Discrete Particle Noise in PIC Simulations of Plasma Microturbulence

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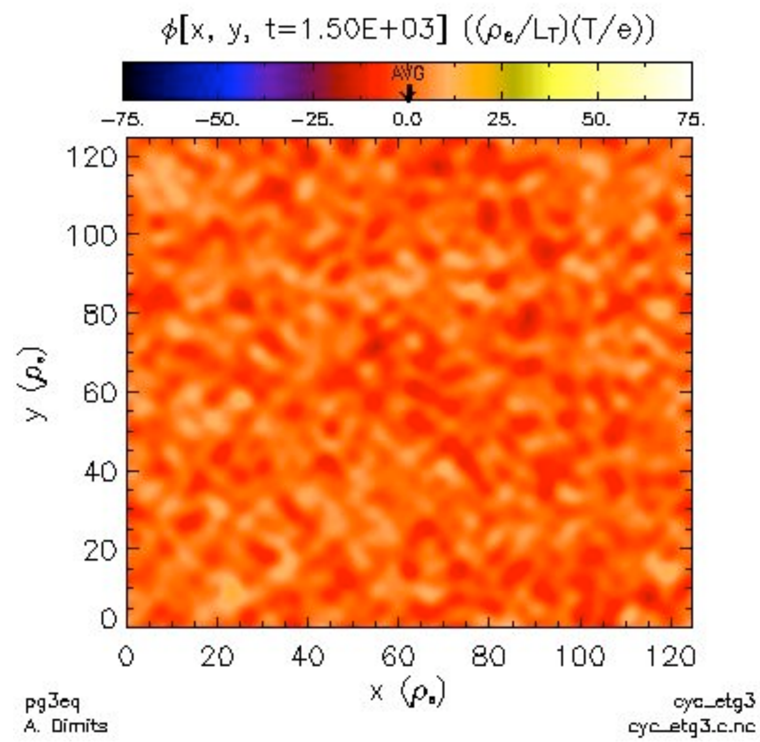
Discrete particle noise should be treated as a code verification issue

- 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 determining when discrete particle noise is a problem

- Can be a problem for:
  - Cyclone base-case-like ETG
  - Cyclone base-case ITG

Cyclone base-case-like ETG
Mid-plane potential



Quantifying Particle Discreteness (1)

The fully uncorrelated fluctuation spectrum

- The gyrokinetic Possion Equation (W.W. Lee, Phys. Fluids '83)

$$\left\{1+\left[1-\Gamma_0(k_\perp^2\rho_{th}^2)\right]\right\}\frac{e\phi_k}{T}=\frac{S_{filter}(k)}{N_p}\sum_i w_i J_o(k_\perp\rho_i)\exp(-i\mathbf{k}\cdot\mathbf{x}_i)$$

$$\frac{e\phi_k}{T}=\frac{S_{filter}(k)}{N_p\left[2-\Gamma_0(k_\perp^2\rho_{th}^2)\right]}\sum_i w_i J_o(k_\perp\rho_i)\exp(-i\mathbf{k}\cdot\mathbf{x}_i)$$

- The fluctuation spectrum

$$\left|\frac{e\phi_k}{T}\right|^2=\frac{S_{filter}^2(k)}{N_p^2\left[2-\Gamma_0(k_\perp^2\rho_{th}^2)\right]^2}\left\{\sum_i\sum_j w_i w_j J_0(k_\perp\rho_i)J_0(k_\perp\rho_j)\exp\left[-i\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)\right]\right\}$$

$$\left\langle\left|\frac{e\phi_k}{T}\right|^2\right\rangle_N=\frac{S_{filter}^2(k)}{\left[2-\Gamma_0(k_\perp^2\rho_{th}^2)\right]^2}\left\{\frac{\Gamma_0(k_\perp^2\rho_{th}^2)\left\langle w_i^2\right\rangle}{N_p}+\frac{1}{N_p^2}\left\langle\sum_{i\neq j}w_i w_j J_0(k_\perp\rho_i)J_0(k_\perp\rho_j)\exp\left[-i\mathbf{k}\cdot(\mathbf{x}_i-\mathbf{x}_j)\right]\right\rangle\right\}$$

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Debye shielding   Polarization   "bare" gyro-center charge density

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assuming particles are uncorrelated

Quantifying Particle Discreteness (2)

(a partially correlated fluctuation spectrum)

- Calculation by G. Hammett (to be presented at 2005 Sherwood Mtg.)
  - Debye shielding in kinetic response
  - Resonance broadening renormalization
    (go to Sherwood to learn more)

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

- The fully uncorrelated spectrum (for comparison)

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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, $\langle |\phi|^2 \rangle(k_x, k_y, z)$

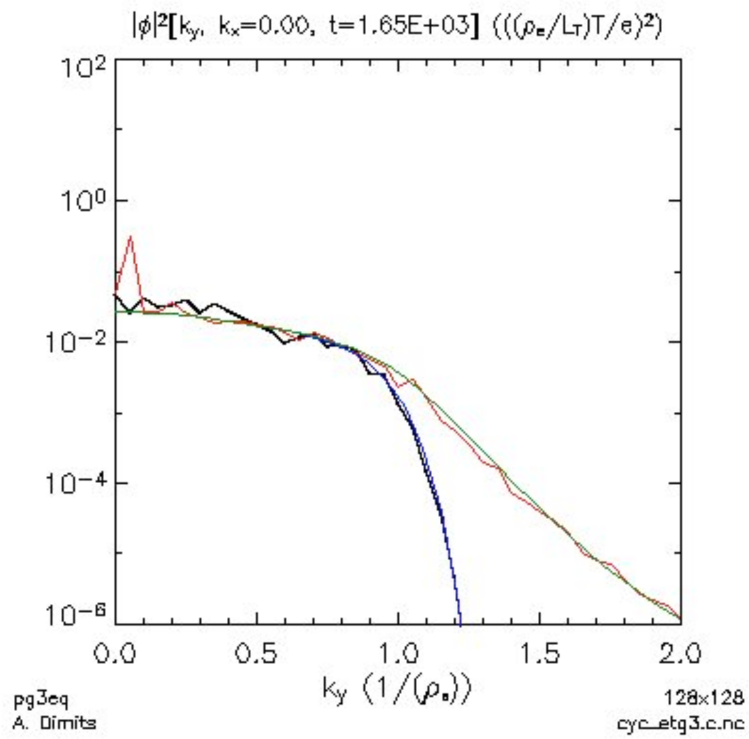
$$\left\langle \left| \frac{e\phi_{k_x,k_y}(z)}{T} \right|^2 \right\rangle = \sum_{k_z} \left\langle \left| \frac{e\phi_{k_x,k_y,k_z}}{T} \right|^2 \right\rangle =$$

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

$\Rightarrow$ Predicted noise spectrum fits the data

$\Rightarrow$ This simulation has a noise problem!

Cyclone base-case-like ETG
Mid-plane potential



Simulation Verification (2)
The Fluctuation Intensity

A less computationally intensive diagnostic

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

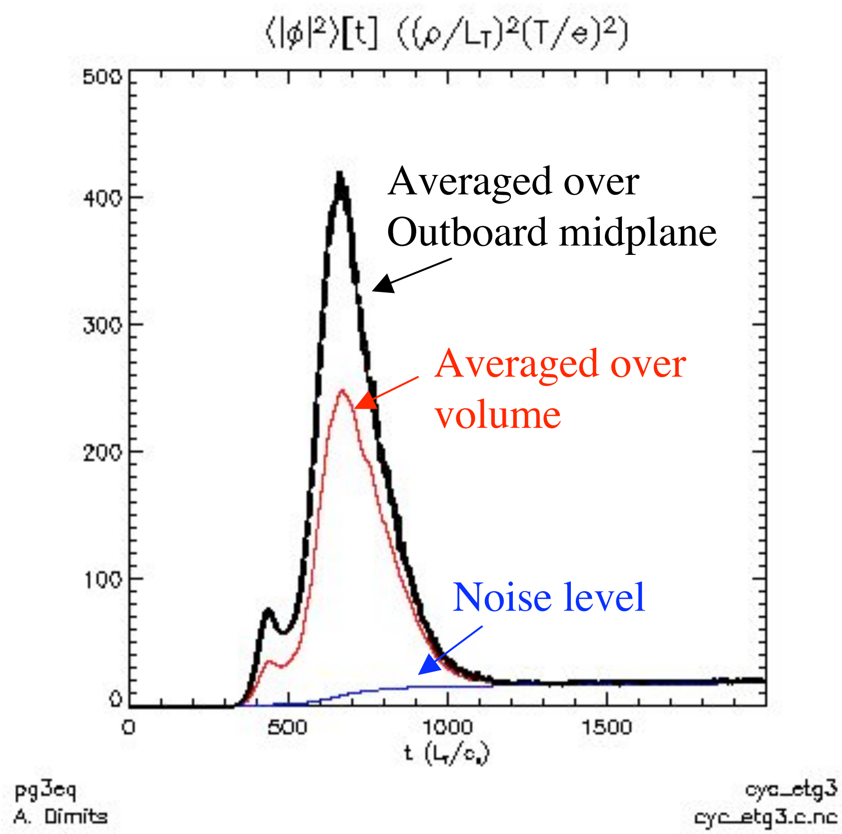
where

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

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

Typically $V_{shield} \approx 30\, \Delta x \Delta y \Delta z$

Cyclone base-case-like ETG
Fluctuation Intensity



Simulation Verification (3)
The Fluctuation Energy Density

Fluctuation energy density may be a more relevant diagnostic:

- Has direct physical significance (energy associated with ExB motion)
- Closely related to transport coefficient $D \approx \langle V_{ExB}{}^2 \rangle \tau_{corr}$

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

where

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

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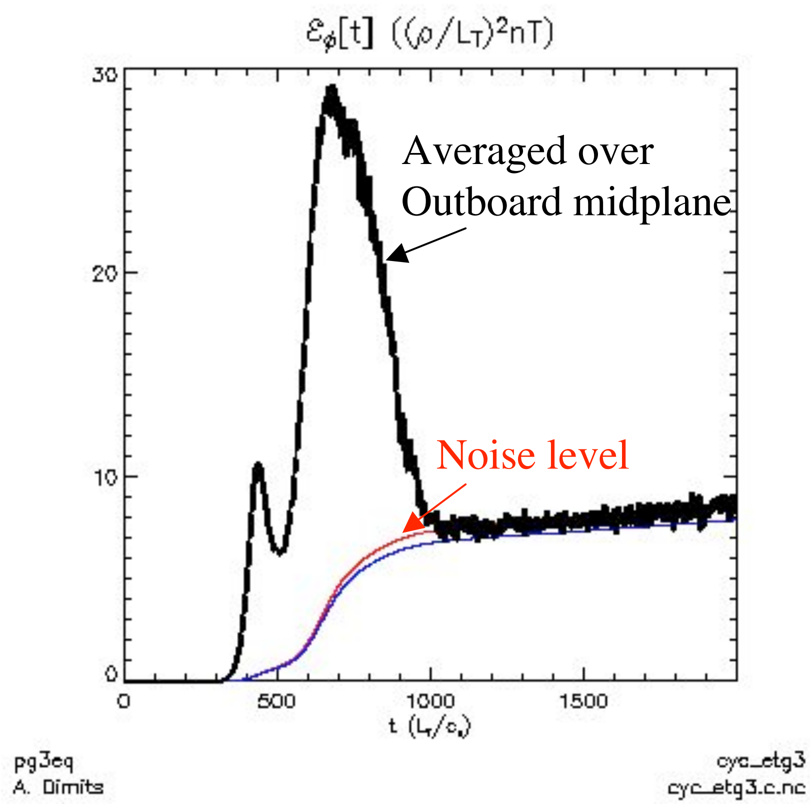
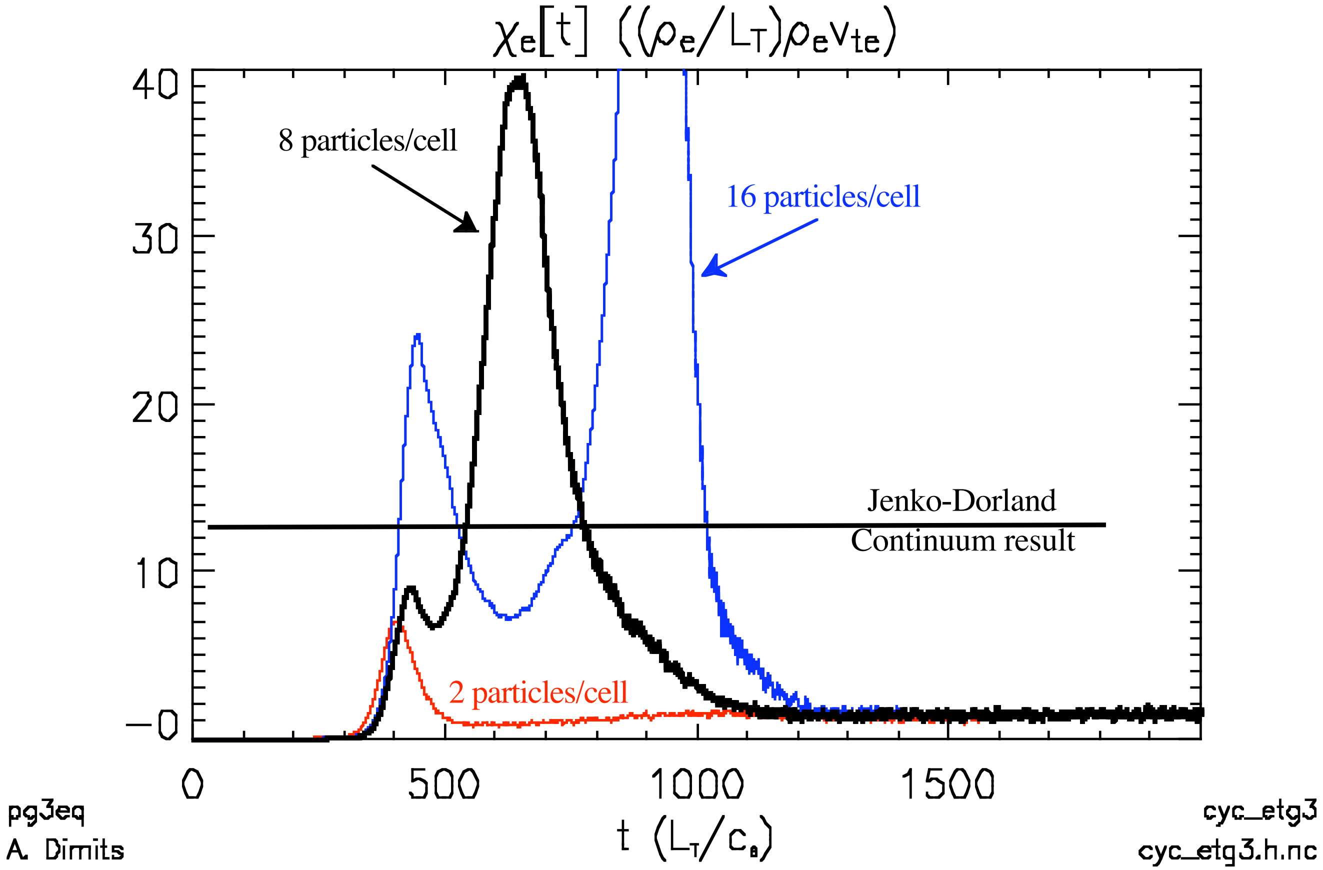
Cyclone base-case-like ETG Fluctuation Energy



Discrete Particle Noise Suppresses Transport In Cyclone-base-case like ETG Simulations



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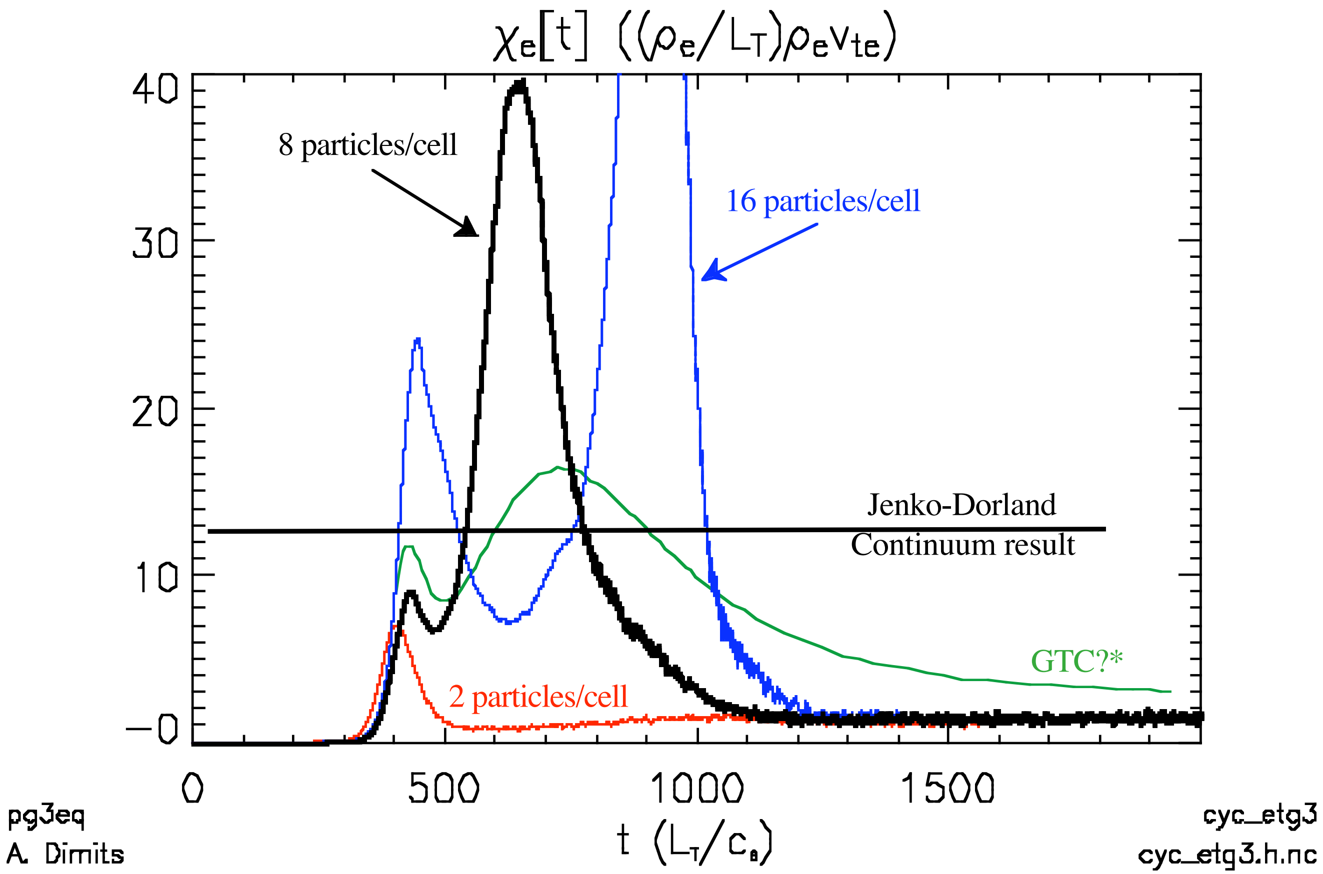
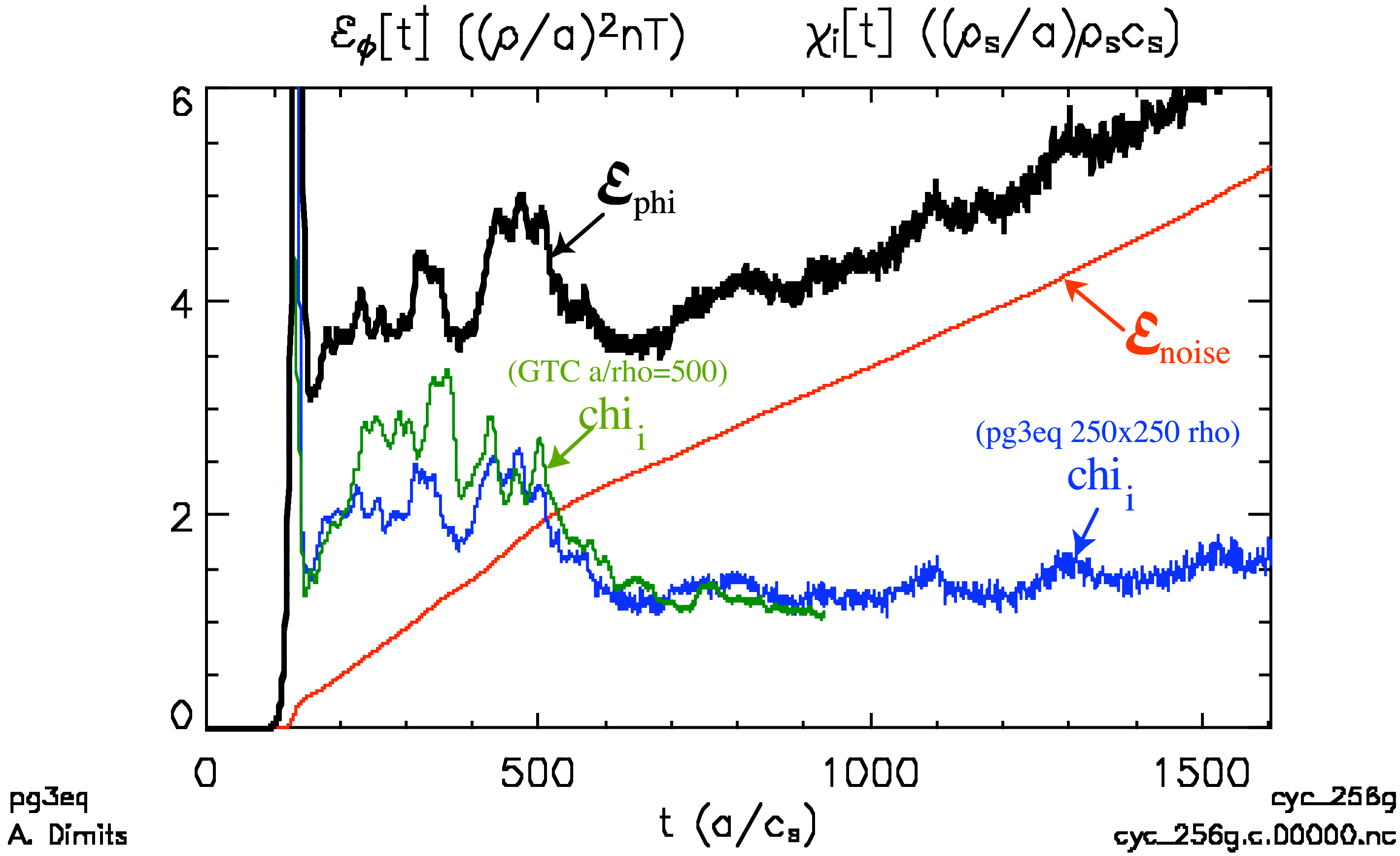


*GTC curve from Slide #13 of Z. Lin's IAEA presentation, which can be found at:
http://www.cfn.ist.utl.pt/20IAEAConf/presentations/T5/2T/5_H_8_4/Talk_TH_8_4.pdf

Discrete particle noise may be a problem in Cyclone base-case ITG turbulence simulations



Summary

- Computed fluctuation spectrum due to discrete particle noise
  - Excellent agreement between computed noise spectrum and simulation
- Proposed three 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 fluctuation energy (noise vs. signal)
- Quantitative comparisons between simulation data and these diagnostics show potentially serious issues for PIC simulations of:
  - ETG turbulence
    (possible resolution of the Jenko-Dorland vs. Lin ETG controversy?)
  - ITG turbulence
    (may help to explain remaining discrepancies in CYCLONE base-case benchmark)

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

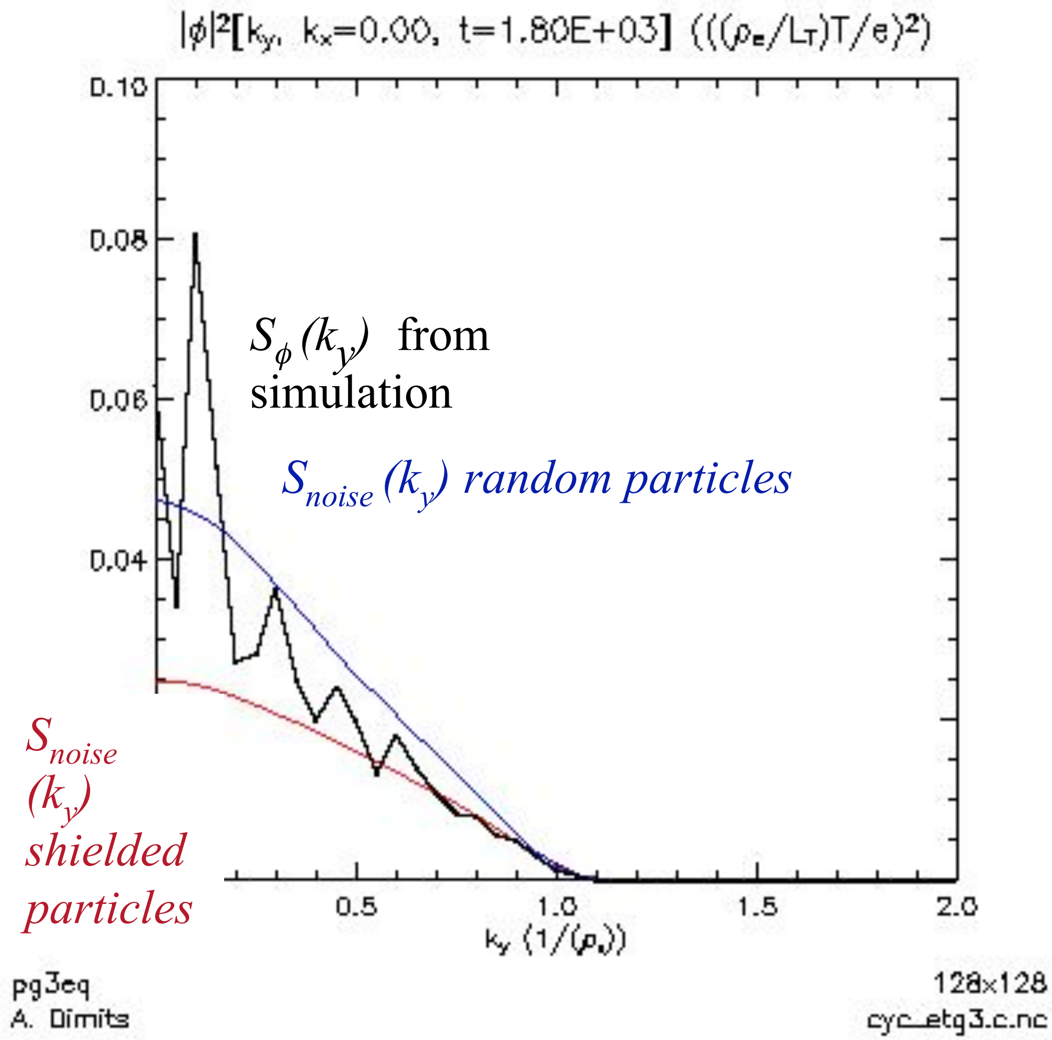
Noise calculation including shielding more accurate.

Simple noise calculation assuming randomly located particles is at most a factor of 2 higher than noise from test-particle superposition principle, including shielding cloud of other particles.

The two noise calculations approach each other for $k_y \rho_e >> 1$, where FLR makes shielding ineffective.

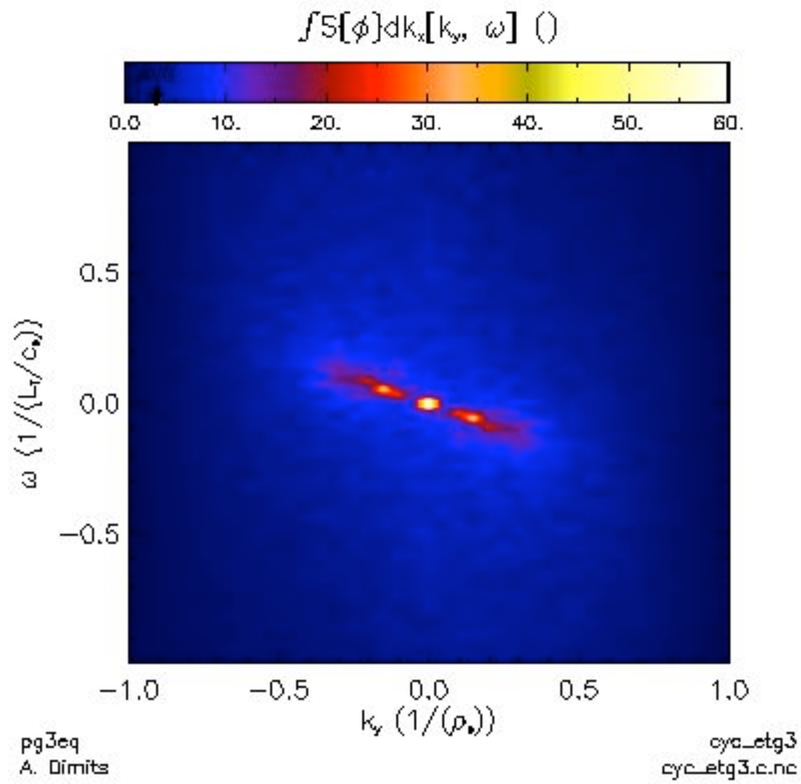
Simple noise from random particles slightly overpredicts observed spectrum.

Noise calculated including shielding from linear gyrokinetic dielectric fits observations better at $k_y \rho_e > 0.5$, provides lower bound on observation.

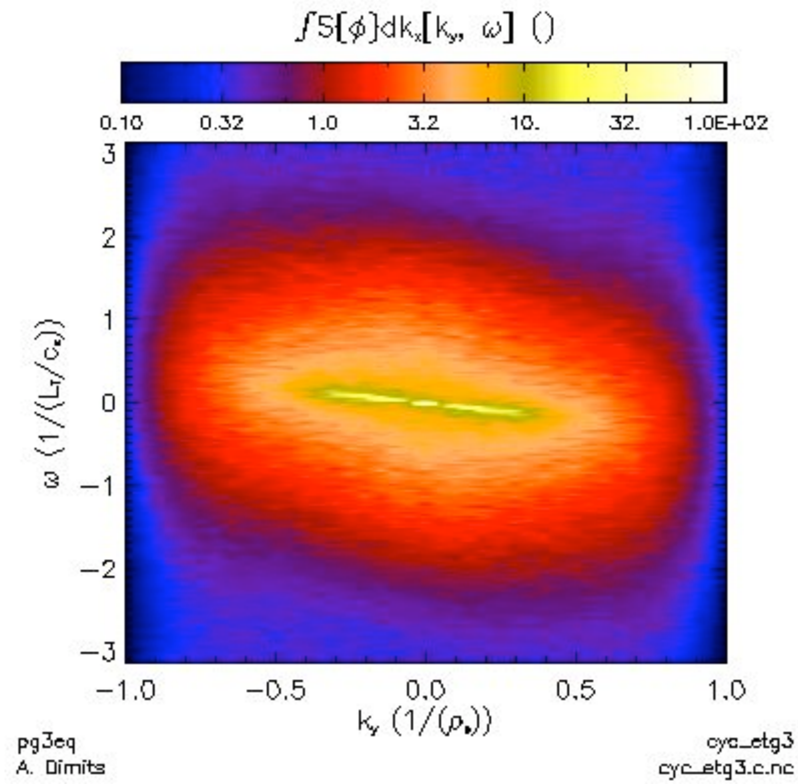


Frequency Spectrum

Drift waves at low-$k_\perp$

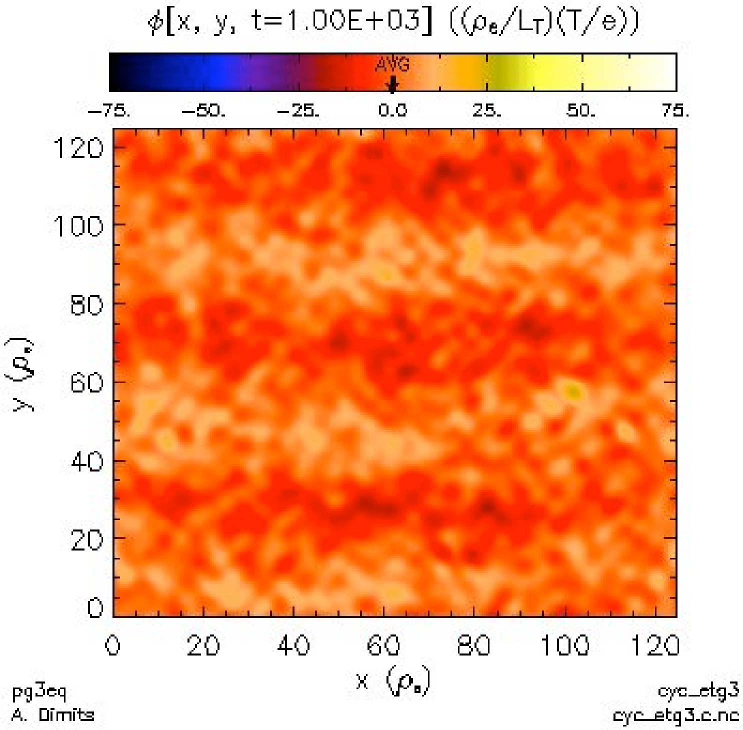


Broad-band noise at high-$k_\perp$

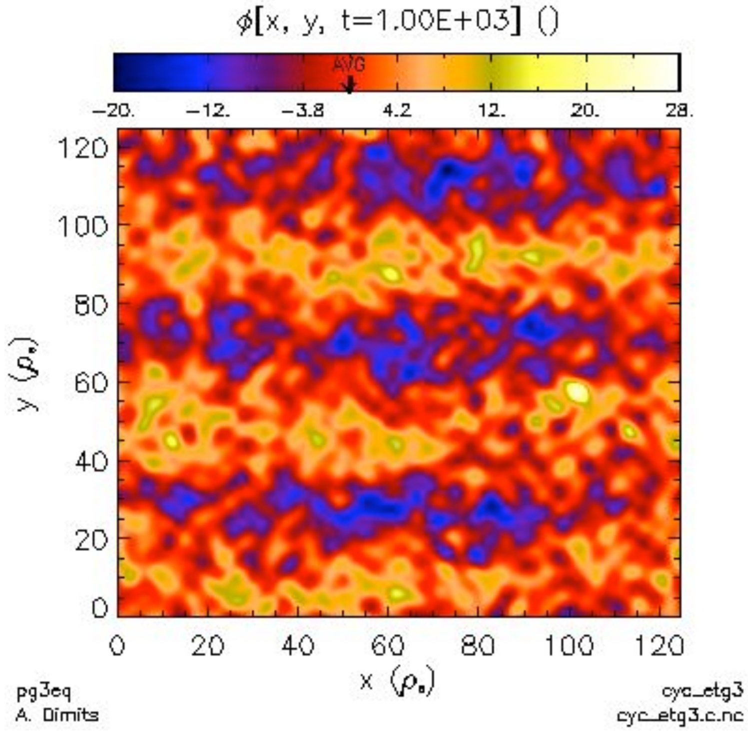


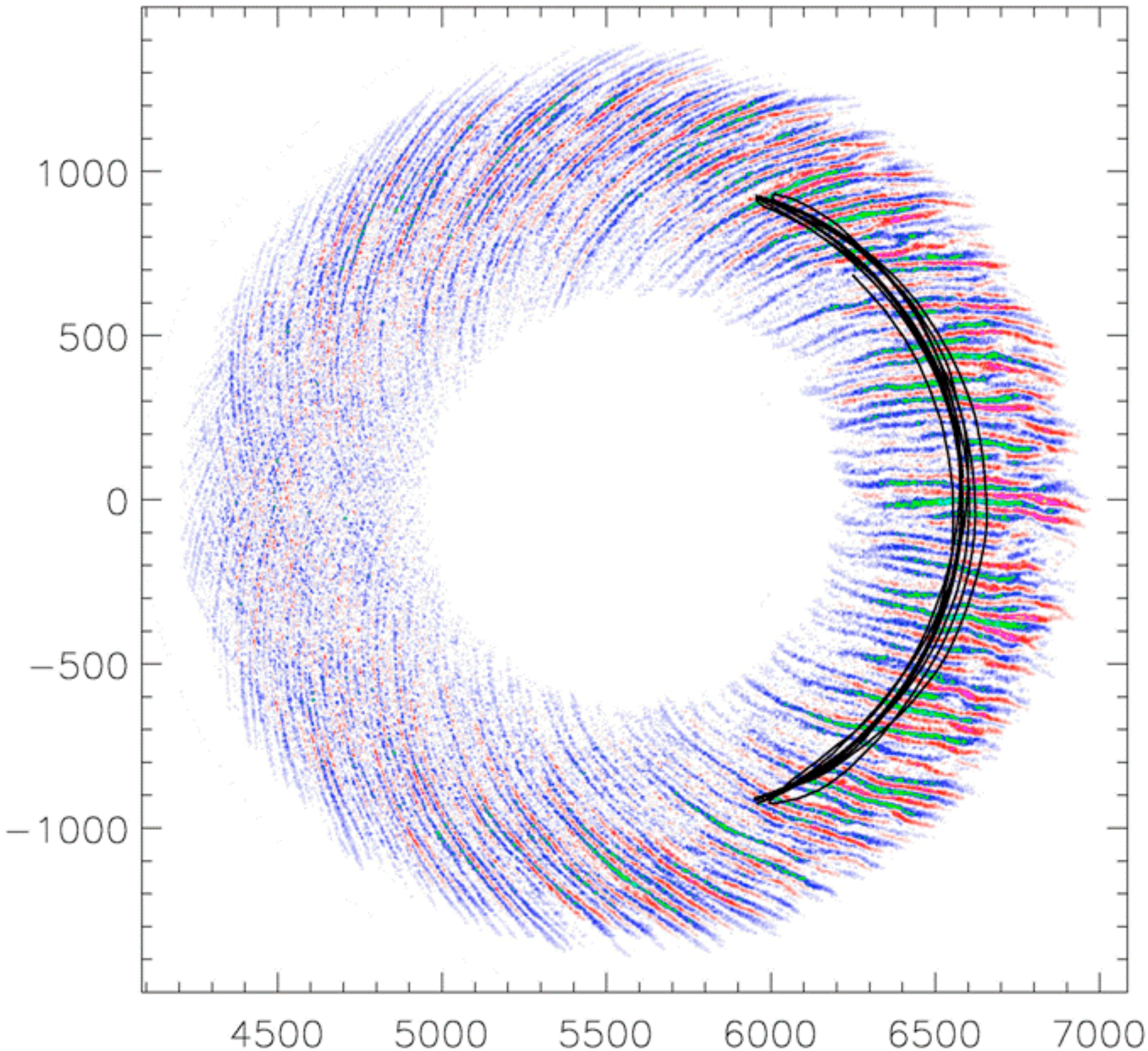
Is the "eyeball" test an accurate measure of the noise level?

Streamers are nearly gone



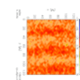
or, are they?
(same data, new color bar)

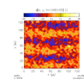




Dimits contour plots at
Same scale as Z. Lin's

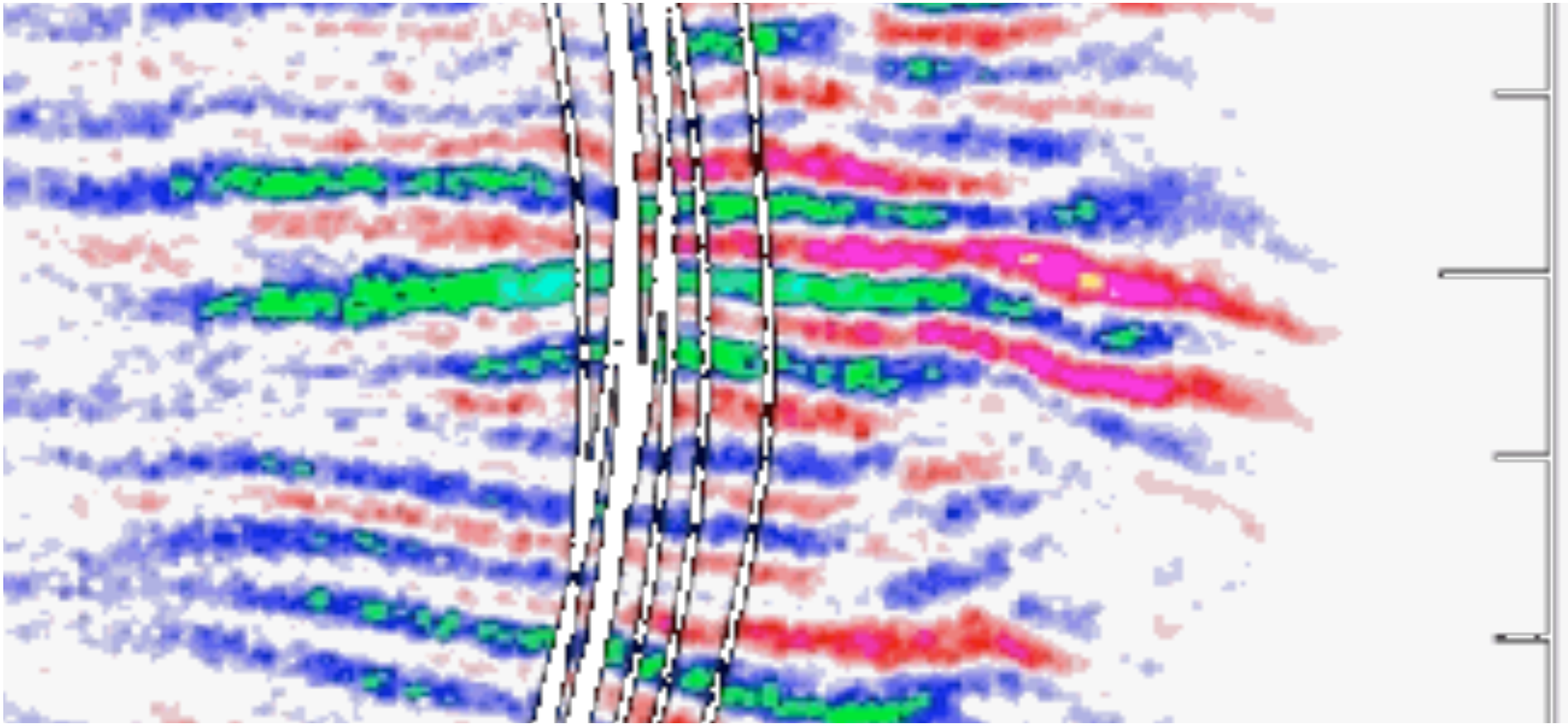
Dimits contour plot with
Re-scaled color bar

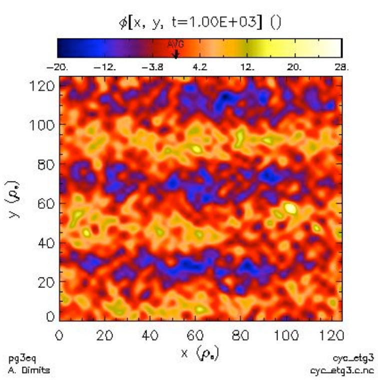


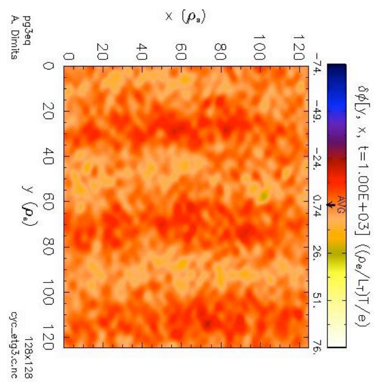


Dimits contour plot at t=1000, when χ_e ~2 x final χ_{noise}. This is when noise effects are strong enough to reduce χ_e to ~1/4th of Jenko-Dorland result, but ETG mode is still apparent.

But if one shrinks the contour plot to the scale used in Z. Lin's plots, then the eye (and the finite resolution of the computer screen) will average out the noise to make it less apparent.







If we blow up Z. Lin's contour plot, then we can see the noise at small scales more easily. It looks roughly comparable to Dimits' contour plot at t=1000 (when $\chi_e \sim 2$ x final $\chi_{noise} \sim 1/4^{th}\ \chi_{Jenko\text{-}Dorland}$.

Eyeball comparisons depend on choice of color table, smoothing in graphics, etc. as illustrated by two versions of Dimits' contour plot to left which differ only in the color table employed. Hence, we need more quantitative measures of noise than the "eyeball test".

Can discrete particle noise cause transport?

$$\frac{\partial P}{\partial t} - D\frac{\partial^2 P}{\partial x^2} = 0$$

$$P(x \mid x_0, t) = \frac{1}{\sqrt{2\pi D t}} \exp\left[-\frac{\left(x - x_0\right)^2}{4Dt}\right]$$

$$\left\langle (x - x_0) \right\rangle (t) = \int (x - x_0) w(x \mid x_0) P(x \mid x_0, t) dx$$

$$w(x \mid x_0) = -(x - x_0)\left[\frac{1}{L_n} + \left(\frac{\varepsilon}{T} - \frac{3}{2}\right)\frac{1}{L_T}\right]$$

$$\left\langle (x - x_0) \right\rangle (t) = -2Dt\left[\frac{1}{L_n} + \left(\frac{\varepsilon}{T} - \frac{3}{2}\right)\frac{1}{L_T}\right]$$

$$\left\langle V_{diffusion} \right\rangle = \frac{d}{dt}\left\langle (x - x_0) \right\rangle = -2D\left[\frac{1}{L_n} + \left(\frac{\varepsilon}{T} - \frac{3}{2}\right)\frac{1}{L_T}\right]$$