Discrete Particle Noise in PIC Simulations of ETG Turbulence

NYU Courant Institute Magneto-Fluid Dynamics Seminar
10/3/2005

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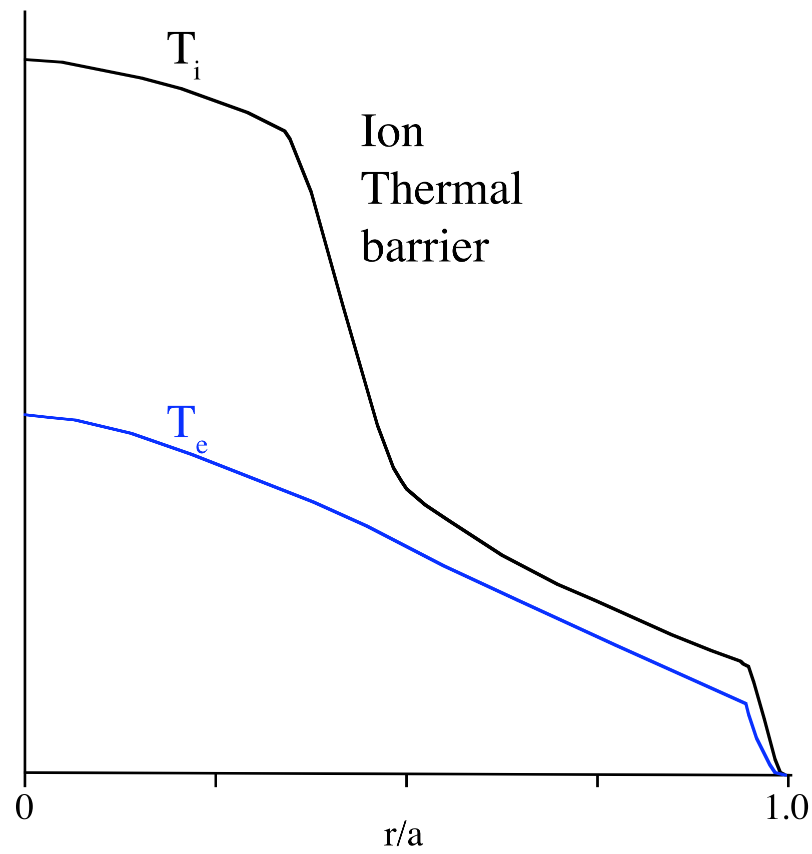
Why do we care about ETG modes?

- Ion Thermal barriers w/o corresponding electron thermal barrier
- Electron thermal transport doesn't always turn off with ion transport
  - □ Mechanisms which transports electrons only:
    - Broken flux surfaces
    - Paleo-classical transport
  - □ Instabilities with $\square \sim \square_e$



Electron Temperature Gradient (ETG) Turbulence has $\lambda \sim \rho_e << \rho_i$

- Electron Heat Transport through ion thermal barriers
  - Need $\chi_e \gtrsim 1 \ m^2/s$
- Isn't ETG transport too weak?
  - (nearly) Isomorphic to ITG but 60× smaller …

$$\chi_e = \Lambda_{e0}\left(\frac{\rho_e}{L_T}\right)\rho_e v_{te} = \Lambda_{e0}\sqrt{\frac{m_e}{M_i}}\left(\frac{\rho_i}{L_T}\right)\rho_i v_{ti}$$

$$\left(\frac{\rho_e}{L_T}\right)\rho_e v_{te} \approx 0.075\left(\frac{T_e}{1\ keV}\right)^{1.5}\left(\frac{B}{1\ Tesla}\right)^{-2}\left(\frac{L_T}{1\ m}\right)^{-1} m^2/s$$

- For ITG, typically $\Lambda_{i0} < 1$

Can $\Lambda_{e0} >> 1$ for ETG???

weak zonal flows ⇒ strong turbulence?

- Previous simulations:
  - Jenko & Dorland, PRL **89**, 225001 (2002)
    flux-tube continuum GK-simulation
    (nearly) Cyclone base-case-like ETG
    $\Lambda_{e0} \approx 13 \Rightarrow \chi_e \approx 1\ m^2/s$
    increases with $s, \nabla T$ …
  - Labit & Ottaviani, Phys. Plasmas **10**, 126 (2003)
    "global" simulations, but $a/\rho_i \sim$ 1-2 dominated by profile variations; model eqs. not full gyro-fluid eqs.
    $\Lambda_{e0} >> \Lambda_{i0}$ (but "small")
  - Li & Kishimoto, Phys. Plasmas **11**, 1493 (2004)
    slab and flux-tube gyro-fluid simulation
    model eqs. not full gyro-fluid eqs
    Λ_{e0} increases with $s, \nabla T$
  - Lin *et al*, 2004 IAEA Mtg. (for example)
    http://www.cfn.ist.utl.pt/20IAEAConf/presentations/T5/2T/5_H_8_4/Talk_TH_8_4.pdf
    global PIC GK simulation
    Cyclone base-case-like ETG
    $\Lambda_{e0} \approx 3 \Rightarrow \chi_e \approx 0.2\ m^2/s$

Cyclone base-case-like ETG Turbulence

- Plasma operating point

  [after Dimits et al, Phys. Plasmas **7**, 969 (March, 2000)]

$$\frac{R_0}{L_T} = 6.9 \qquad q = 1.4$$

$$\frac{R_0}{L_n} = 2.2 \qquad \hat{s} \equiv \frac{r}{q}\frac{dq}{dr} = 0.79$$

$$\frac{T_e}{T_i} = 1.0$$

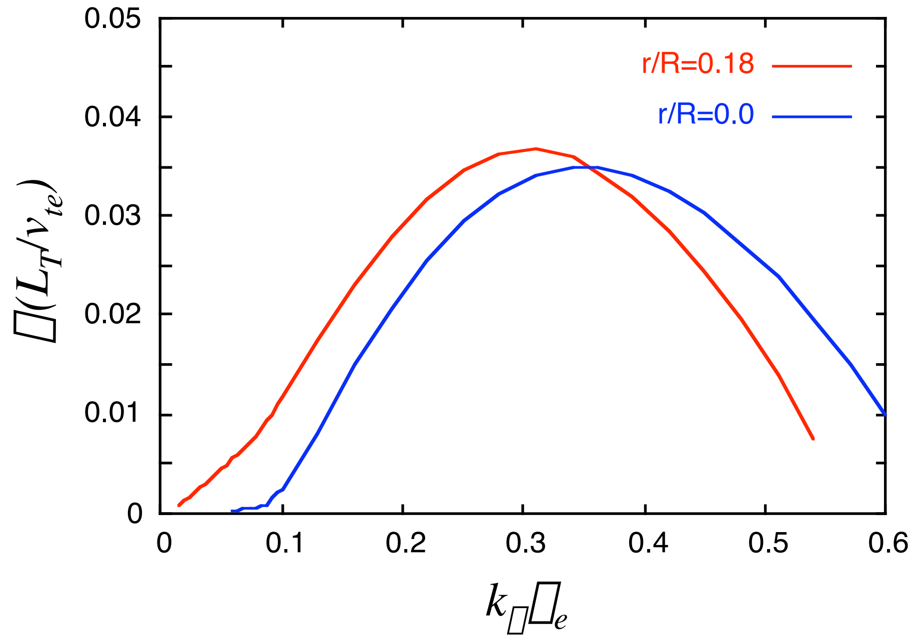
(J&D)

$$\left(\frac{r}{R_0}\right) = 0$$

(Lin)

$$\left(\frac{r}{R_0}\right) \approx 0.18$$

Linear growth rate
with *(r/R₀)=0.18* and without *(r/R₀)=0*
magnetic trapping



Why do Jenko & Dorland ($\square_{e0}\approx 13$) get different results than Lin et al ($\square_{e0}\approx 3$)?

- Different operating point???

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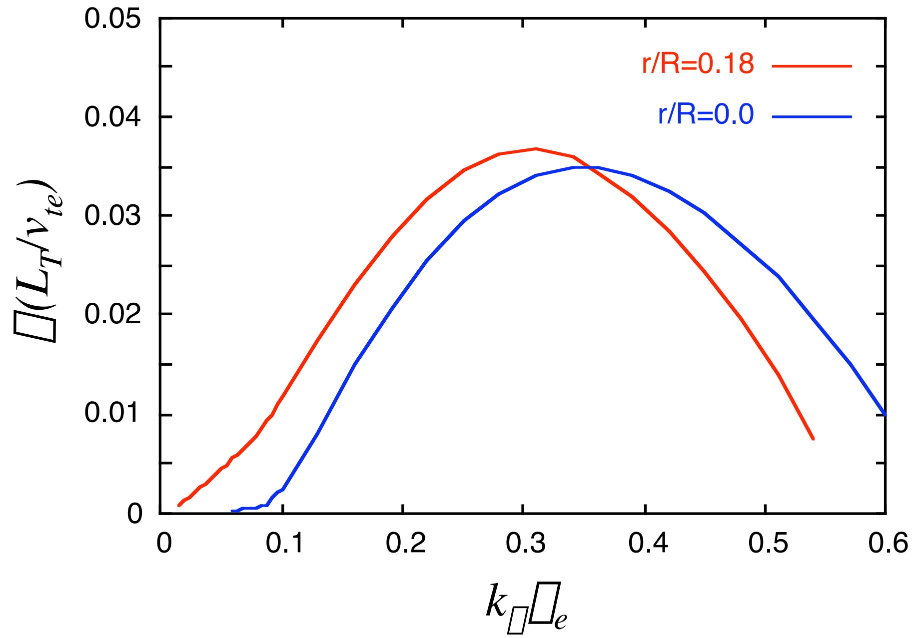

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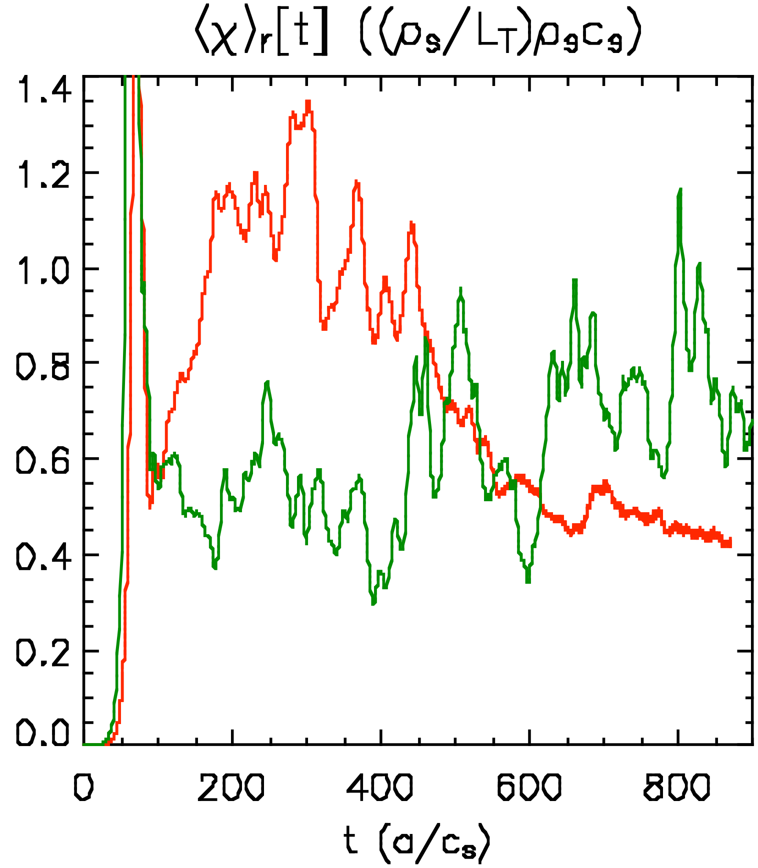
- Different operating point???
- Global vs. flux tube???
- PIC vs. Continuum???
  - Same codes get χ_{i0} within ±30% for Cyclone ITG benchmark

Cyclone ITG Benchmark



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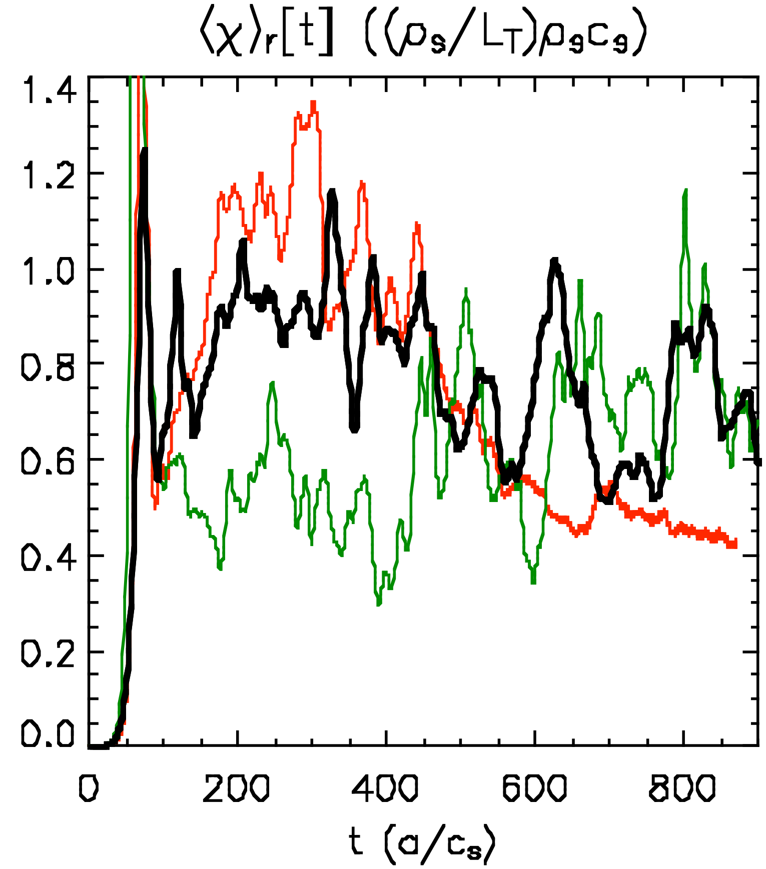

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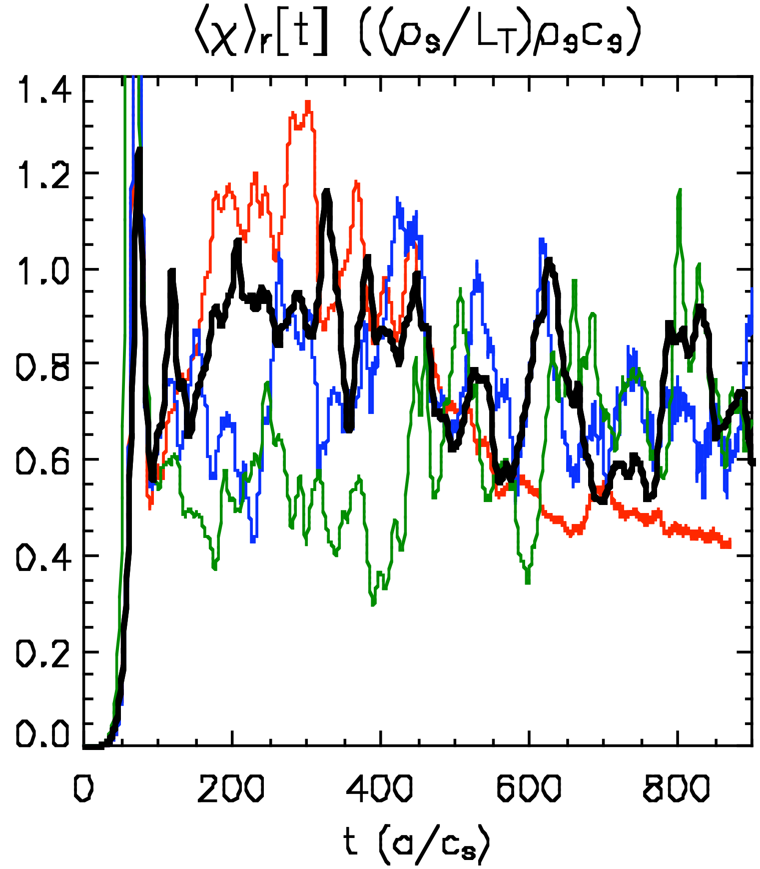

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- Different operating point???
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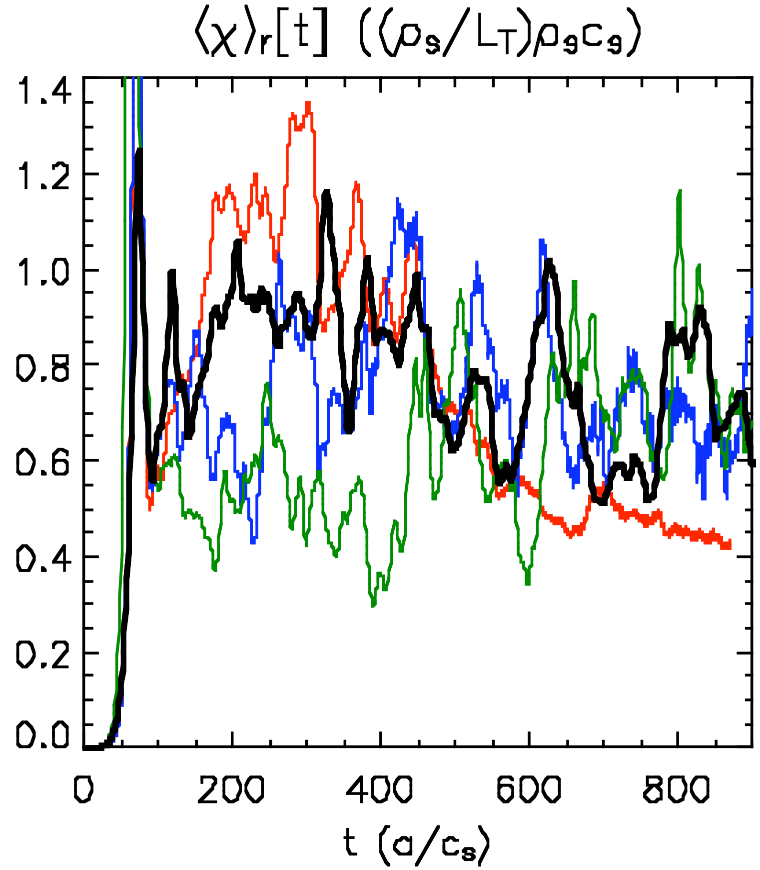
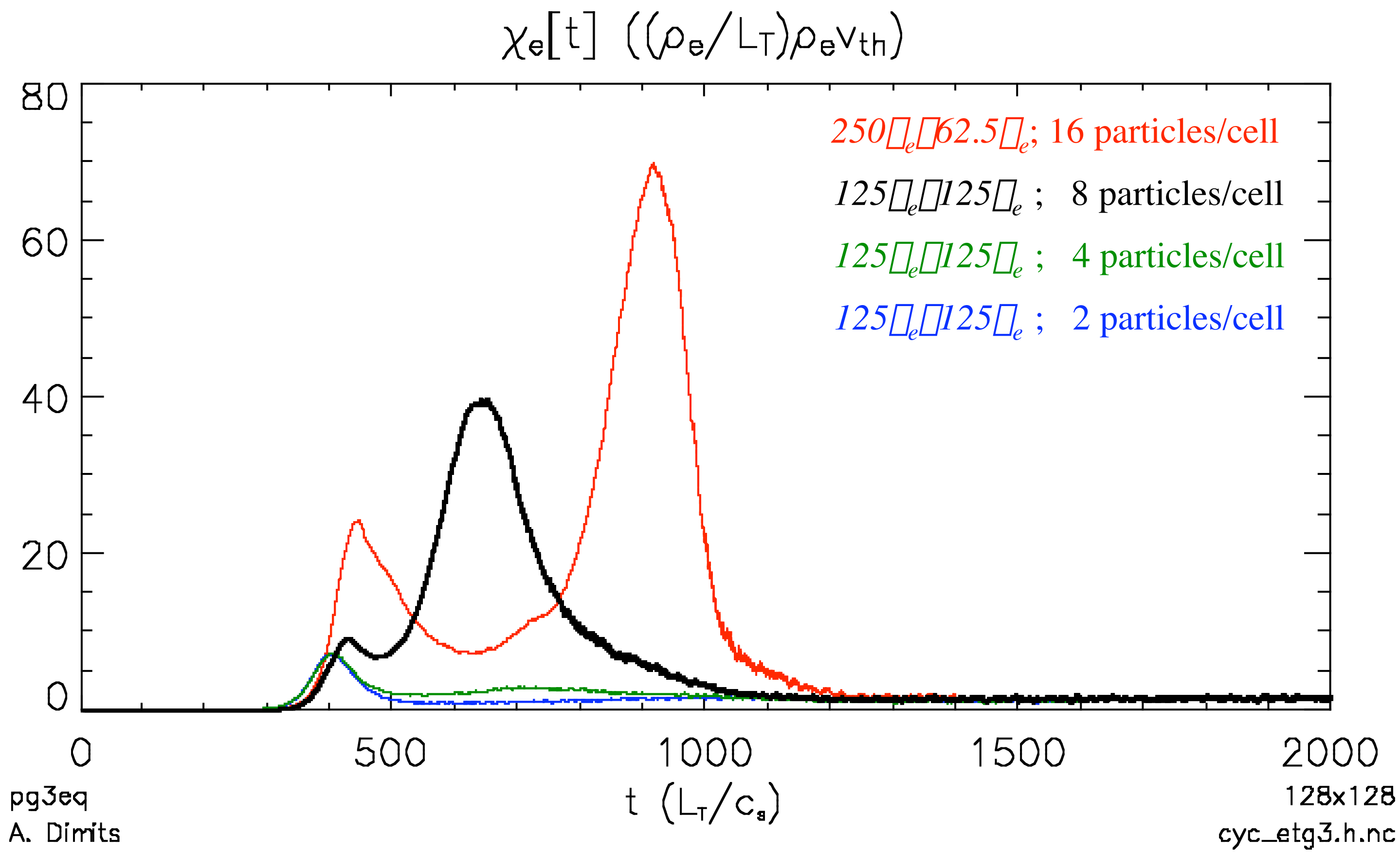
  - Same codes get χ_{i0} within ±30% for Cyclone ITG benchmark
- Compare both Jenko/Dorland and Lin *et al* with PG3EQ
  - LLNL/UCLA code
    - Flux tube
    - PIC
  - PG3EQ agreed with GTC, GS2 in Cyclone ITG benchmark

Cyclone ITG Benchmark



PG3EQ Convergence tests without magnetic trapping ($r/R_0=0$)



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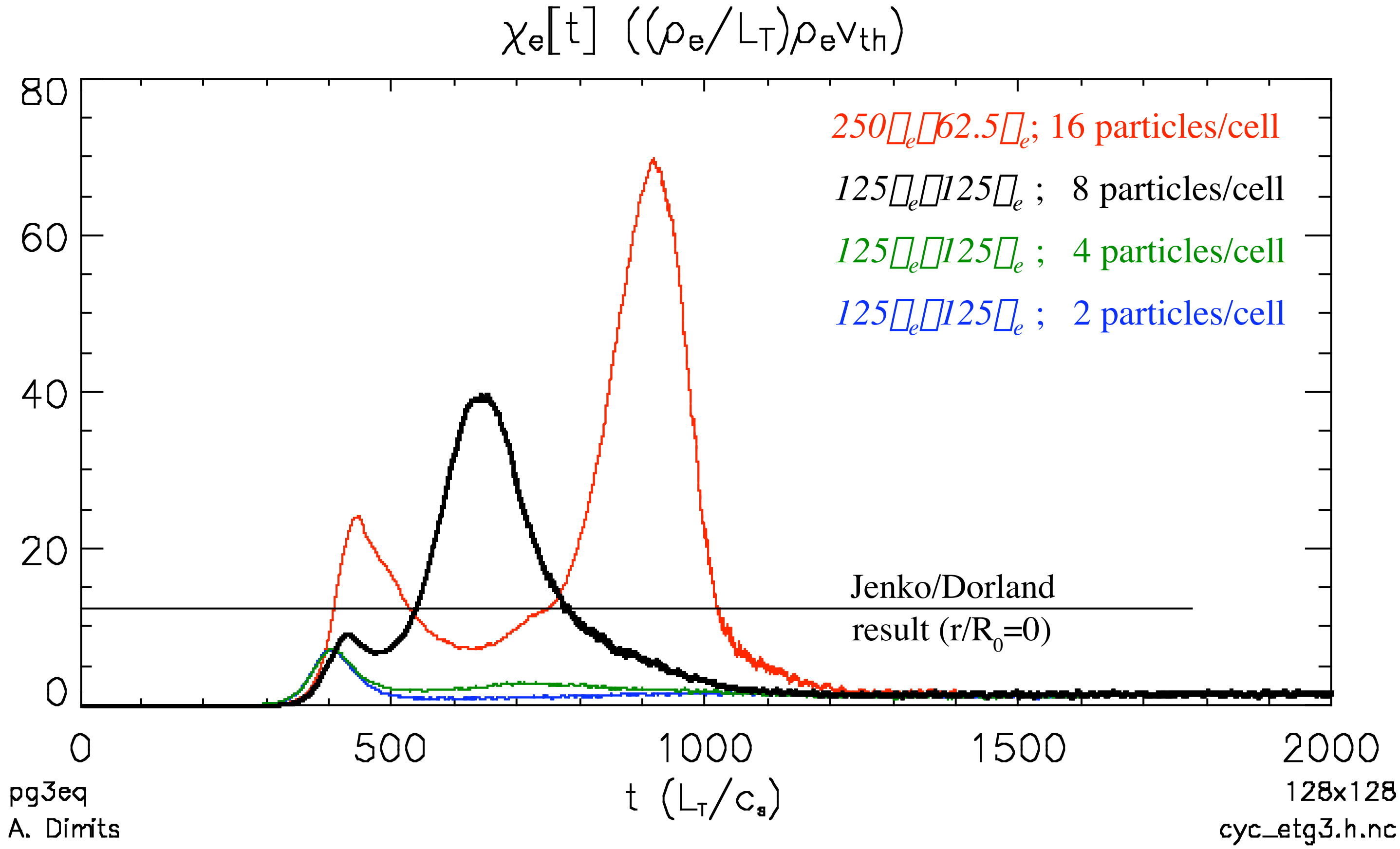

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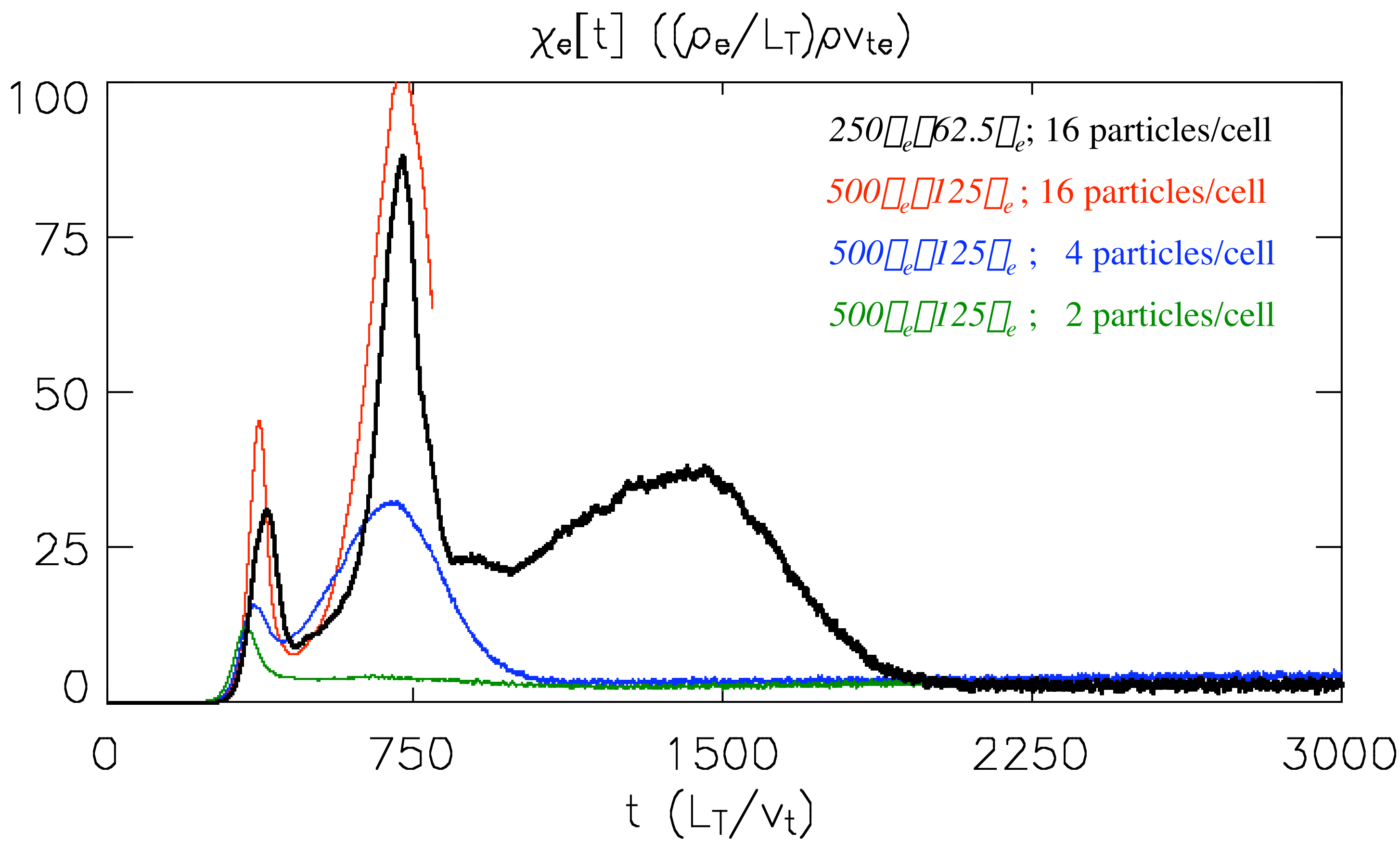

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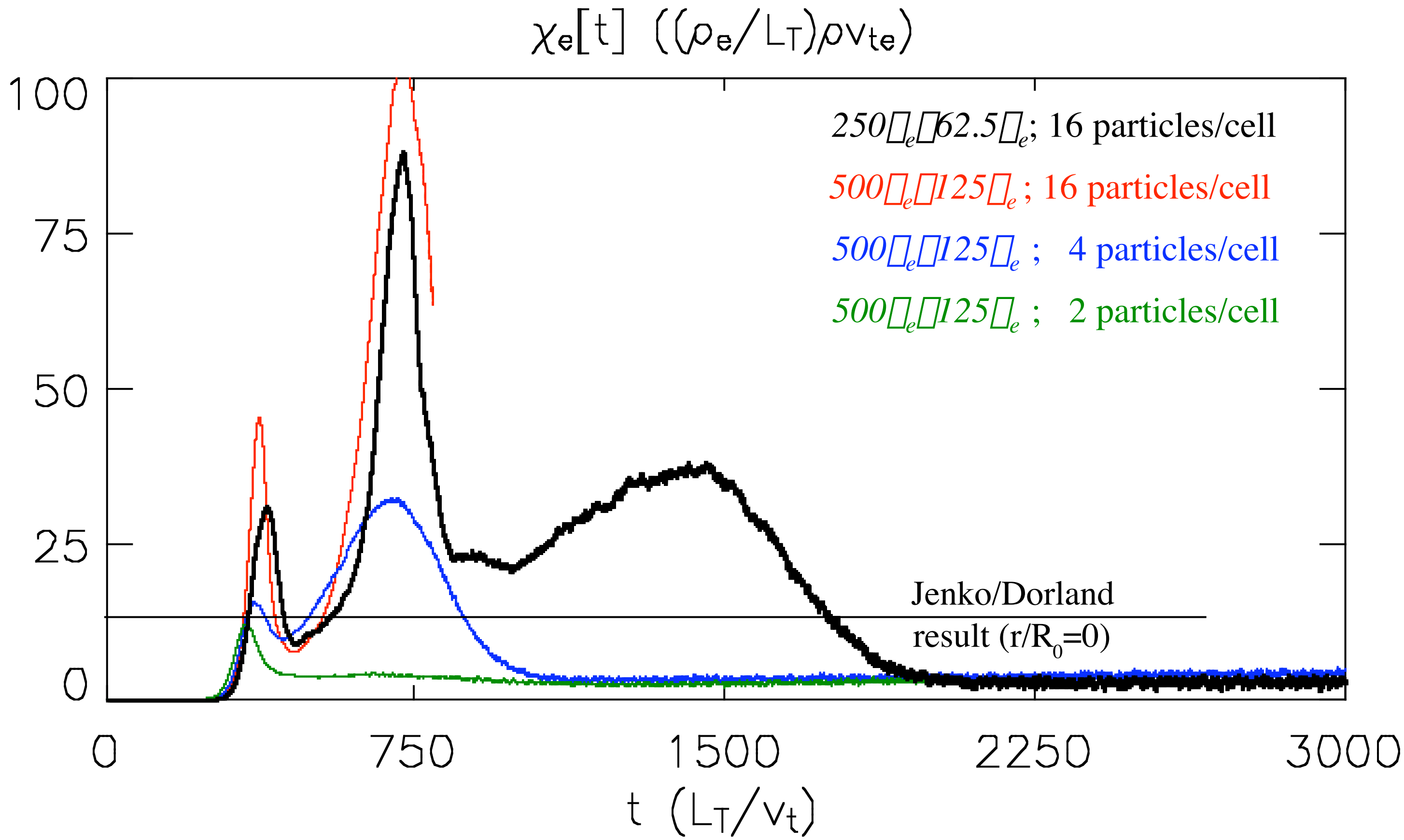

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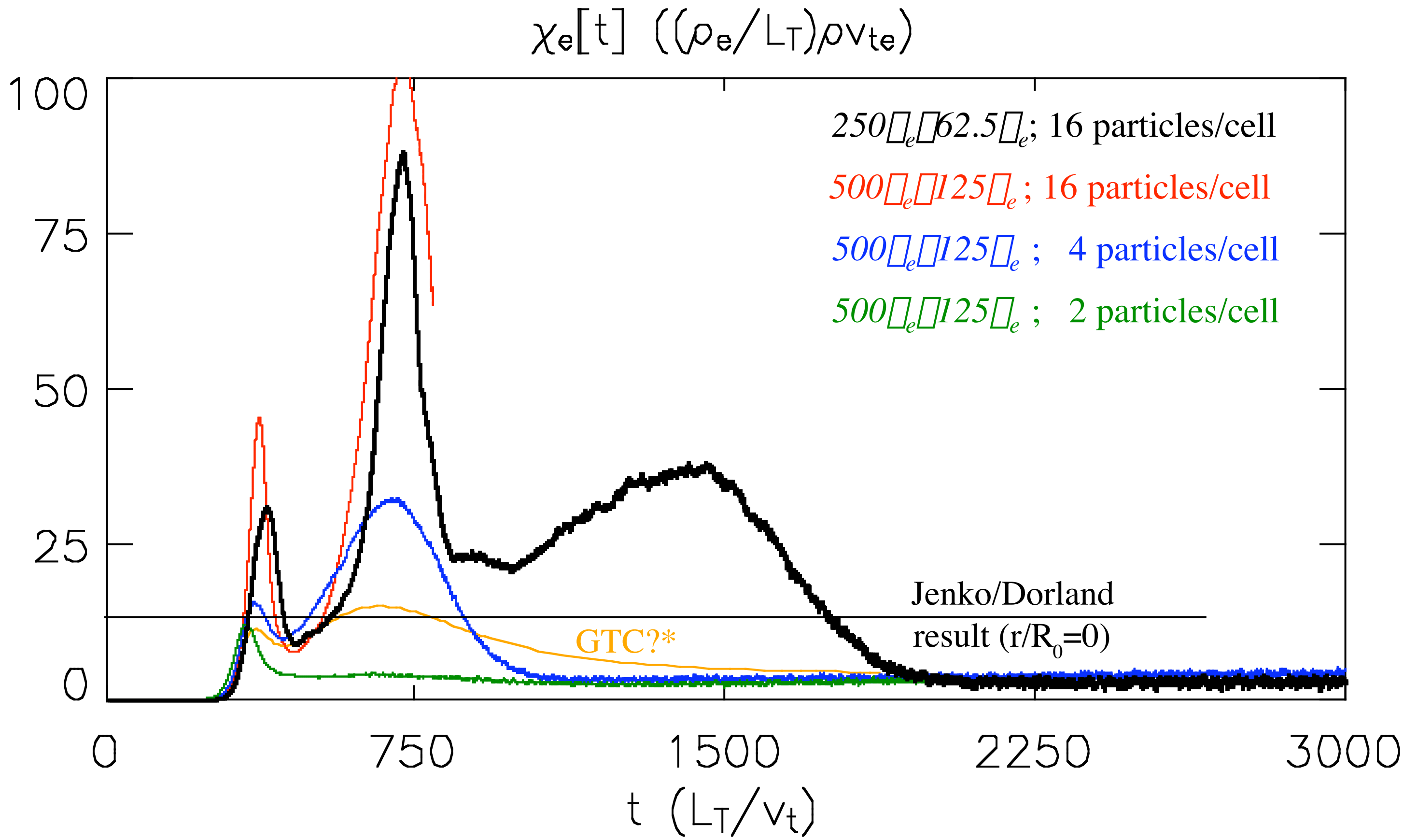
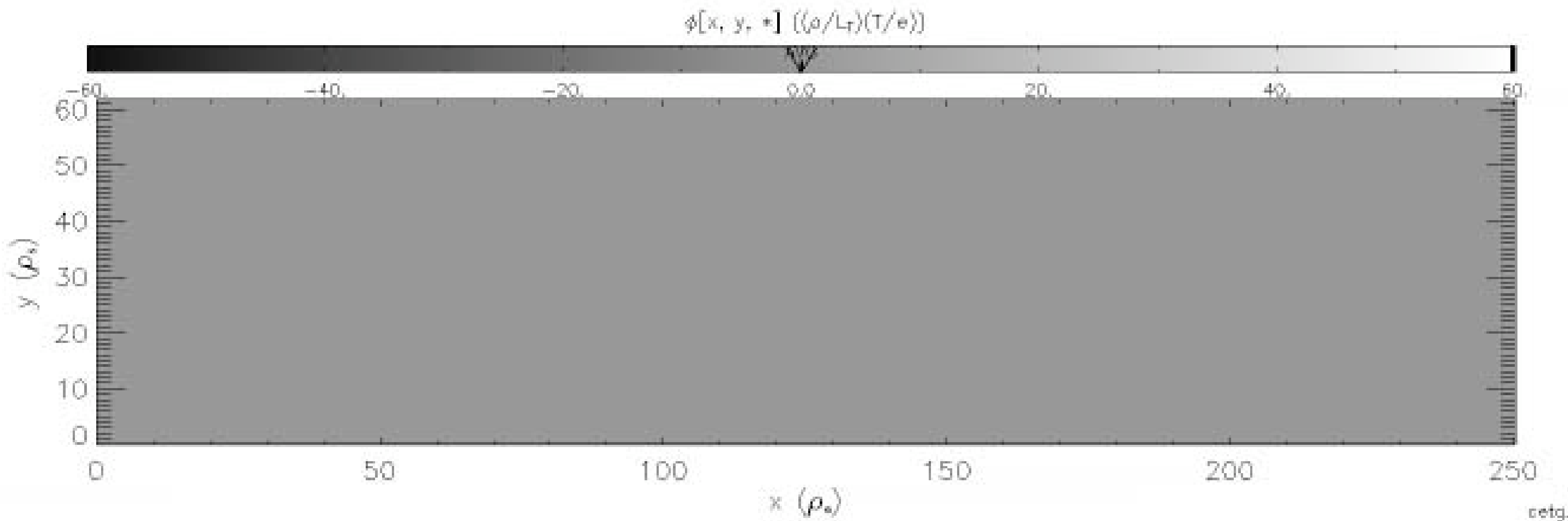


*GTC curve after Slide #13 of Z. Lin's IAEA presentation, which can be found at:
http://www.cfn.ist.utl.pt/20IAEAConf/presentations/T5/2T/5_H_8_4/Talk_TH_8_4.pdf

The mid-plane potential

(r/R$_0$=0.18; 250□$_e$□62.5 □$_e$; 16 particles/cell*)*

- Starts out looking like we've verified results of Lin et al:
  - Characteristic ETG "streamers"
  - Cascade to long wave length
  - □$_{e0}$≈3 (at late times)



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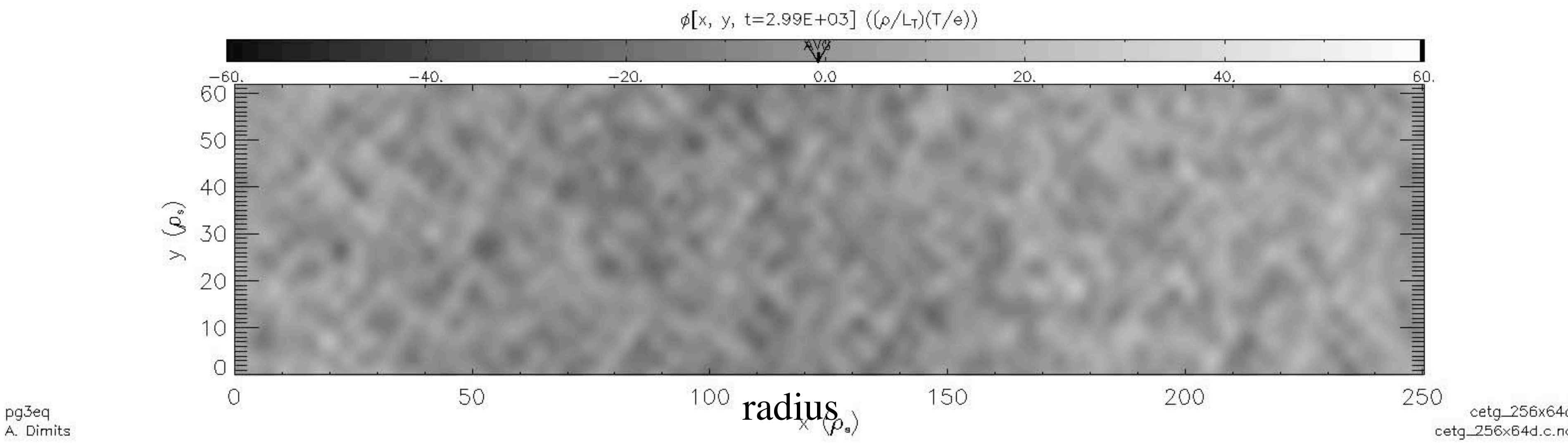
(r/R_0=0.18; 250ρ_e×62.5 ρ_e; 16 particles/cell*)*

- Starts out looking like we've verified results of Lin et al:
  - Characteristic ETG "streamers"
  - Cascade to long wave length
  - χ_{e0}≈3 (at late times)
- Ends up looking like somebody disconnected the TV antenna

⇒ Perhaps we're seeing discrete particle noise?



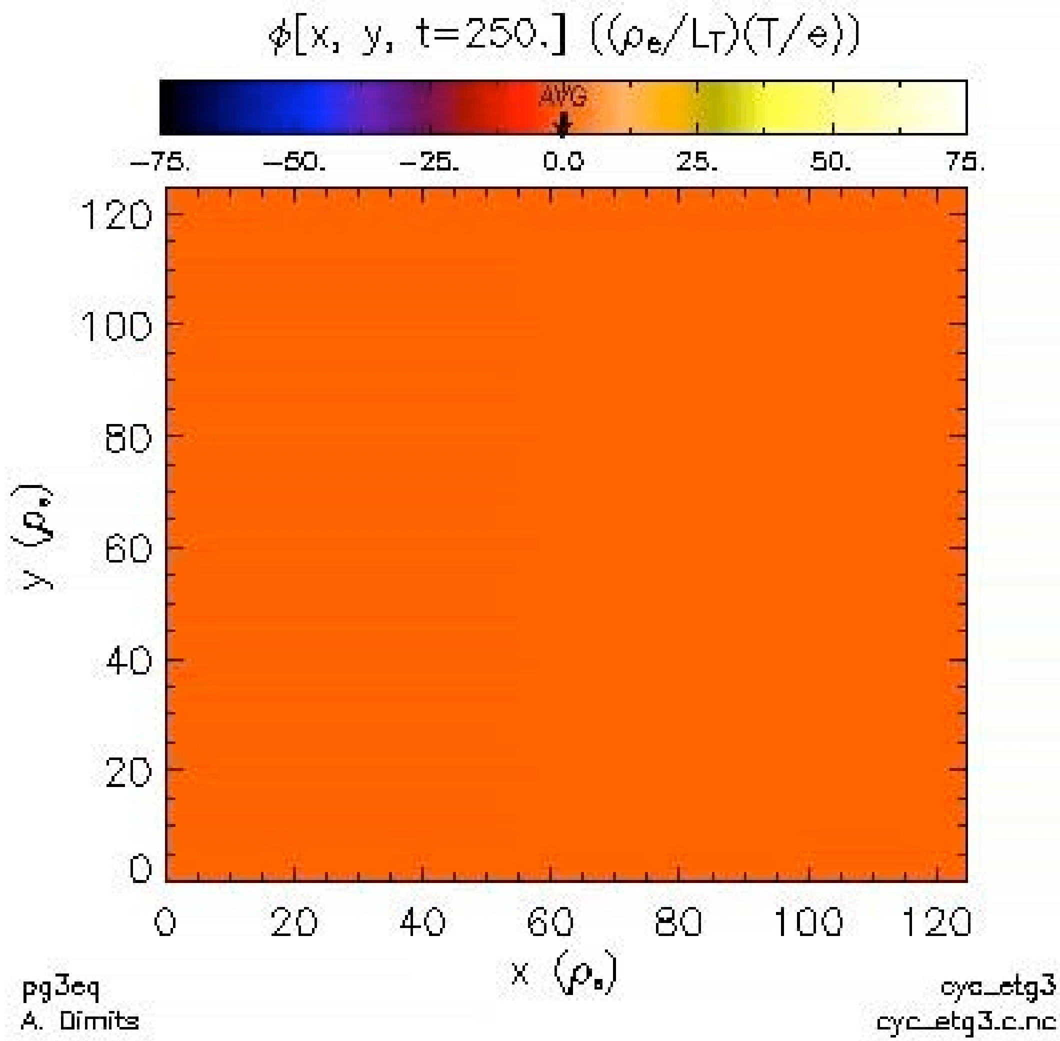
What's known about discrete particle noise in δf PIC codes?

- The major source of controversy between PIC and Continuum GK-simulation communities
- It's quantifiable — a literature on particle discreteness in PIC codes:
  - Langdon '79 – Birdsall&Langdon '85
  - Krommes '93 – Hammett '05

⇒ We can develop objective criteria to determine when discrete particle noise is a problem

- Can be a problem for:
  - Cyclone base-case-like ETG
  - Some Cyclone base-case ITG (mainly longer simulations)

Cyclone base-case-like ETG
Mid-plane potential



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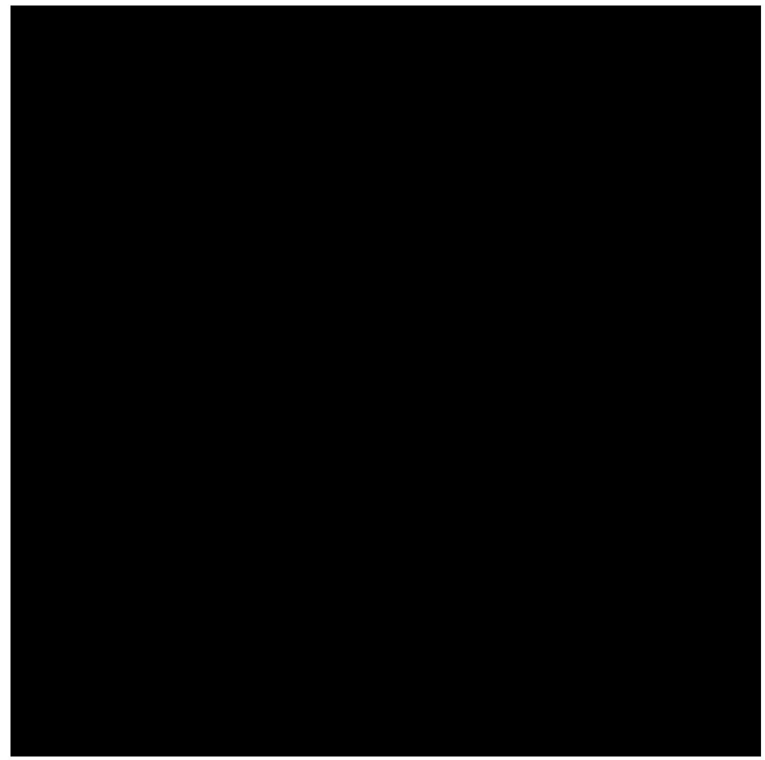


Why Particle Weights Grow in Time

$$\frac{\partial f}{\partial t} + \left(\mathrm{v}_{\parallel} + \mathrm{v}_{ExB}\right) \cdot \nabla f + \frac{q}{m} E_{\parallel} \frac{\partial f}{\partial \mathrm{v}_{\parallel}} = 0$$

$$\frac{Df}{Dt} = 0$$

Clever δf algorithm to reduce noise: f = smooth f_0 + particles δf

$$\frac{D}{Dt}\delta f = -\frac{D}{Dt} f_0 \approx -\mathrm{v}_{ExB} \cdot \nabla f_0$$

$$\delta f = \sum_i w_i(t)\, \delta\!\left(x - x_i(t)\right) \delta\!\left(\mathrm{v} - \mathrm{v}_i(t)\right)$$

$$\delta f \approx \left(x - x_0\right) \frac{df_0}{dx}$$

f = constant along particle's trajectory. But as particle moves to position where local f_0 is different than the f where particle started, weight grows to represent difference.

$$\frac{dw_{rms}^2}{dt} = \frac{d}{dt} \frac{\left\langle (\delta f)^2 \right\rangle}{f^2} \approx \frac{2\chi_{tot}}{L_T^2}$$

entropy balance in steady state
W.W. Lee & W. Tang 88

Simple Estimate of Noise: Randomly Positioned Particles

Fourier conventions: $$\phi(\vec{x}) = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}\,\tilde{\phi}_{\vec{k}}$$

$$\tilde{\phi}_{\vec{k}} = \frac{1}{V}\int_V d^3x\, e^{-i\vec{k}\cdot\vec{x}}\,\phi(\vec{x})$$

Quasineutrality: Adiabatic species + polarization density = “bare” guiding center contribution

Gyrokinetic Poisson Eq:
(W.W. Lee, Phys. Fluids ’83)

$$n_0\frac{e\phi}{T} + n_0 k_\perp^2\rho^2\frac{e\phi}{T} = S_{filt}\int d^3\mathrm{v}\, J_0\,\delta f$$

$$= S_{filt}\sum_i w_i J_{0i}\,\delta(\vec{x}-\vec{x}_i)$$

Fourier transform:

$$n_0\left(2-\Gamma_0\right)\frac{e\tilde{\phi}_k}{T} = \frac{S_{filt}}{V}\sum_i w_i J_{0i} e^{-i\vec{k}\cdot\vec{x}_i}$$

$$\left|\frac{e\tilde{\phi}_k}{T}\right|^2 = \frac{S_{filt}^2}{n_0^2 V^2 (2-\Gamma_0)^2}\sum_i\sum_j w_i w_j J_{0i} J_{0j} e^{-i\vec{k}\cdot\left(\vec{x}_i-\vec{x}_j\right)}$$

Averages to zero unless i=j

Simple Estimate of Noise: Randomly Positioned Particles (II)

Average over uncorrelated random particles:

$$\left\langle \left| \frac{e\tilde{\phi}_k}{T} \right|^2 \right\rangle_N = \frac{S_{filt}^2}{n_0^2 V^2 (2\,\square\,\square_0)^2} \sum_i w_i^2 J_{0i}^2$$

$$= \frac{S_{filt}^2\left(\vec{k}\right)}{\left(n_0 V\right)^2 (2\,\square\,\square_0)^2}\, n_0 V \left\langle w_i^2 \right\rangle \square_0$$

$$\left\langle \left| \frac{e\phi(\vec{x})}{T} \right|^2 \right\rangle = \sum_k \left\langle \left| \frac{e\tilde{\phi}_k}{T} \right|^2 \right\rangle_N$$

$$= \frac{\left\langle w_i^2 \right\rangle}{n_0 V} \sum_k \frac{S_{filt}^2}{(2\,\square\,\square_0)^2} \square_0 = \frac{\left\langle w_i^2 \right\rangle}{n_0 V_{smooth,N}}$$

Noise scales with 1/(Number of particles per smoothing volume)

V_{smooth} ~ 150 cells ~ $(5.3)^3$ cells for Dimits' smoothing parameters

Quantifying Particle Discreteness (2)

(a partially correlated fluctuation spectrum)

- More detailed calculation following Krommes93 gyrokinetic test-particle superposition calculation, including dielectric shielding in kinetic response, numerical filtering/interpolation factors, resonance broadening renormalization:

$$\left\langle \left| \frac{e\phi_k}{T} \right|^2 \right\rangle_H = \frac{V^2 \left\langle w_i^2 \right\rangle S_{filter}^2(k) S^2(k) \Gamma_0(k_\perp^2 \rho_{th}^2)}{N_p \left[2 - \Gamma_0(k_\perp^2 \rho_{th}^2) \right] \left[2 - \left(1 - S_{filter} S^2 d_{\|}(k) \right) \Gamma_0(k_\perp^2 \rho_{th}^2) \right]} \xrightarrow{k \to 0} \frac{V^2 \left\langle w_i^2 \right\rangle}{2 N_p}$$

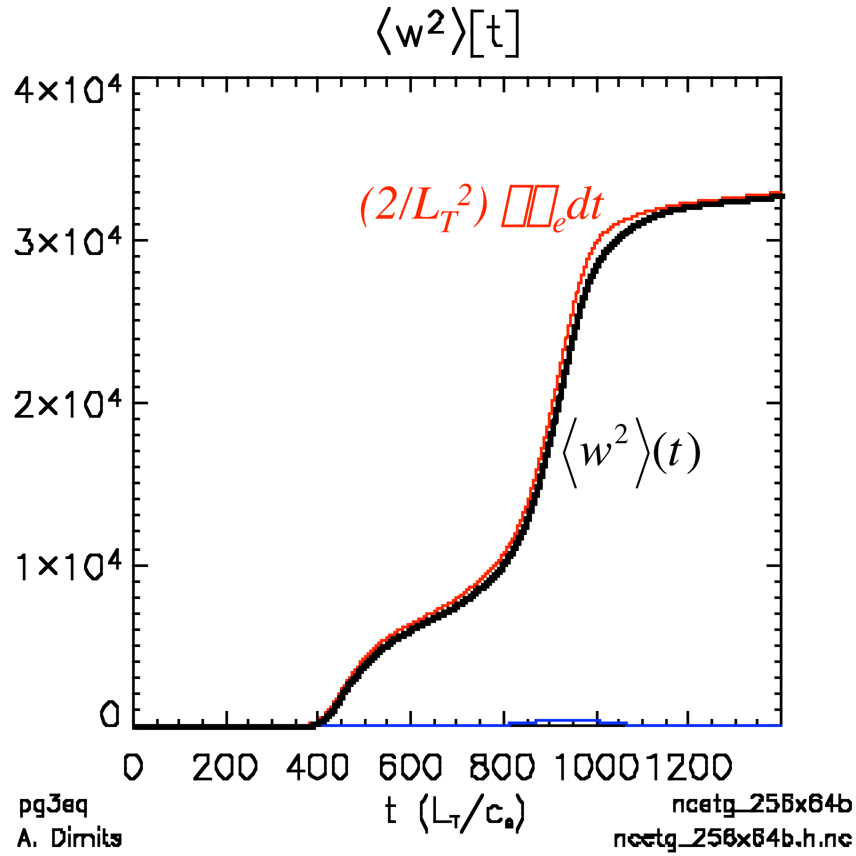
- Only difference with simple fully uncorrelated spectrum is factor of 2 at long wavelengths from Debye shielding by discrete particles:

$$\left\langle \left| \frac{e\phi_k}{T} \right|^2 \right\rangle_N = \frac{V^2 \left\langle w_i^2 \right\rangle S_{filter}^2(k) S^2(k) \Gamma_0(k_\perp^2 \rho_{th}^2)}{N_p \left[2 - \Gamma_0(k_\perp^2 \rho_{th}^2) \right]^2} \xrightarrow{k \to 0} \frac{V^2 \left\langle w_i^2 \right\rangle}{N_p}$$

In δf PIC simulations $\langle w^2 \rangle$ and the discrete particle noise increase in time

- Computing $\langle |\phi_k(t)|^2 \rangle_{noise}$ requires:
  - Information about the code
    - $S_G(k)$
    - $S(k)$
    - $\Gamma_0(k_\perp^2 \rho^2)$
    - $d_{||}(k)$
  - Information about the run
    - N_p
    - N_G
  - The time-series $\langle w^2 \rangle(t)$ (which quantifies the "noise")
- Best to get $\langle w^2 \rangle(t)$ from the code (as in all examples shown here)
- If unavailable, can use the Lee/Tang Entropy theorem:

$$\left\langle w^2 \right\rangle(t) \Box \frac{2}{L_T^2} \int_0^t \Box_e(t)\,dt$$



Simulation Verification (1)
The Transverse (to *B*) Fluctuation Spectrum

Requires:

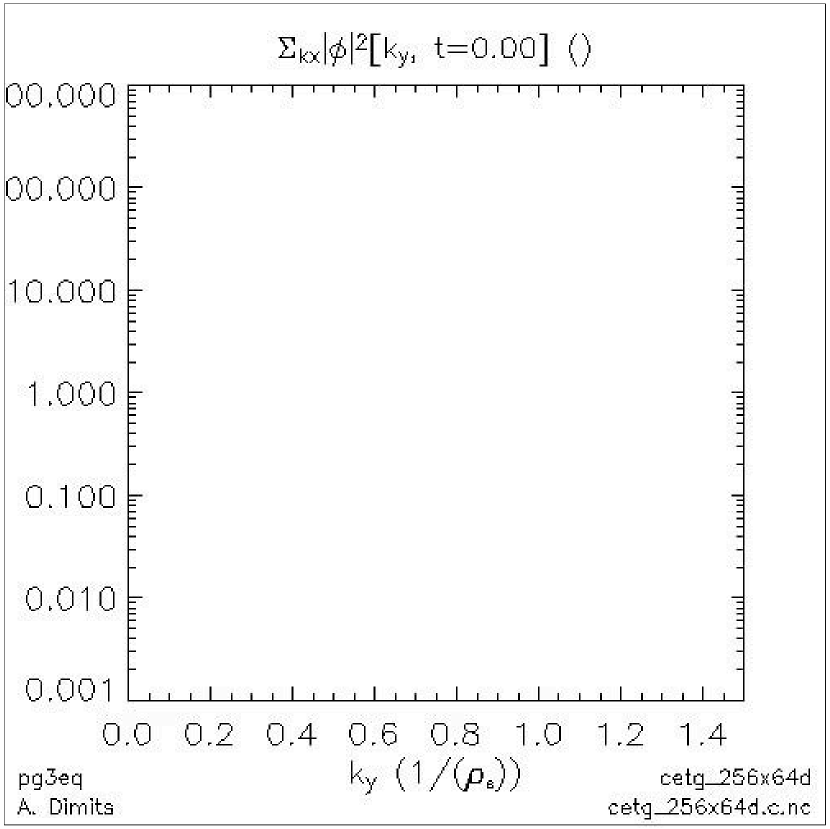
- From Simulation,
  - Fluctuation data in plane $\perp$ to $\boldsymbol{B}$
  - The time-series $\langle w^2 \rangle(t)$
  - Numerical details about the field-solve
- A mixed representation, $\langle |\phi_{k_y}|^2 \rangle_{x,z}$

$$\left\langle \left| \frac{e\phi_{k_y}}{T} \right|^2 \right\rangle_{x,z} = \sum_{k_x k_z} \left\langle \left| \frac{e\phi_{k_x,k_y,k_z}}{T} \right|^2 \right\rangle =$$

$$\approx \frac{\langle w^2 \rangle}{n_p (L_y \Delta x \Delta z)} \left[\frac{\Delta x \Delta z}{(2\pi)^2} \int_{-\pi/\Delta x}^{\pi/\Delta x} \int_{-\pi/\Delta z}^{\pi/\Delta z} \frac{S_{filter}^2 \Gamma_0 \, dk_x dk_z}{[2 - \Gamma_0][2 - (1 - S_{filter} d_{\parallel}) \Gamma_0]} \right]$$

- Predicted noise spectrum fits the data
- This simulation has a noise problem!

Cyclone base-case-like ETG
Mid-plane potential



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- A mixed representation, $\langle\langle |\phi_{ky}|^2 \rangle\rangle_{x,z=0}$

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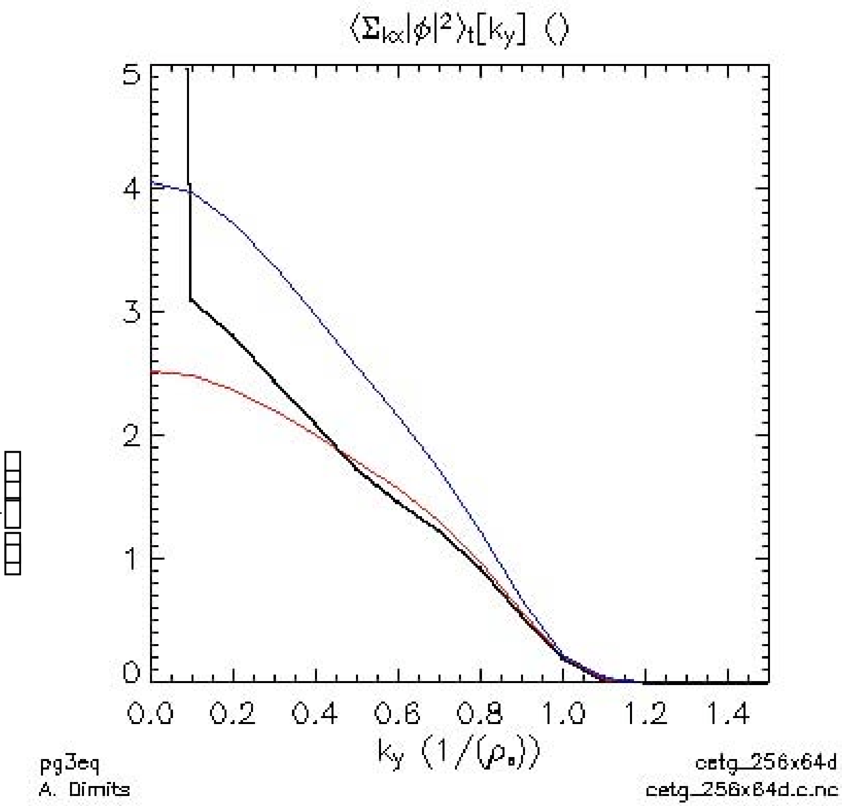


Simulation Verification (2)
The Fluctuation Intensity

A less computationally intensive diagnostic

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

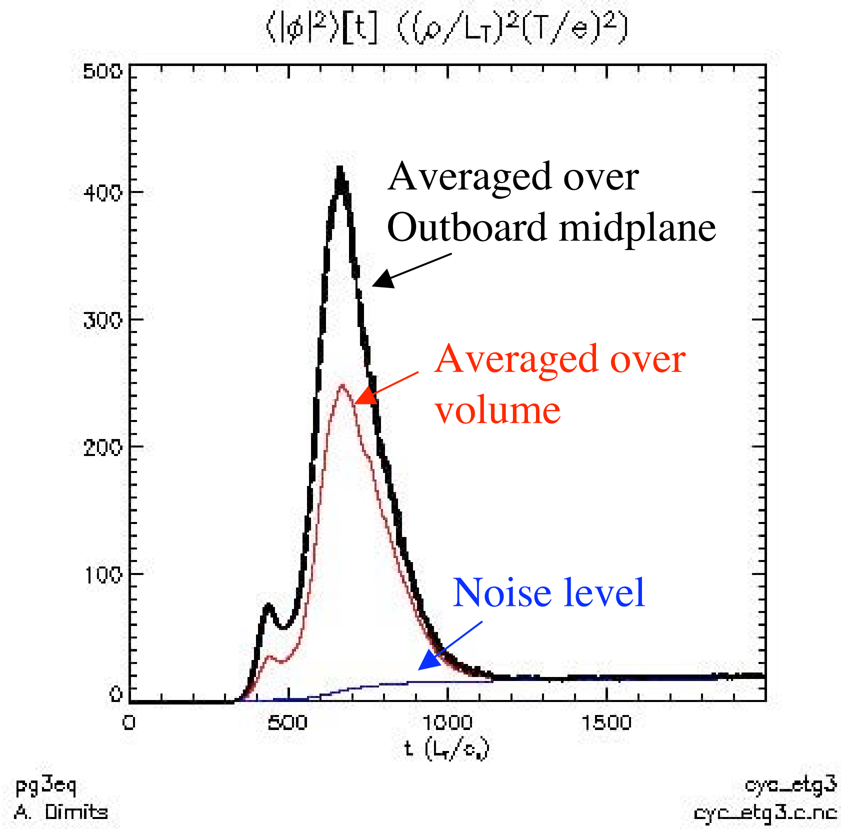
where

$$V_{shield}^{(H)} \equiv \left[\frac{1}{(2\pi)^3} \int d^3k \frac{S_{filter}^2 \Gamma_0 (k_\perp^2 \rho_{th}^2)}{[2 - \Gamma_0]\left[2 - \left(1 - S_{filter} d_\parallel\right)\Gamma_0\right]} \right]^{-1}$$

$$V_{shield}^{(N)} \equiv \left[\frac{1}{(2\pi)^3} \int d^3k \frac{S_{filter}^2 \Gamma_0 (k_\perp^2 \rho_{th}^2)}{\left[2 - \Gamma_0 (k_\perp^2 \rho_{th}^2)\right]^2} \right]^{-1}$$

Typical $V^{(H)}{}_{shield}$ ~ *150 ΔxΔyΔz* for Dimits PIC filtering parameters

Cyclone base-case-like ETG
Fluctuation Intensity



Simulation Verification (3)
The $E \times B$ Energy Density

$E \times B$ energy density may be a more relevant diagnostic:

- Closely related to transport coefficient $D \approx \langle V_{ExB}^2 \rangle \tau_{corr}$

$$\frac{\omega_p^2}{\Omega_c^2}\left\langle \frac{|\nabla_\perp \phi|^2}{4\pi} \right\rangle = nT \frac{\langle w^2 \rangle}{n_p V_{shield}} \left\langle K_\perp^2 \phi^2 \right\rangle_{noise}$$

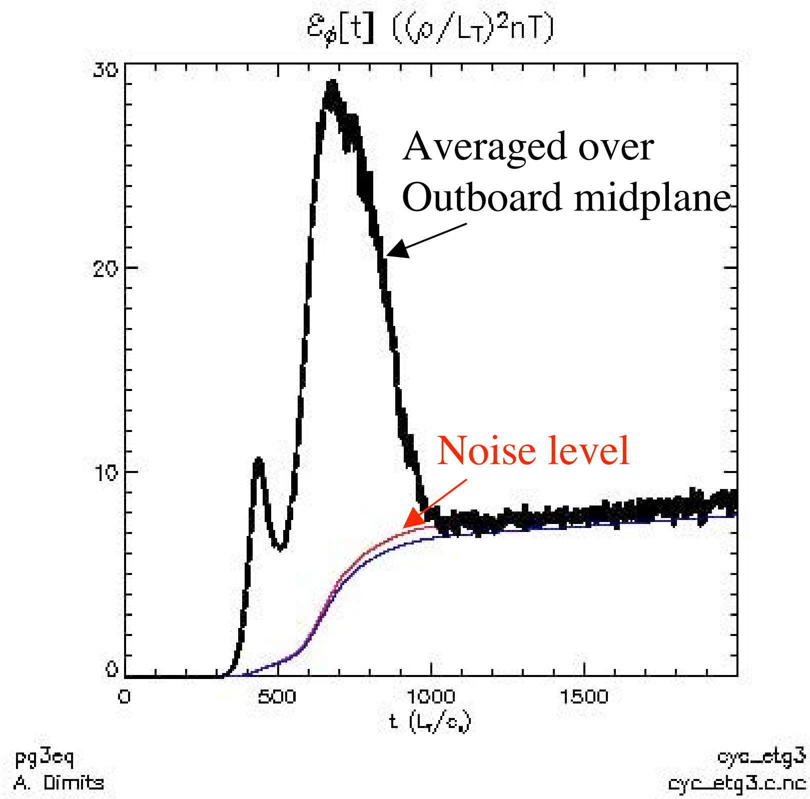
where

$$\left\langle K_\perp^2 \phi^2 \right\rangle_{noise}^{(H)} \equiv \left(\frac{V_{shield}}{(2\pi)^3} \int d^3k \frac{K_\perp^2(k)\phi^2 S_{filter}^2(k)\Gamma_0(k_\perp^2\rho_{th}^2)}{[2-\Gamma_0]\left[2-\left(1-S_{filter}d_\parallel\right)\Gamma_0\right]} \right)$$

$$\left\langle K_\perp^2 \phi^2 \right\rangle_{noise}^{(N)} \equiv \left(\frac{V_{shield}}{(2\pi)^3} \int d^3k \frac{K_\perp^2(k)\phi^2 S_{filter}^2(k)\Gamma_0(k_\perp^2\rho_{th}^2)}{\left[2-\Gamma_0(k_\perp^2\rho_{th}^2)\right]^2} \right)$$

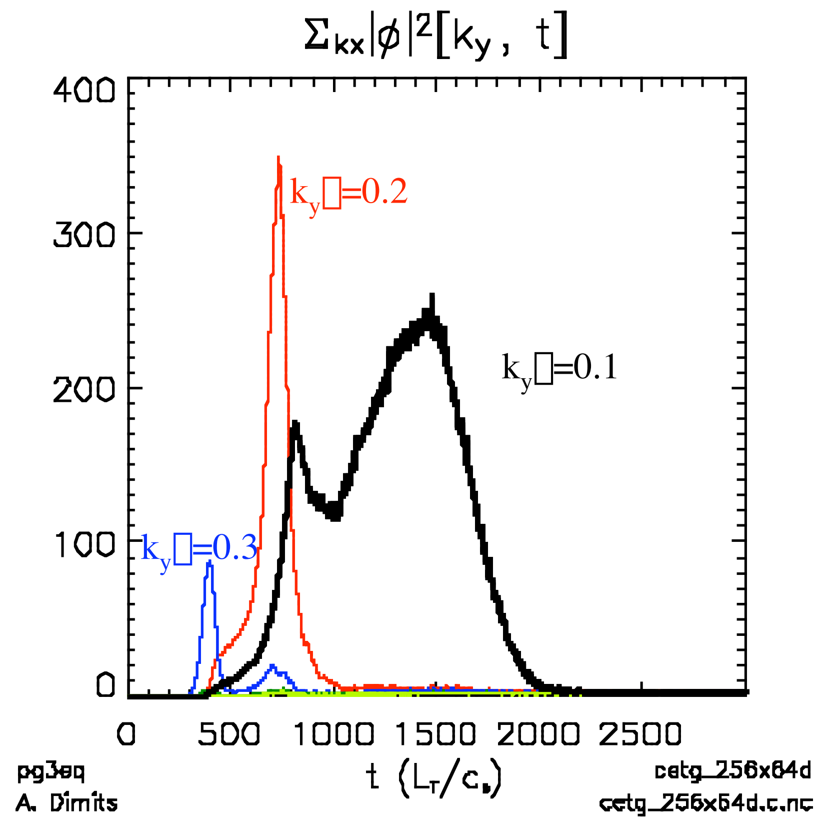
Cyclone base-case-like ETG

$E \times B$ Energy



Discrete Particle Noise Suppresses ETG turbulence and associated transport???

- What happened in simulations?
  - Burst of ETG turbulence
  - Discrete particle noise grows (as measured by $\langle w^2 \rangle$)
  - ETG turbulence goes away
- Nevins at TTF Mtg.:
  "Discrete particle noise suppresses ETG turbulence"
  - As n_p increases burst lasts longer, but disappears at same noise level, $\langle w^2 \rangle n_P$
- Lin at TTF Mtg.:
  Decay of ETG turbulence has nothing to do with discrete particle noise
  - Proof: Bolton/Lin "noise test"



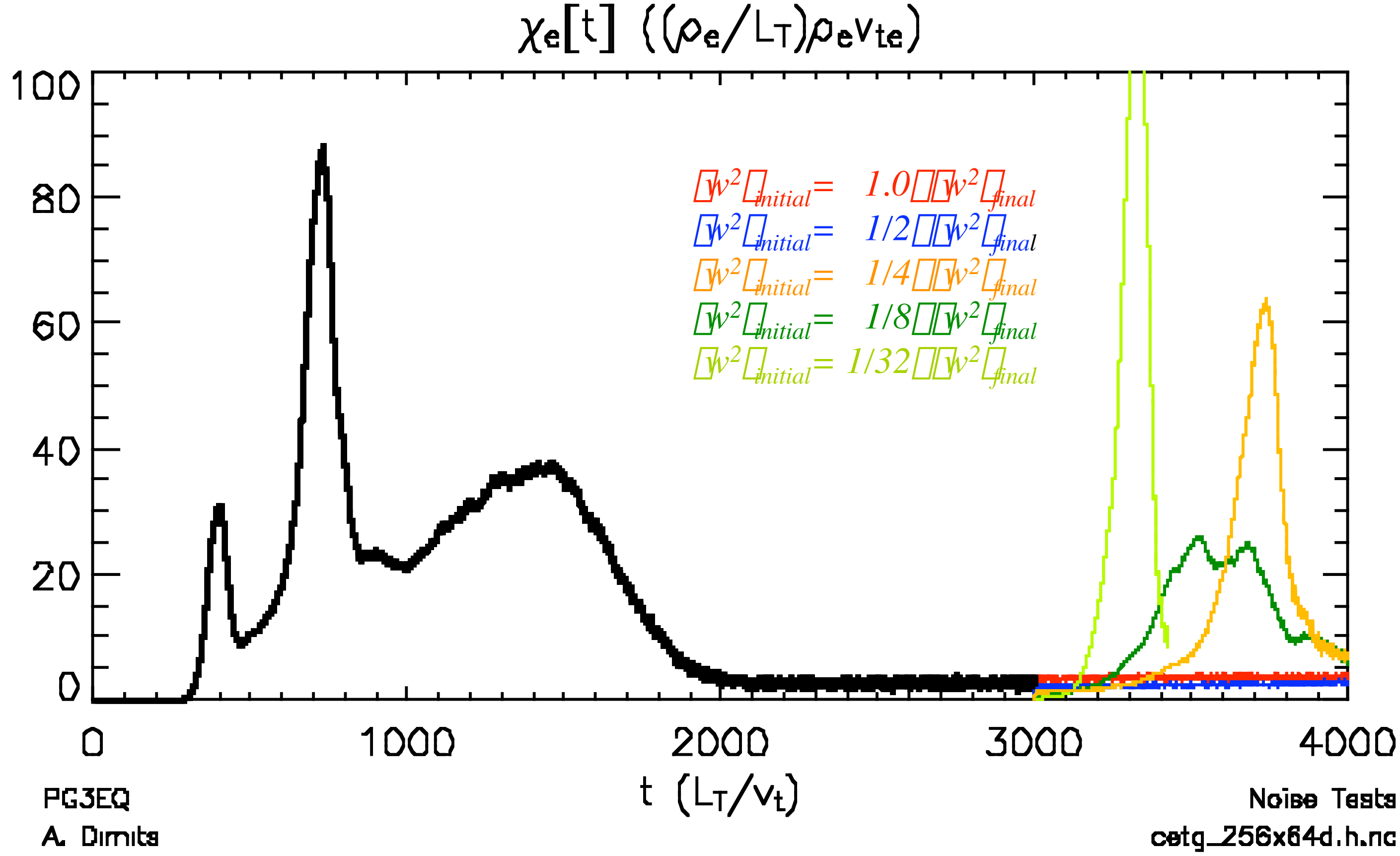
The Bolton/Lin "Noise Test"

- Select reference simulation:
  - *r/R_0=0.18*
  - *$250\rho_e \times 62.5\ \rho_e$*
  - *16* particles/cell
- Determine $\langle w^2 \rangle$ at end of simulation ($\langle w^2 \rangle_{final} = 7.8 \times 10^4$)
- Restart simulation with:
  - Same physics operating point
  - Same simulation parameters
  - New particle positions
  - New particle weights, $\{w_i\}$ chosen by random number generator such that new $\langle w^2 \rangle_{initial}$ proportional to old $\langle w^2 \rangle_{final}$

$\Rightarrow$ Only "memory" in GK simulations encoded in particle weights/positions

- If noise suppresses of ETG:
  - $\langle w^2 \rangle_{initial} = \langle w^2 \rangle_{final}$
    - $\langle \phi^2 \rangle \approx$ constant
    - $\chi_e \approx$ constant
  - $\langle w^2 \rangle_{initial} < \langle w^2 \rangle_{final}$
    - Exponential growth of $\langle \phi^2 \rangle$
    - γ increases as $\langle w^2 \rangle_{initial}$ decreases
    - χ_e starts low, grows with $\langle \phi^2 \rangle$
- If noise does not suppress ETG:
  - No dependence on $\langle w^2 \rangle_{initial}$
  - New runs similar to previous run:
    - Bust of ETG turbulence
    - χ_e independent of $\langle w^2 \rangle_{initial}$

The Bolton/Lin "Noise Test":
Discrete particle noise suppresses ETG transport



Why does discrete particle noise suppress ETG?

Discrete particle noise ⇒ (computer) particle diffusion

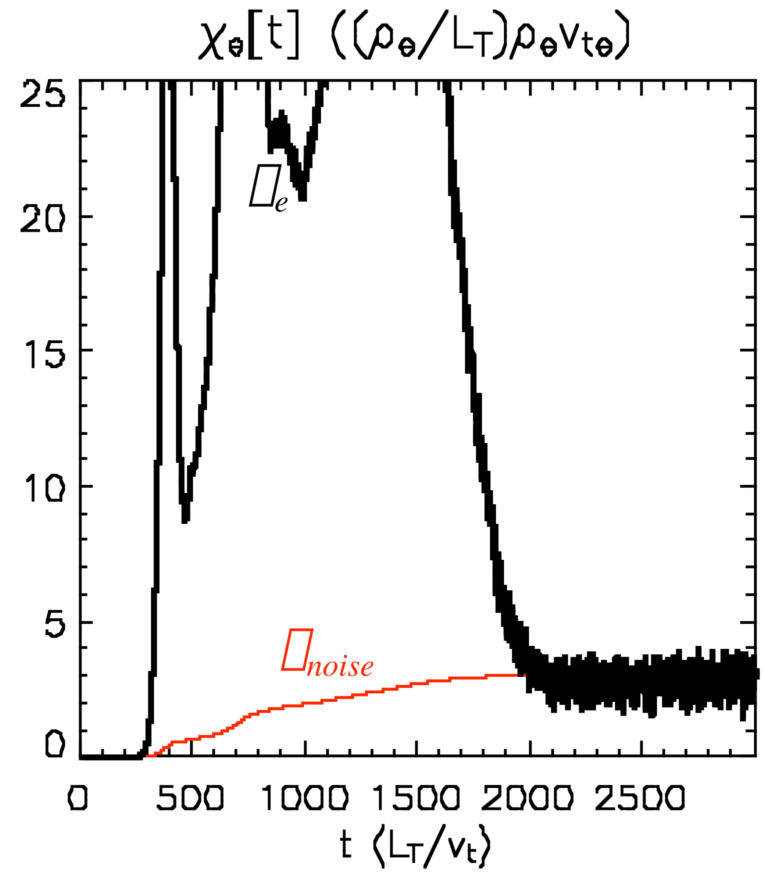
- No velocity scattering
  ("partially linearized" simulations)
- $E \times B$ motion leads to diffusion:

$$D_{noise} = \frac{1}{12}\left(\frac{cT}{eB}\right)^2 \left\langle \left|\frac{e\phi}{T}\right|^2 \right\rangle_{noise}$$

$$\approx \frac{V_{Shield}^{(H)} k_{\perp N}^2}{V_{Sh,2}} \frac{3.05}{k_{\|\max} v_{te}\sqrt{2}}$$

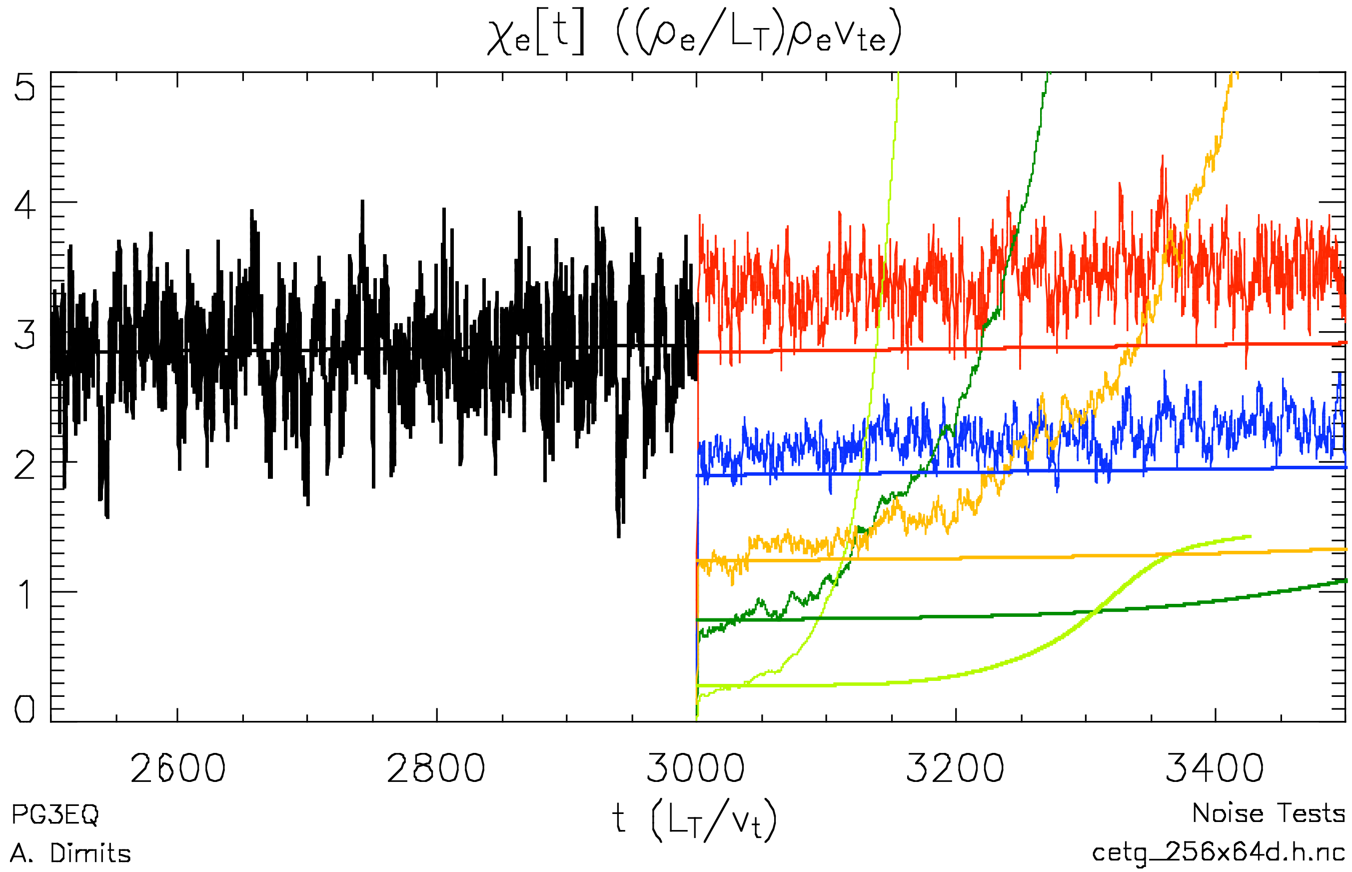
$$\times \log\left[1 + \frac{k_{\|\max} v_{te}\sqrt{2}}{3.05\left(D_{noise} k_{\perp N}^2 + \gamma_*\right)}\right]$$

$$\chi_{noise} \equiv \tfrac{3}{2} D_{noise}$$



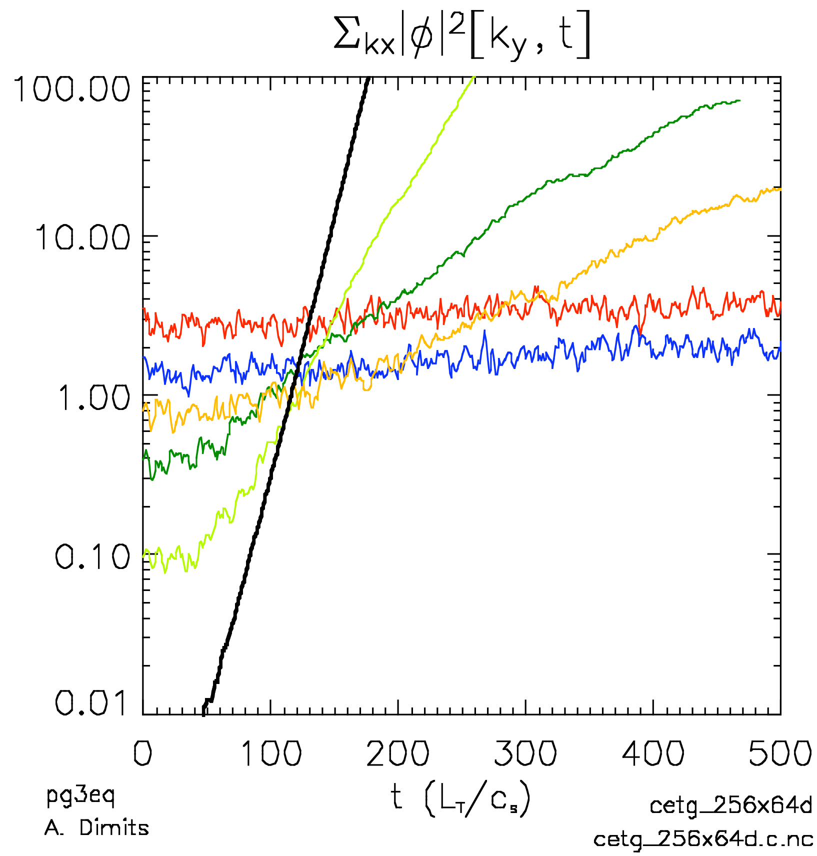
For details see
http://www.mfescience.org/mfedocs/ucrl-jrnl-212536.pdf

Predicted $\chi_{noise} \approx$ measured χ_e for every $\langle w^2 \rangle_{initial}$ in "noise" test

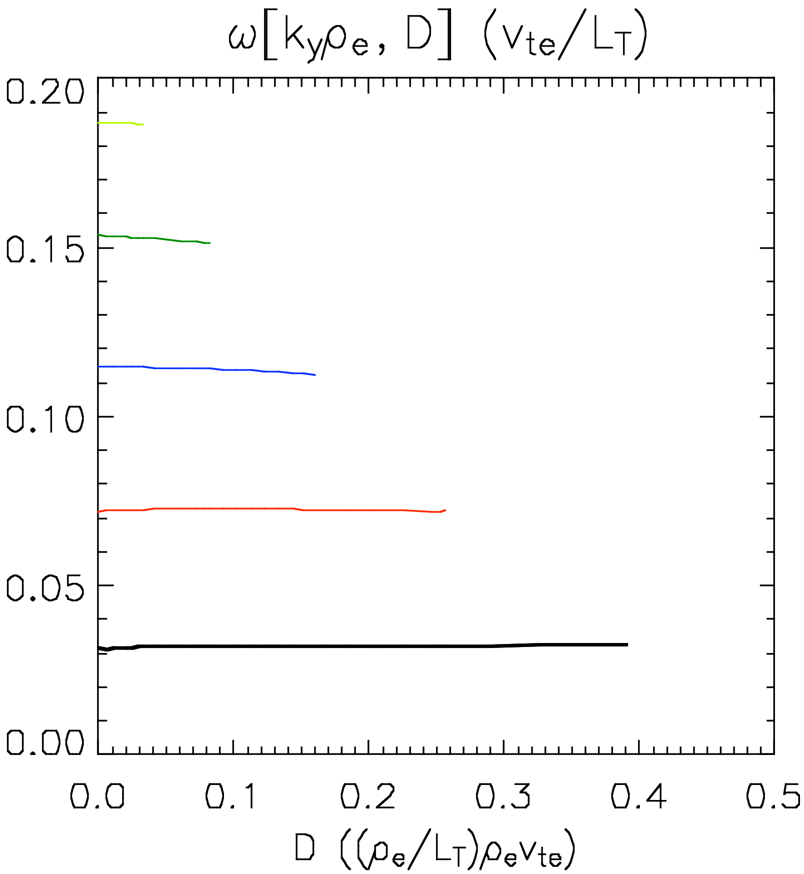


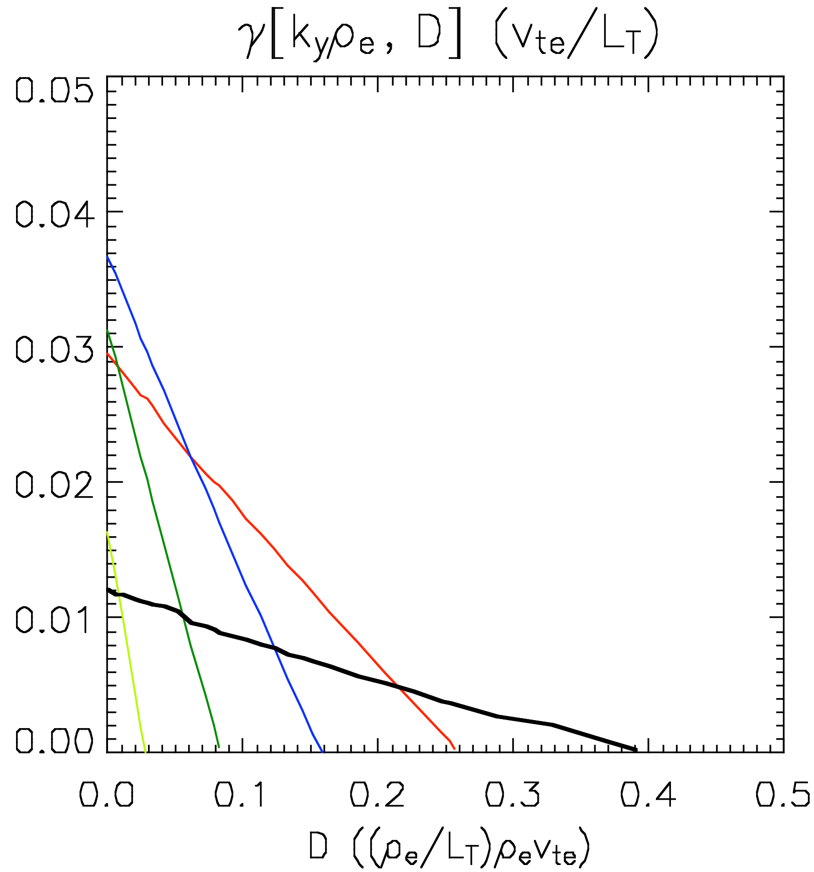
The Bolton/Lin "Noise Test":
"Noise" suppresses linear growth of ETG modes

- Growth-rate of fastest-growing mode can be measured after each restart
  - 1/2 slope of $Ln(|\phi_{ky}|^2)$ $vs.$ t
  - Data of sufficient quality to provide good estimates of γ_{max}
- Clear trend:
  - Increasing $\langle w^2\rangle_{initial}$
  - $\Rightarrow$ Decreasing γ_{max}
- $\gamma_{max} \approx 0$ for $\langle w^2\rangle_{initial} = \langle w^2\rangle_{final}$



Why does noise suppress growth of ETG modes?
noise-induced particle diffusion

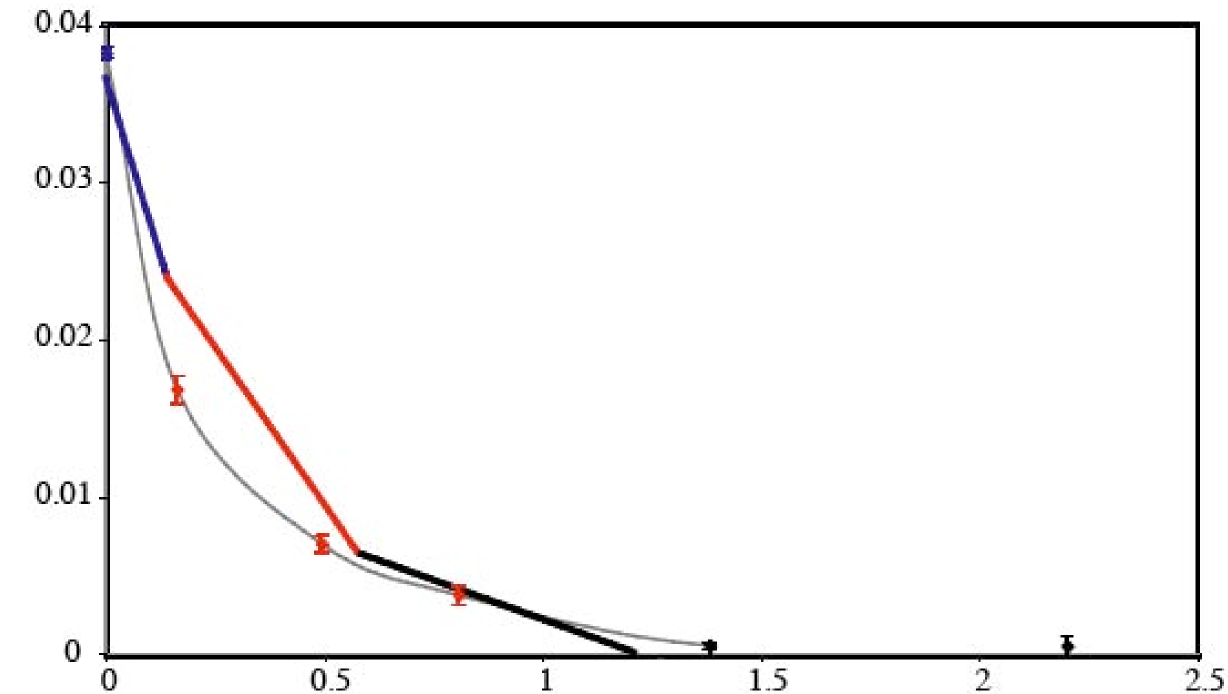




Data from GS2 kinetic solution of linear initial-value problem

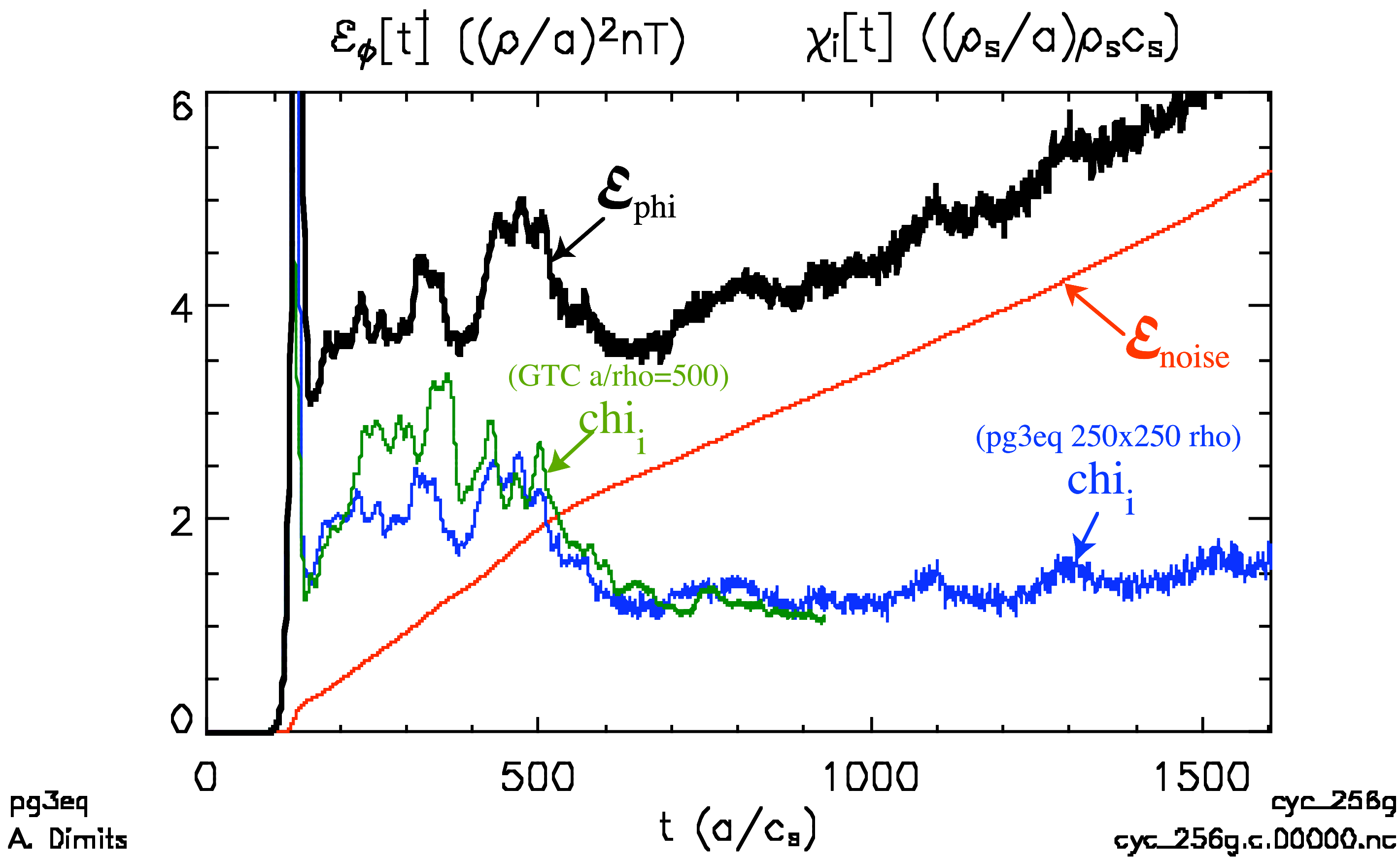
$$\gamma(D_{noise}) \approx \gamma(D_{noise}=0) - k_y^2 D_{noise}$$

γ_{max} (v_{te}/L_T)



D_{noise} $((\rho_e/L_T)\rho_e v_{te})$

Discrete particle noise is a problem in some Cyclone base-case ITG turbulence simulations



Summary: discrete particle noise

- Computed fluctuation spectrum due to discrete particle noise
  - Excellent agreement between computed noise spectrum and simulation
- Proposed five diagnostics for use in quantifying the noise level in PIC simulations of plasma microturbulence
  - The perpendicular fluctuation spectrum (noise vs. signal)
  - The fluctuation intensity (noise vs. signal)
  - The $E\times B$ energy (noise vs. signal)
  - The transport level (χ_{noise} vs. signal)
  - Noise decorrelation compared with growth rates ($\chi_{noise}\, k_{\perp}^2$ vs. $\gamma(k_y)$)
- Quantitative comparisons between simulation data and these diagnostics show potentially serious issues for PIC simulations of:
  - ETG turbulence
    (resolution of the Jenko-Dorland vs. Lin ETG controversy)
  - ITG turbulence
    (may help to explain remaining discrepancies in CYCLONE base-case benchmark)

Summary: discrete particle noise

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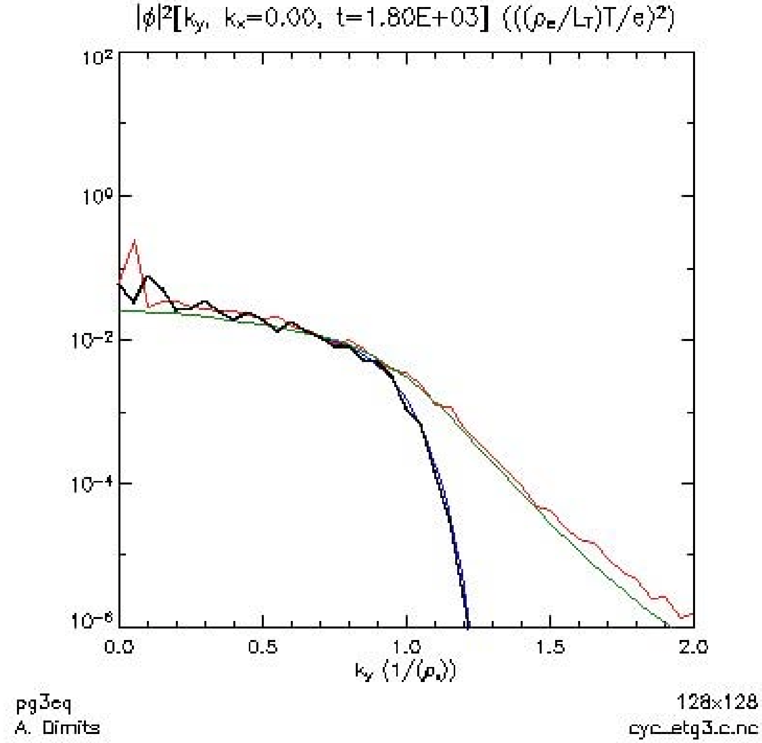
$\Rightarrow$ Perhaps PIC code-development effort should focus on noise reduction?

Conclusions



- Simple calculation of spectrum of noise fluctuations due to random uncorrelated particles, agrees within a factor of 2 of more complicated derivation.

- Detailed calculation of noise spectrum (extending Krommes 93 calculation to include filters, etc.) agrees very well (no free parameters) with observed spectrum at late times in Dimits' gyrokinetic ETG simulations (chosen with parameters similar to Z. Lin's simulations), confirming that noise grows to dominate those ETG results.

- Renormalized calculation of $\square_{noise}$ also agrees very well with PIC simulations.

- ETG simulations require many more particles for convergence than ITG. Motivates search for additional methods of reducing noise (such as the Vadlamani-Parker weight resetting algorithm). Have to be careful that the artificial dissipation introduced by these methods isn't too big…

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