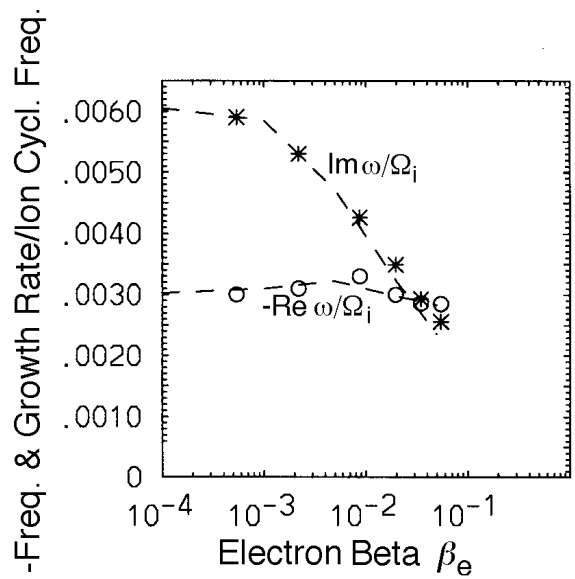




- The Hybrid II algorithm gives good results for $\beta m_i/m_e > 1$ and any skin depth, while the standard δf simulation fails *except* for $\beta m_i/m_e \le 1$ and $\Delta y < c/\omega_{pe}$.

Hybrid II Code – Slab ITG Instability Accurate for $\beta m_i/m_e$>1

- 2D Hybrid II simulations of shearless ITG accurate for $\beta m_i/m_e > 1$ and no constraint on the skin depth, i.e., c/ω_{pe} relative to the cell size Δx. Accommodates finite η_e.



- 2D slab simulations with no shear, θ=0.01, T_e=T_i, η_i =η_e=4, ρ_s/L_n=0.1, Ω_e/ω_{pe}=1, m_i/m_e=1836, ρ_s=2Δx, 32×32 grid. Frequency and growth rates for the (0,1) mode ($k_y\rho_s \approx \pi/8$) vs. $\beta_e = (\omega_{pe}\Delta x/c)^2(\rho_s/\Delta x)^2(m_e/m_i)(\omega_{pe}/\Omega_e)^2$ theory (- - -) (J. Cummings, Ph.D. Thesis, 1995) (±10% error bars in obs. Re ω)

Hybrid II Code – Shear-Alfvén Instability for $\beta m_i/m_e$<1

- Consider the consequences of the explicit backward differencing of the inertia term in the Ohm's law, which leads to a numerical instability at low β:

$$en_{0e}\vec{E}\cdot\hat{b}^{(0)} = -\nabla_{\|}P_{\|e} + \frac{\delta\vec{B}_{\perp}}{B}\cdot\nabla en_{0e}\phi - n_{0e}m_e(\partial/\partial t + \vec{v}_{ExB}\cdot\nabla)u_{\|e}, \ldots. \partial u_{\|e}/\partial t = \Delta t^{-1}(u_{\|e}^{n} - u_{\|e}^{n-1})$$

- A heuristic stability analysis yields the following dispersion relation for shear-Alfvén waves:

$$(\lambda^{-1} + \omega_{pe}^2/k_{\perp}^2c^2)(\lambda-1)^2/4\lambda = \omega_h^2\Delta t^2/4, \ldots \lambda \equiv \exp(-i\omega\Delta t)$$

- Limits---

  Electrostatic: $\omega_{pe}^2/k_{\perp}^2c^2 = (\beta_e m_i/m_e)/k_{\perp}^2\rho_s^2 << 1 \;\rightarrow \lambda = 1/(1\pm\omega_h\Delta t)$

  |λ|>1 ***instability*** !!

  Electromagnetic: $\omega_{pe}^2/k_{\perp}^2c^2 = (\beta_e m_i/m_e)/k_{\perp}^2\rho_s^2 >> 1$ and $k_{\|}v_A\Delta t/2 < 1$

  stability with $\omega\Delta t/2 = \pm\frac{1}{2}k_{\|}v_A\Delta t(1-\varepsilon/2) - i\varepsilon(\frac{1}{2}k_{\|}v_A\Delta t)^2, \varepsilon \equiv k_{\perp}^2c^2/\omega_{pe}^2 << 1$

  General dispersion relation is a cubic (for a cold plasma), and there is numerical ***stability*** for $\omega_{pe}^2/k_{\perp}^2c^2 = (\beta_e m_i/m_e)/k_{\perp}^2\rho_s^2 > O(1)$.

Hybrid II Code – Implicit Solution of $u_{||e}$ to Improve Numerical Stability

- If we Introduce implicit time differencing of $u_{||e}$ in the electron inertia term in Ohm's law, then

$$en_{0e}\vec{E}\cdot\hat{b}^{(0)} = -\nabla_{||}P_{||e} + \frac{\delta\vec{B}_{\perp}}{B}\cdot\nabla en_{0e}\phi - n_{0e}m_e(\partial/\partial t + \vec{v}_{ExB}\cdot\nabla)u_{||e}, \ldots. \partial u_{||e}/\partial t = \Delta t^{-1}(u_{||e}^{n+1} - u_{||e}^{n})$$

- Next solve for $A_{||}^{n+1}$ in terms of $u_{||e}^{n+1}$ and substitute into Ampere's law to obtain an elliptic equation for $u_{||e}^{n+1}$

$$(-\nabla_{\perp}^2 + \omega_{pe}^2/c^2)u_{||e}^{n+1} = -\nabla_{\perp}^2(\ldots)^n$$

- We would expect this modification of the hybrid algorithm to have improved numerical stability for smaller values of $\omega_{pe}^2/k_{\perp}^2c^2 = (\beta_e m_i/m_e)/k_{\perp}^2\rho_s^2$. How much smaller?

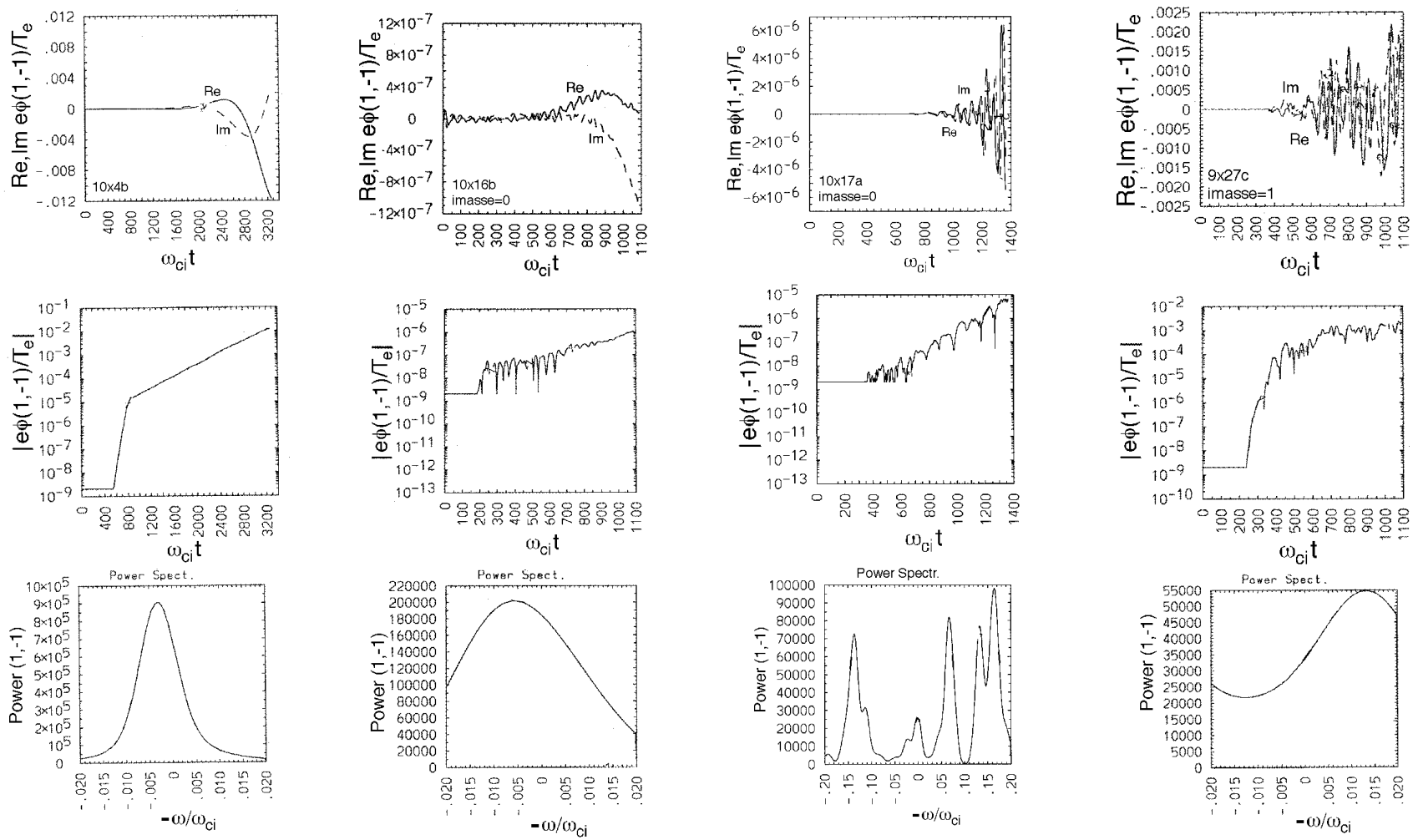
- However, the hybrid algorithm will remain ***poorly posed*** as $\beta \to 0$ because of the presence of $A_{||}$ and use of Ampere's law which becomes a statement of 0=0.

Hybrid II Has Trouble with Sheared-Slab Electron Resonant Response

- The Hybrid II algorithm uses a perturbation expansion around an adiabatic fluid representation for the electron response. In a sheared slab near a mode rational surface, the electron response transitions from hydrodynamic to adiabatic locally in space (with an intermediate region where kinetic corrections are ***not*** perturbative). The following sheared slab ITG results illustrate the failure of the algorithm.

$T_e=T_i$, $\eta_i=\eta_e=4$, $\rho_s/L_n=0.05$, $L_s/L_n=200$, $\Omega_e/\omega_{pe}=1$, $m_i/m_e=1836$, $\rho_s=3\Delta x$, 128×32 grid. $\Delta x_e\sim1.5\Delta x$

adiabatic electrons | massless fluid electrons $\beta_e=2\times10^{-4}$ | kin. electrons $\beta_e=2\times10^{-4}$ | kin. electrons $\beta_e=.02$

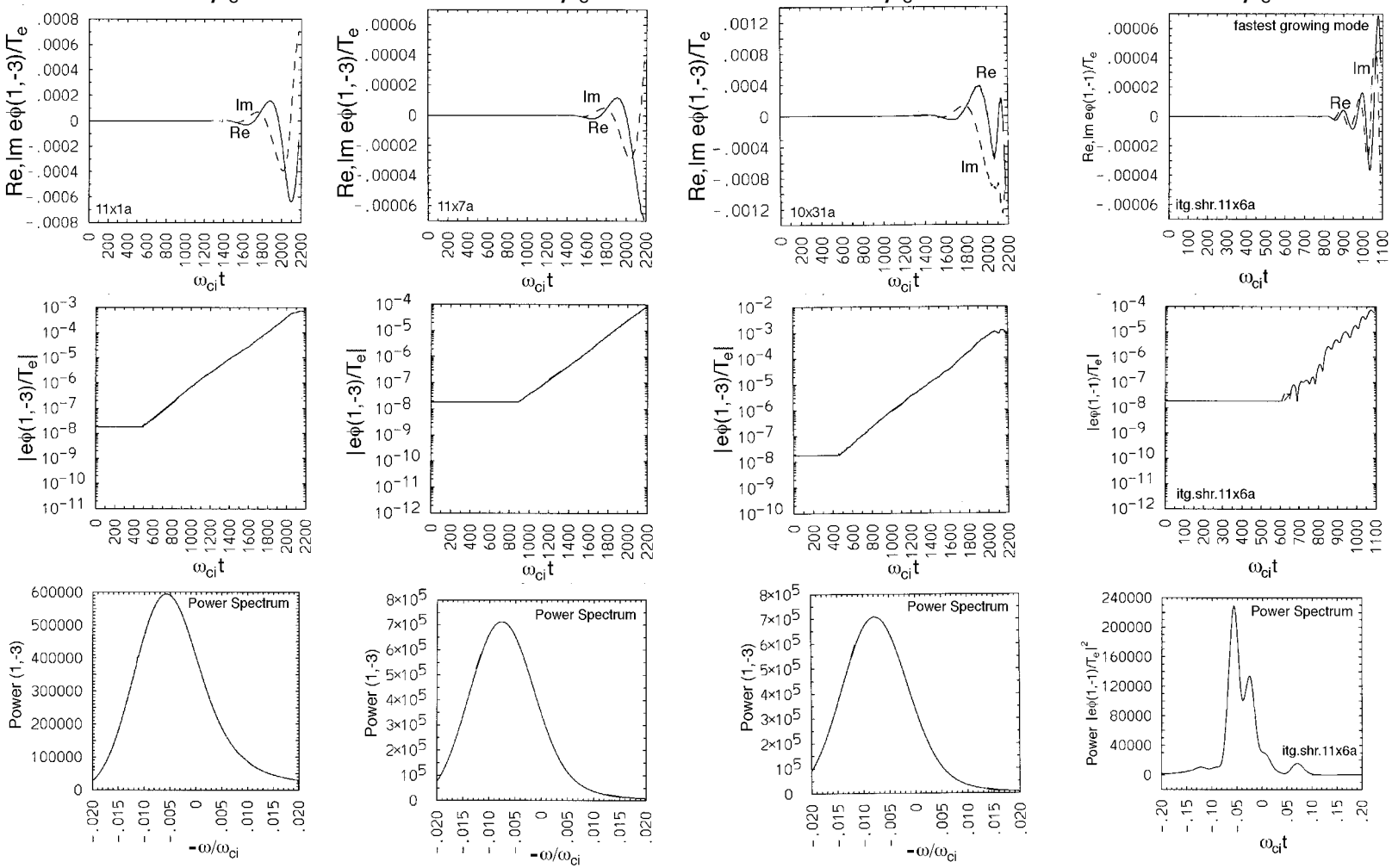


ITG: $\omega/\Omega_i=.003+i.003$ | ITG: $\omega/\Omega_i=.005+i.004$ | ITG: $\omega/\Omega_i=??+i.008$ | Alfvén noise & no ITG

Hybrid II Sheared-Slab Simulation: Example Suite #2 (unresolved electron layer)

- The Hybrid II simulation suite addressing a sheared slab. If we deliberately do *not* resolve the layer near the mode rational surface where the electron response transitions from hydrodynamic to adiabatic locally in space, what happens to the simulation results? The following sheared slab ITG results indicate that the algorithm produces systematic errors when there are kinetic electrons. $T_e=T_i$, $\eta_i=\eta_e=4$, $\rho_s/L_n=0.05$, $L_s/L_n=200$, $\Omega_e/\omega_{pe}=1$, $m_i/m_e=1836$, $\rho_s=\Delta x$, 128×32 grid. $\Delta x_e \sim \Delta x$, imasse=0

fluid electrons $\beta_e=2\times10^{-5}$ | fluid electrons $\beta_e=.002$ | kin. electrons $\beta_e=2\times10^{-5}$ | kin. electrons $\beta_e=.002$

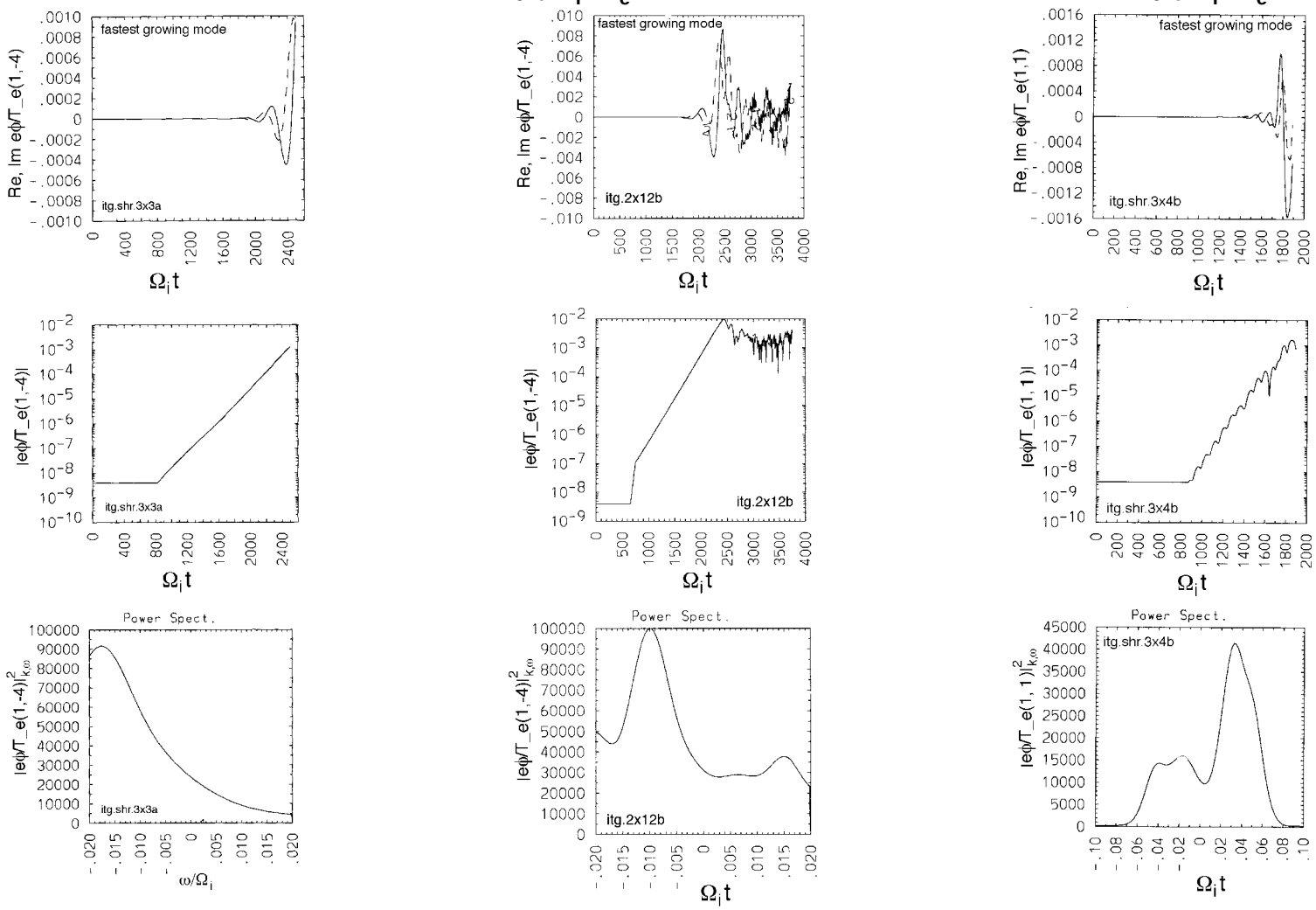


ITG: ω/ω_{ci}=0.0059+i0.0069 ω/ω_{ci}=0.0075+i0.0066 ω/ω_{ci}=0.008+i0.0069 ω/ω_{ci}=0.06+i0.018

Hybrid II Sheared-Slab Simulation: Example Suite #3

- The Hybrid II simulation suite addressing a sheared slab. Here we resolve the electron resonance layer near the mode rational surface by using a smaller mass ratio: m_i/m_e=400. These sheared-slab ITG results indicate that Hybrid II again produces systematic errors when there are kinetic electrons. $T_e=T_i$, $\eta_i=\eta_e=4$, $\rho_s/L_n=0.05$, $L_s/L_n=200$, $\Omega_e/\omega_{pe}=1$, $m_i/m_e=400$, $\rho_s=\Delta x$, 128×32 grid. $\Delta x_e \sim 10\Delta x$, imasse=1

adiab. elect.(sheared) **kin. elect. $\beta_e m_i/m_e$=2 (unsheared, θ=0.01)** **kin. elect. $\beta_e m_i/m_e$=2 (sheared)**



linear modes: ω/Ω_i=.017+i.0073 ω/Ω_i=.017+i.0064 ω/Ω_i=-.032+i.013

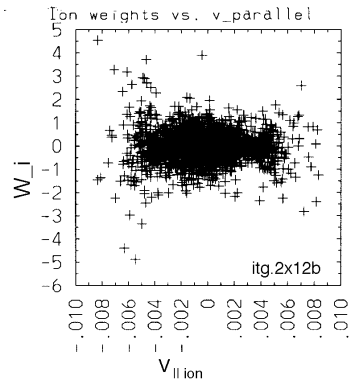
Hybrid II Sheared-Slab Simulation: Example Suite #3 (cont'd)

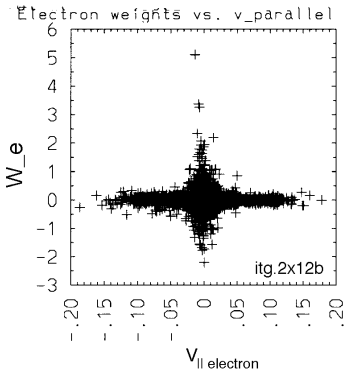
- The Hybrid II simulation produces a systematic error in the electron resonance layer leading to anomalously large electron weights.

- Compare electron and ion weights in unsheared and sheared slab simulations for ITG. The electron weights $|W_e| \sim 10|W_i|$ in the sheared case.

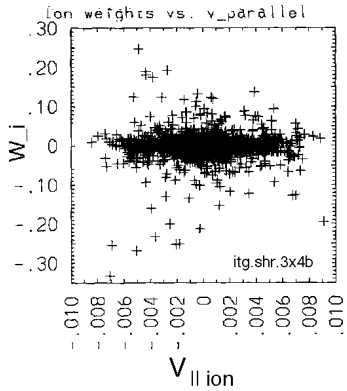
$T_e=T_i$, $\eta_i=\eta_e=4$, $\rho_s/L_n=0.05$, $L_s/L_n=200$, $\Omega_e/\omega_{pe}=1$, $m_i/m_e=400$, $\rho_s=\Delta x$, 128×32 grid, imasse=1

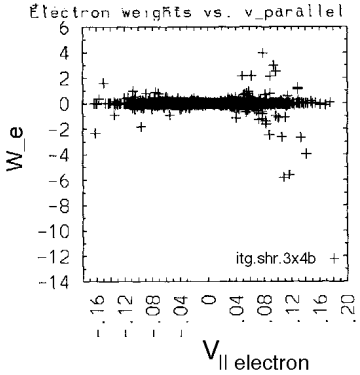
Unsheared ITG (saturated regime with $|W_e|\sim|W_i|$)





Sheared ITG (linear regime with $|W_e|\sim10|W_i|$)





Hybrid II Algorithm Breaks Near Mode Rational Surfaces

- **Hybrid II algorithm (and Lin-Chen) is predicated on a perturbative expansion of the electrons relative to their adiabatic fluid response:**

  Ohm's Law: $en_{0e}\vec{E}\cdot\hat{b}^{(0)} = -\nabla_{\|}P_{\|e} + \frac{\delta\vec{B}_{\perp}}{B}\cdot\nabla en_{0e}\phi - n_{0e}m_e(\partial/\partial t + \vec{v}_{ExB}\cdot\nabla)u_{\|e}$

  ---------- dominant ---------- perturbation

  Split-weight electrons: $f_e = f_M(\vec{x},\vec{v}) + \left(\delta n_e^{(0)} / n_{0e}\right) f_M(\vec{v}) + h_e(\vec{x},\vec{v})$

- **2 significant errors in electron physics description in electron resonant layers.**
  (1) When $\omega >> k_{\|}v_e$, dominant terms in Ohm's law are electron inertia and parallel electric field force, and parallel pressure is a correction. Iterating inertia term as an explicit correction to an adiabatic response is grossly in error.
  (2) The lowest-order fluid solution of fluid equations (sans kinetic increment) used in algebraic reduction of dW^e/dt electron weight evolution equation is invalid, and the electron kinetic correction h_e to the perturbed electron distribution when integrated over velocity space is NOT small compared to $\delta n^{(0)}$ (the lowest-order fluid approximation).

- **Conclusions:**
  -The Hybrid II electron description breaks near mode rational surface inside the electron resonance layer: $\Delta x_e / \Delta x = \frac{\omega/\Omega_i}{k_y\rho_s}\sqrt{\frac{m_e}{m_i}}\frac{L_s}{\Delta x}$
  -Anomalous growth of the electron weights, Alfvénic noise, and lack of finite-β stabilization observed in ITG simulations in sheared slab and toroidal simulations are probable manifestations of the Hybrid II algorithm breaking.

Toroidal Flux-tube Implementation of the Hybrid II Algorithm

- Determine the parallel electric field from the modified electron momentum equation (Ohm's law) including toroidicity (ref: P. Snyder and G. Hammett)

$$en_{0e}\vec{E}\cdot\hat{b}^{(0)} = -\nabla_{||}P_{||e} + \frac{\delta\vec{B}_{\perp}}{B}\cdot\nabla en_{0e}\phi - n_{0e}m_e(\partial/\partial t + \vec{v}_{ExB}\cdot\nabla)u_{||e}$$

$$-\left(\tfrac{1}{2}\delta P_{\perp e} - \delta P_{||e}\right)\hat{b}^{(0)}\cdot\nabla\ln B$$

where $\nabla_{||}P_{||e} = \nabla_{||}P_{||e}^{(0)} + T_{||e}^{(0)}\nabla_{||}(\delta n_e - \delta n_e^K) + n_{0e}\nabla_{||}\delta T_{||e}$ with $\nabla_{||}(T_{||e}^{eq} + \delta T_{||e}) = 0$.

- Use Ohm's law to advance $A_{||}$, $\partial A_{||}/c\partial t = (\vec{E} + \nabla\phi)\cdot\hat{b}^{(0)} = \ldots$
- With the updated $A_{||}$ use Ampere's law to determine parallel electron flux: $\Gamma_{||e} = n_{0e}u_{||e} = \frac{c^2}{4\pi e}\nabla_{\perp}^2\frac{A_{||}}{c} + \overline{\Gamma}_{||i}$, where $\overline{\Gamma}_{||i}$ is the gyrokinetic parallel ion current.
- Use the electron continuity equation to advance the total electron density:

$$\frac{\partial\delta n_e}{\partial t} + n_{0e}(\vec{B}^{(0)} + \delta\vec{B}_{\perp})\cdot\nabla\frac{u_{||e}}{B} + \vec{v}_{E\times B}\cdot\nabla n_e$$

$$+\frac{1}{m_e\Omega_e B^2}(\vec{B}\times\nabla B)\cdot\nabla(\tfrac{1}{2}\delta P_{\perp e} + \delta P_{||e}) + \frac{2n_{0e}}{B^3}(\vec{B}\times\nabla B)\cdot\nabla\phi = 0$$

Hybrid II Toroidal Electromagnetic Algorithm (cont'd)

- Determine the electric potential ϕ from the quasineutrality relation using the updated electron and gyrokinetic ion densities:

$$\nabla^2\phi - \frac{\tau(\phi-\tilde{\phi})}{\lambda_D^2} = 4\pi e\left(\delta\overline{n}_i - \delta n_e\right)$$

- Advance the gyrokinetic ions and the drift-kinetic electrons including the toroidal drifts: $\vec{v}_{gs} = v_{\|}\hat{b} + \vec{v}_{E\times B} + \vec{v}_{ds}$, $\vec{v}_{ds} = \frac{v_{\|}^2 + v_{\perp}^2/2}{\Omega_s B^2}\vec{B}\times\nabla B$, $\Omega_s \equiv q_s B_0 / m_s c$ and mirroring.

$$\dot{v}_{\|} = (q_s/m_s)\hat{b}\cdot\vec{E} - (\mu_s/m_s)\hat{b}\cdot\nabla B + v_{\|}(\hat{b}\cdot\nabla\hat{b})\cdot\vec{v}_{E\times B}$$

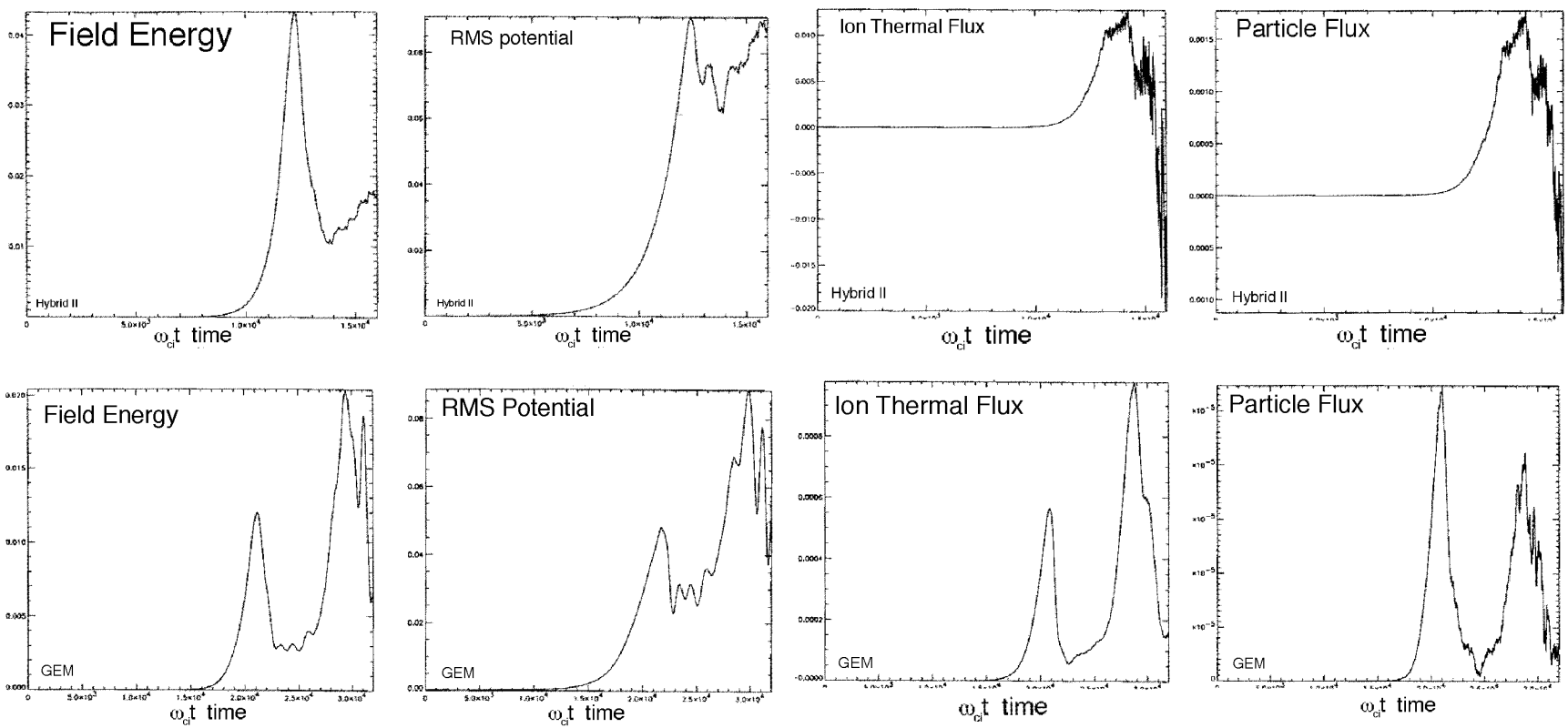
- From drift-kinetic equation for electrons with split-weights (after cancellations)

$$\begin{aligned}\frac{d}{dt}w_i^e &= (\kappa_e - \kappa_{ne})\hat{x}\cdot(\vec{v}_{E\times B} + v_{\|}\hat{b}) - \vec{v}_{de}\cdot\nabla\delta n_e / n_{0e} + \vec{B}\cdot\nabla(u_{\|e}/B) + (v_{\|}/v_e^2)(\tfrac{\partial}{\partial t} + \vec{v}_{E\times B}\cdot\nabla)u_{\|e} \\ &+ v_{\|}(\hat{b}^{(0)}\cdot\nabla\ln B)(\tfrac{1}{2}\delta p_{\perp e} - \delta p_{\|e})/(n_{0e}T_e^{(0)}) + \vec{v}_{E\times B}\cdot(\varepsilon_{\|}\hat{b}\cdot\nabla\hat{b} + \tfrac{1}{2}\varepsilon_{\perp}\nabla\ln B)/T_e^{(0)} \\ &+ (n_{0e}m_e\Omega_e B^2)(\vec{B}\times\nabla B)\cdot\nabla(\delta p_{\|e} + \tfrac{1}{2}\delta p_{\perp e}) + (2c/B^3)(\vec{B}\times\nabla B)\cdot\nabla\phi\end{aligned}$$

- Use flux-tube coordinates: $x=r-r_0$, $y=(r_0/q_0)(q\theta-\zeta)$, $z=q_0R_0\theta$

Initial Comparison Run of Toroidal Hybrid II and GEM Codes

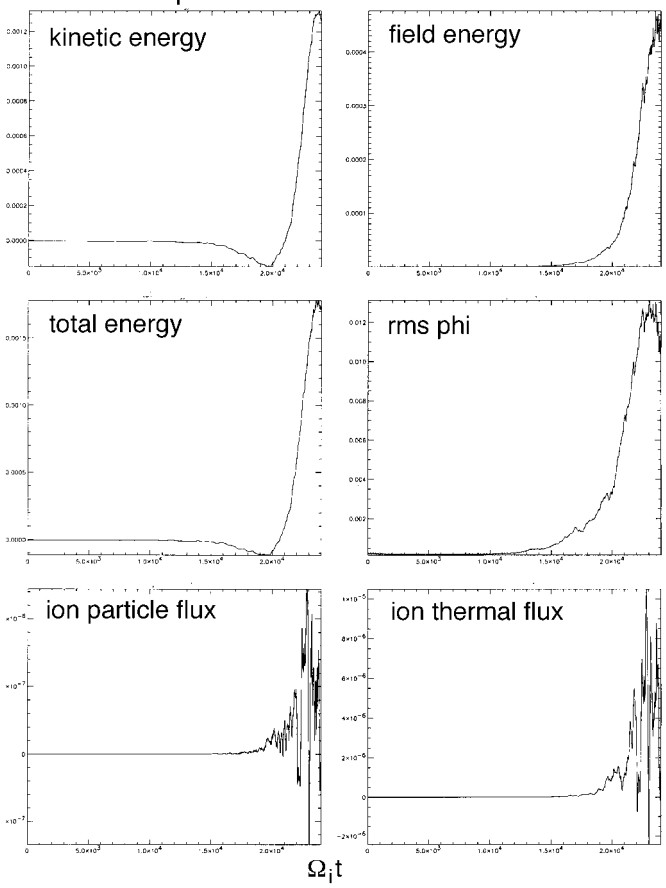
- Toroidal ITG simulations with 32x32x32 grid, $\beta=5\times10^{-4}$, $\eta_\iota=3.5$, $q_0=1.4$, kinetic electrons and ions, $m_i/m_e=1837$, comparing GEM (conventional low-β code) to toroidal Hybrid II preliminary results. Toroidal Hybrid II results are dubious. Electric fields look reasonable, but the thermal and particle fluxes and total energy in Hybrid II simulation are too large.



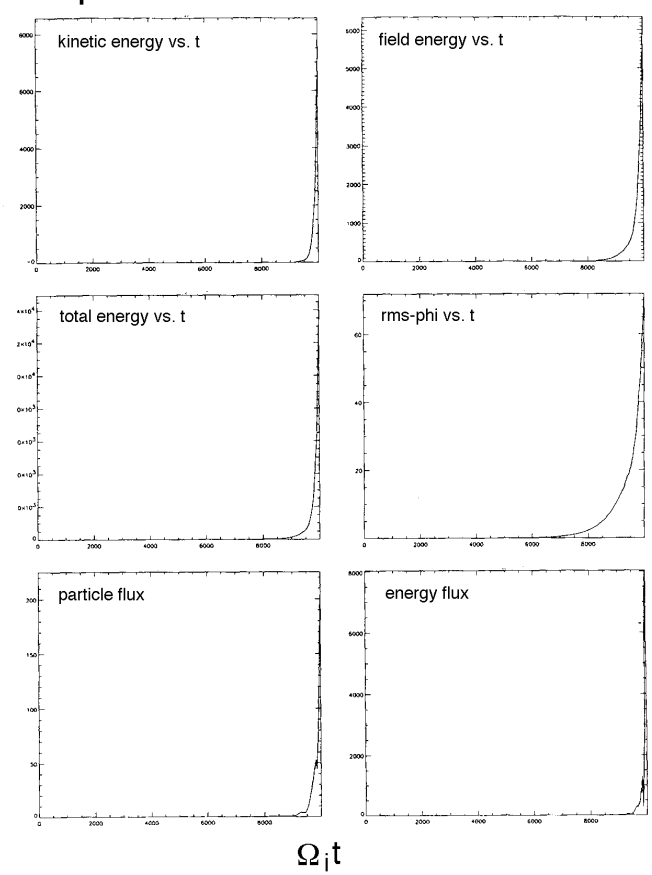
3D Slab Hybrid II Simulations With and Without Kinetic Electrons Codes

- 3D Slab ITG simulations with 32x32x32 grid, $\beta=2.5\times10^{-3}$, $\eta_\iota=5$, tor=0, $m_i/m_e=400$, comparing hybrid simulation (fluid electrons) to kinetic simulation (Hybrid II). The hybrid simulation is well behaved, but the kinetic simulation shows anomalous growth. This suggests that misrepresentation of the electron kinetic resonant layers is fatal.

hps.032 fluid electrons tor=0



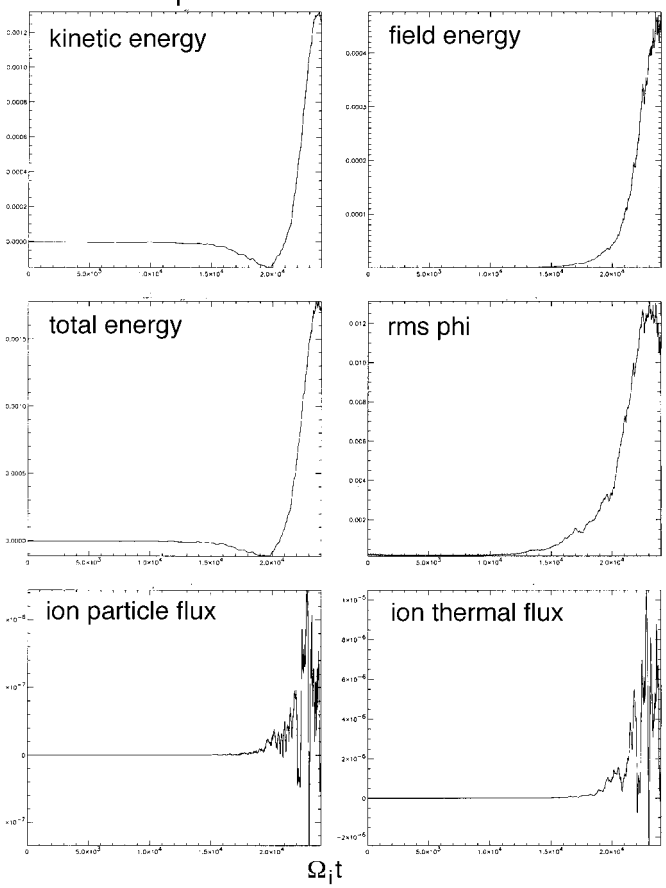
hps.031 kinetic electrons tor=0



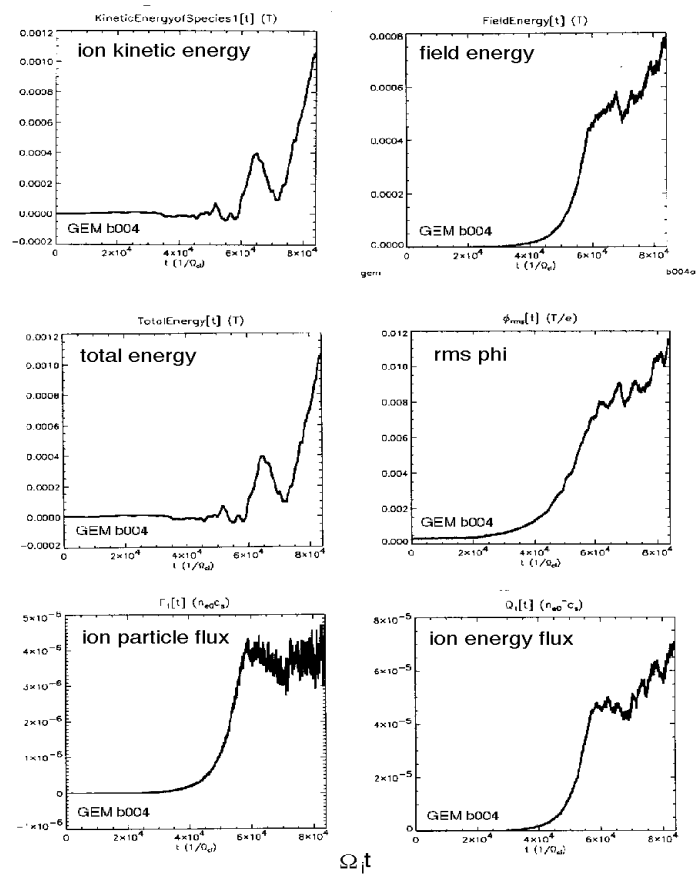
3D Slab Hybrid II & GEM Simulations Without/With Kinetic Electrons

- 3D Slab ITG simulations with 32x32x32 grid, $\beta=2.5\times10^{-3}$, $\eta_i=5$, tor=0, $m_i/m_e=400$, comparing Hybrid simulation (fluid electrons) to kinetic simulation (GEM, drift-kinetic electrons). Both simulations behave, but disagree significantly (particularly fluxes), suggesting that non-adiabatic electron response near rational surfaces is important.

hps.032 fluid electrons tor=0



gem.b004 drift-kinetic electrons tor=0



A Kinetic Electron Closures for Electromagnetic Simulation -- Summary

- The Hybrid II kinetic closure works very well for systems without magnetic shear for $\beta m_i / m_e > 1$ in simulations of shear-Alfvén waves and electromagnetic drift-wave and ITG instabilities with drift-kinetic electrons (two-dimensional, unsheared slab).
- Hybrid II sheared-slab and toroidal simulations with mode rational surfaces fail because the algorithm does not give correct physics in electron resonance layers. (We expect that the very similar Lin-Chen algorithm would have the same difficulties.)
- The more direct GEM δf PIC gyrokinetic Vlasov-Maxwell algorithm of Y. Chen et al. can resolve electron resonances and does not have the same difficulties. The continuum Vlasov-Maxwell codes GS2 and GYRO have not reported any difficulties of this kind.