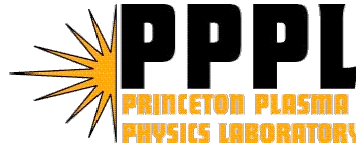


# Discrete Particle Noise in PIC Simulations of Plasma Microturbulence



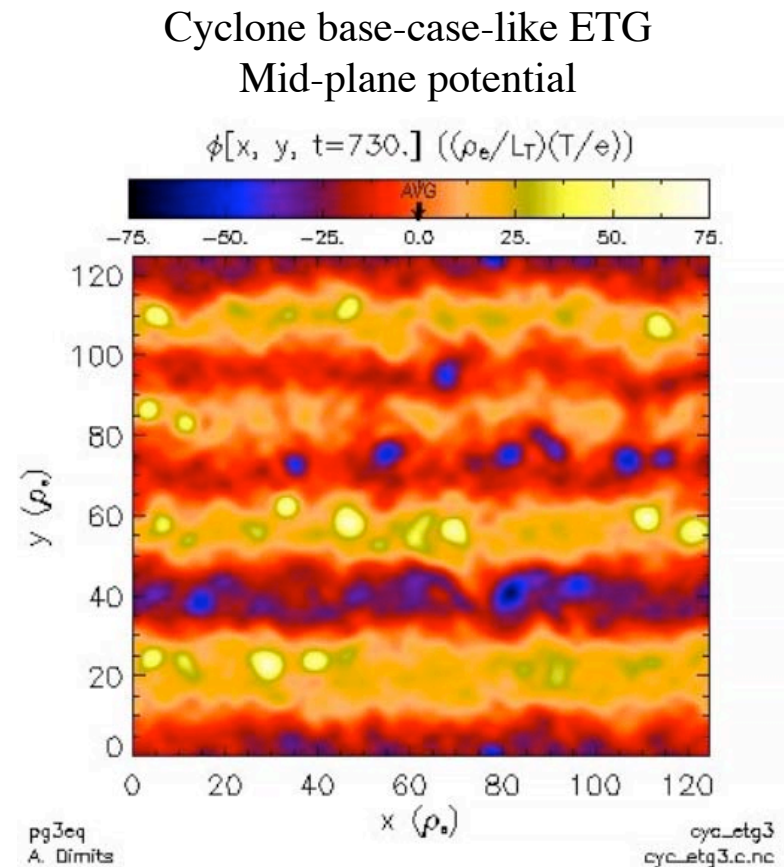
W.M. Nevins and A. Dimits  
LLNL, Livermore, CA

G. Hammett  
PPPL, Princeton, NJ



# 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



# Quantifying Particle Discreteness (1)

The fully uncorrelated fluctuation spectrum

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

$$\left\{1 + \left[1 - \Gamma_0(k_\perp^2 \rho_{th}^2)\right]\right\} \frac{e\phi_k}{T} = \frac{S_{filter}(k)}{N_p} \sum_i w_i J_0(k_\perp \rho_i) \exp(-i\mathbf{k} \cdot \mathbf{x}_i)$$

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

- The fluctuation spectrum

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

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

# Quantifying Particle Discreteness (1)

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$$\overset{\text{Debye}}{\text{shielding}} \left\{ 1 + \left[ 1 - \overset{\text{Polarization}}{\Gamma_0(k_{\perp}^2 \rho_{th}^2)} \right] \right\} \frac{e\phi_k}{T} = \frac{S_{filter}(k)}{N_p} \sum_i \overset{\text{"bare" gyro-center charge density}}{w_i J_0(k_{\perp} \rho_i) \exp(-i\mathbf{k} \cdot \mathbf{x}_i)}$$

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

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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)

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

- The fully uncorrelated spectrum (for comparison)

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

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# Simulation Verification (1)

## The Transverse (to $\mathbf{B}$ ) Fluctuation Spectrum

Requires:

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

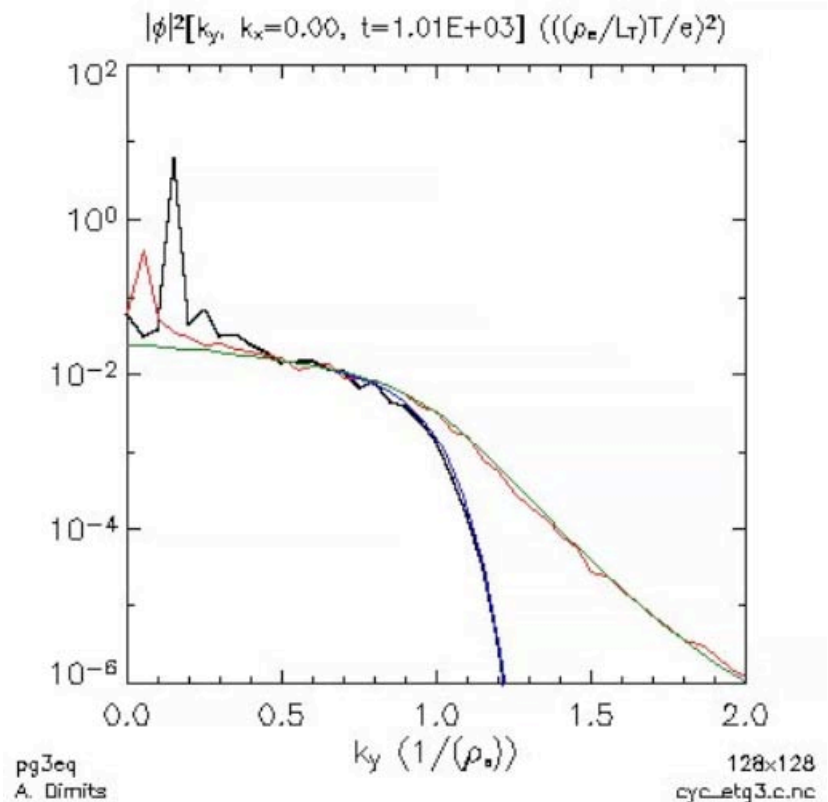
$$\left\langle \left| \frac{e\phi_{k_x, k_y}(z)}{T} \right|^2 \right\rangle = \sum_{k_z} \left\langle \left| \frac{e\phi_{k_x, k_y, k_z}}{T} \right|^2 \right\rangle =$$

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

⇒ Predicted noise spectrum fits the data

⇒ This simulation has a noise problem!

Cyclone base-case-like ETG





# 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

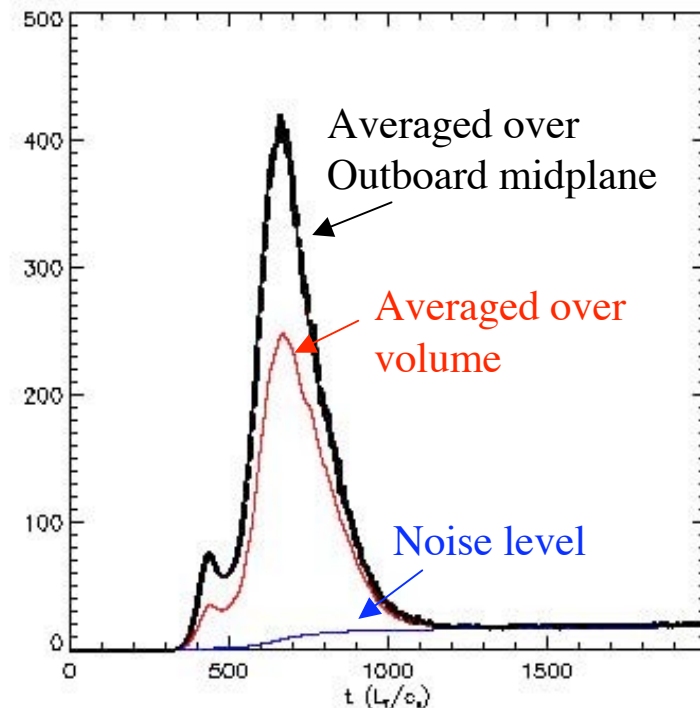
$$V_{shield}^{(H)} \equiv \left\{ \frac{1}{(2\pi)^3} \int d^3k \frac{S_{filter}^2 \Gamma_0(k_{\perp}^2 \rho_{th}^2)}{[2 - \Gamma_0][2 - (1 - S_{filter} d_{\parallel}) \Gamma_0]} \right\}^{-1}$$

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

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

Cyclone base-case-like ETG  
Fluctuation Intensity

$\langle |\phi|^2 \rangle [t] \left( (\rho/L_T)^2 (T/e)^2 \right)$



pg3eq  
A. Dimits

cyc\_etg3  
cyc\_etg3.c.nc

# 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  
 $D \approx \langle V_{ExB}^2 \rangle \tau_{corr}$

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

where

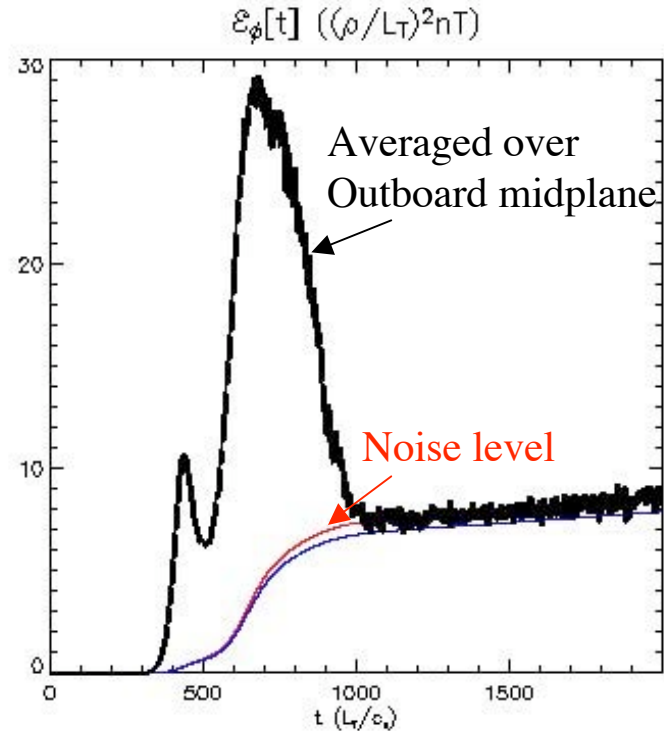
$$\langle K_{\perp}^2 \rho^2 \rangle_{noise}^{(H)} \equiv \left\{ \frac{V_{shield}}{(2\pi)^3} \int d^3k \frac{K_{\perp}^2(k) \rho^2 S_{filter}^2(k) \Gamma_0(k_{\perp}^2 \rho_{th}^2)}{[2 - \Gamma_0][2 - (1 - S_{filter} d_{\parallel}) \Gamma_0]} \right\}$$

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

4/8/2005

TTF Mtg. Napa, CA

Cyclone base-case-like ETG  
Fluctuation Energy

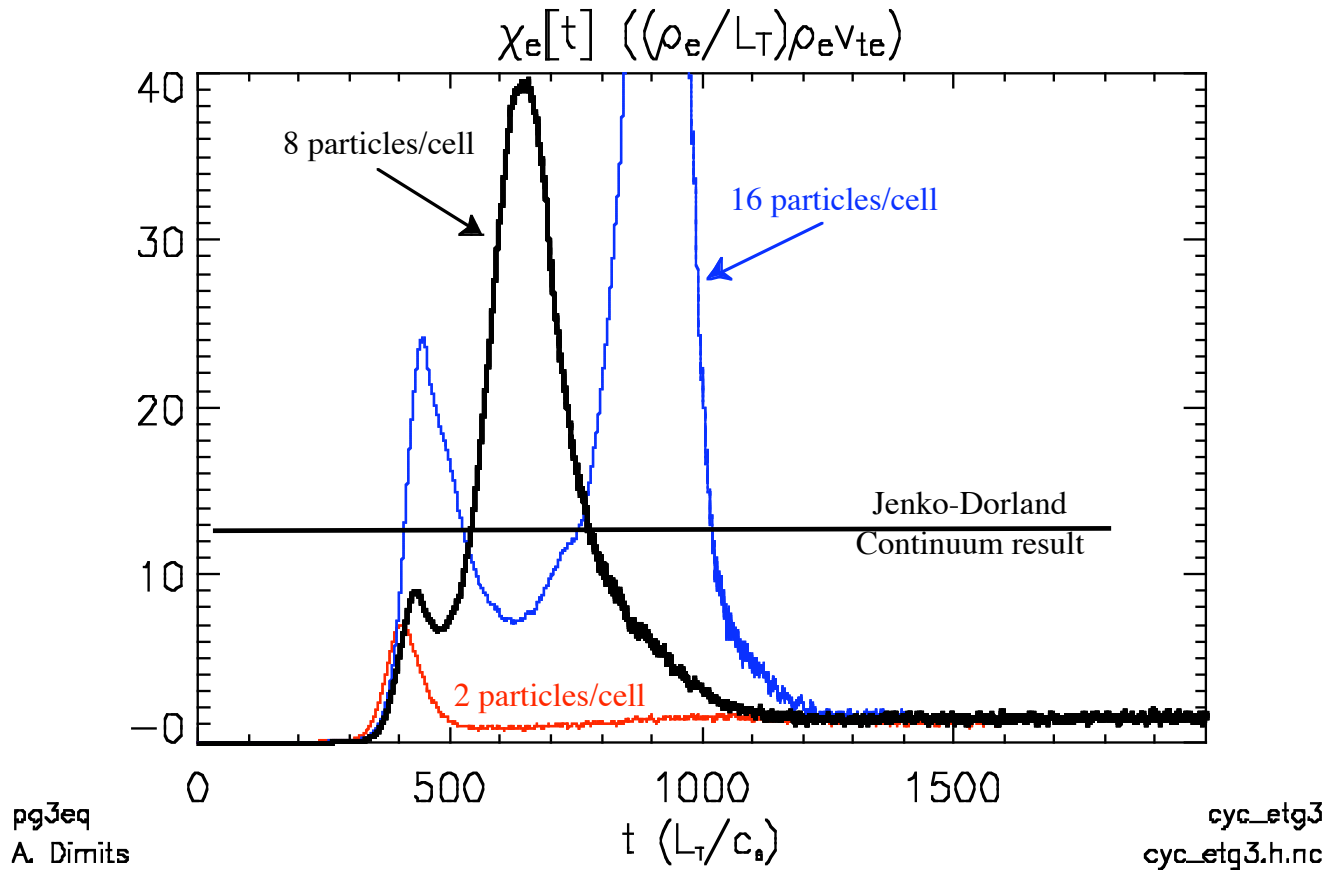


pg3eq  
A. Dimits

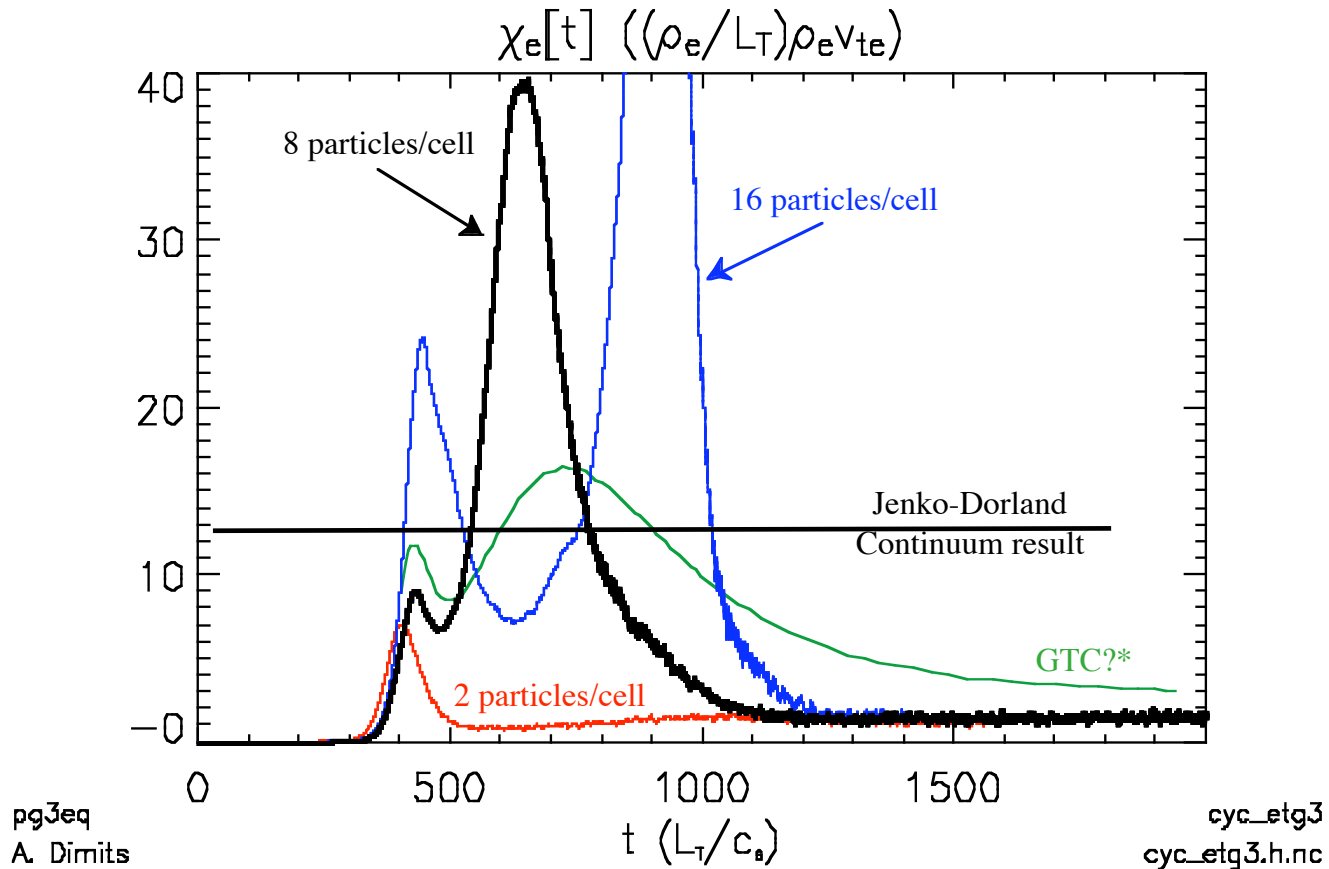
cyc\_etg3  
cyc\_etg3.c.nc

10

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

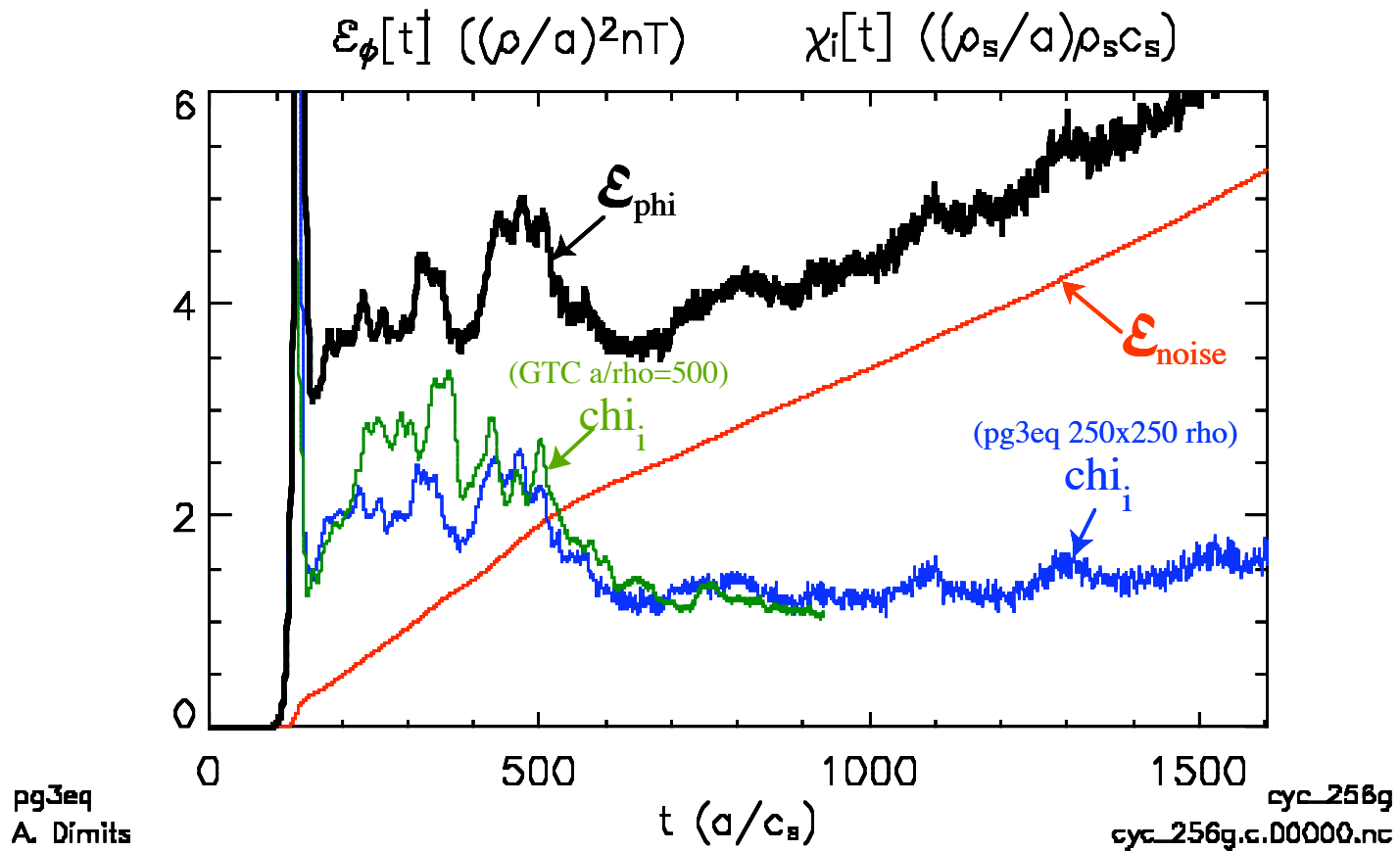


# Discrete Particle Noise Suppresses Transport In Cyclone-base-case like ETG Simulations



\*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](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)

# Summary

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(may help to explain remaining discrepancies in CYCLONE base-case benchmark)

⇒ Perhaps PIC code-development effort should focus on noise reduction?

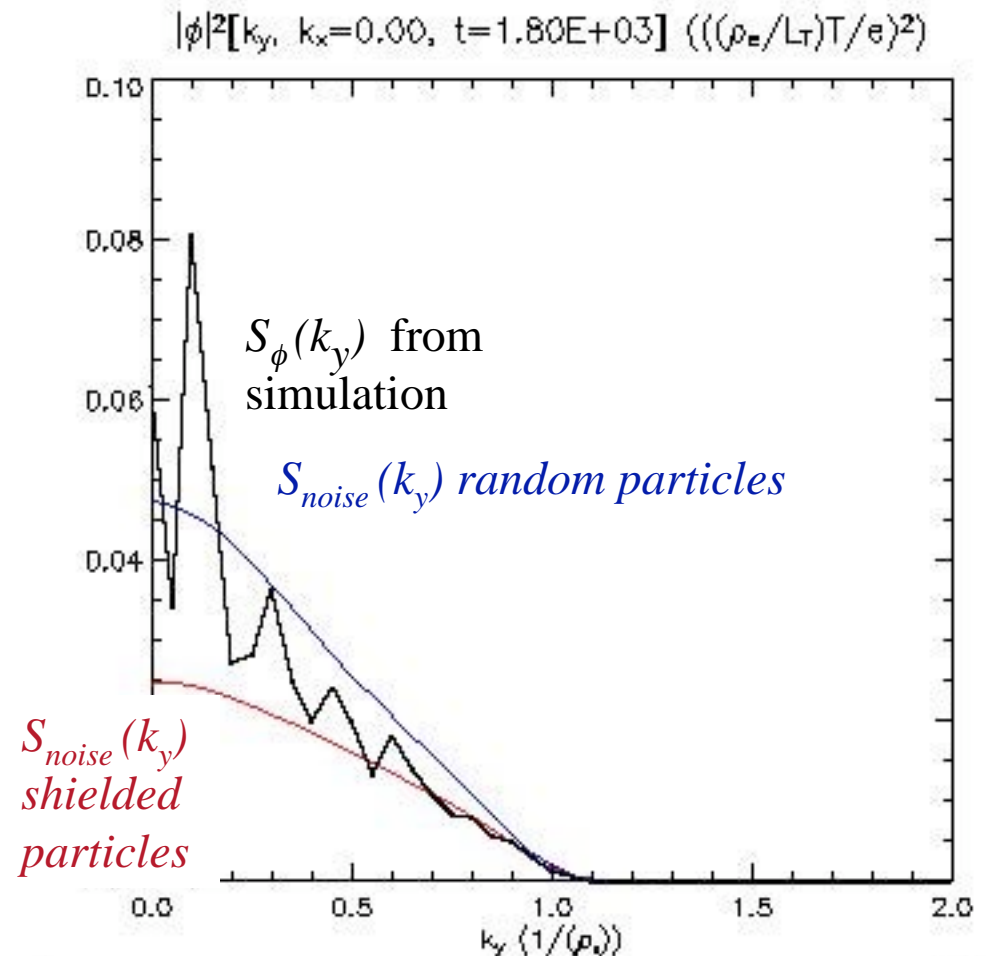
# Noise calculation including shielding more accurate.

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  $k_y \rho_e \gg 1$ , 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.



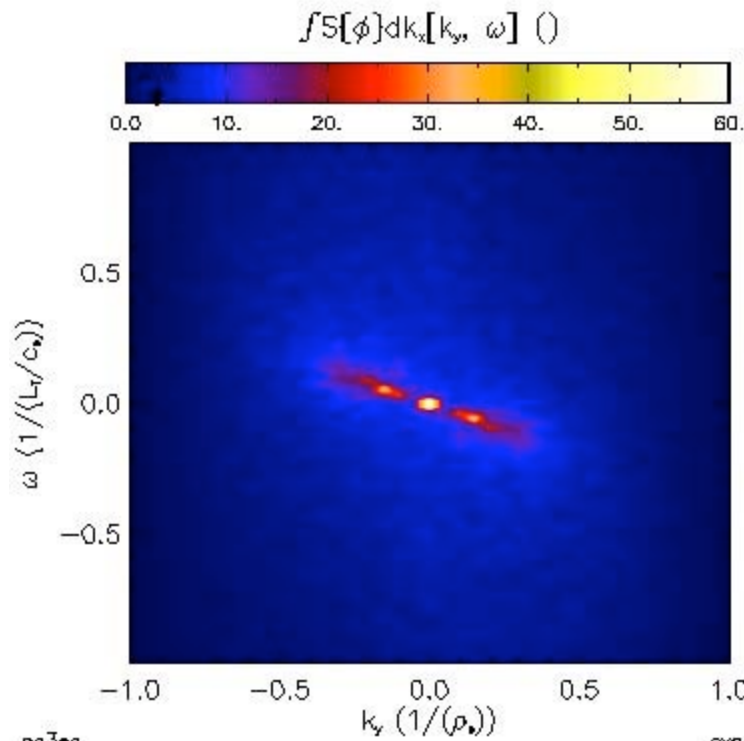
pg3eq  
A. Dimits

128x128  
cyc\_etg3.c.nc



# Frequency Spectrum

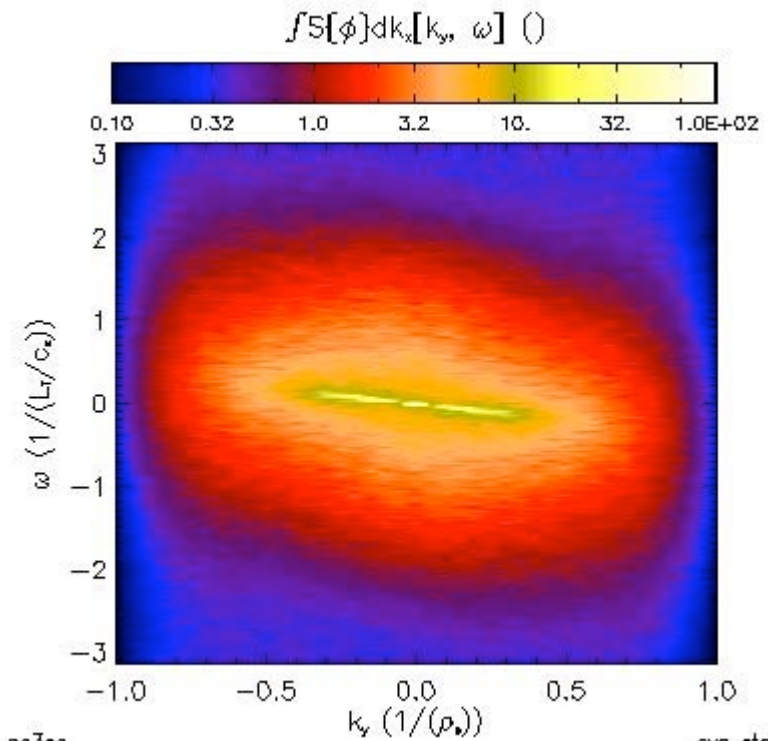
Drift waves at low- $k_{\perp}$



pg3eq  
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cyc\_etg3  
cyc\_etg3.c.nc

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

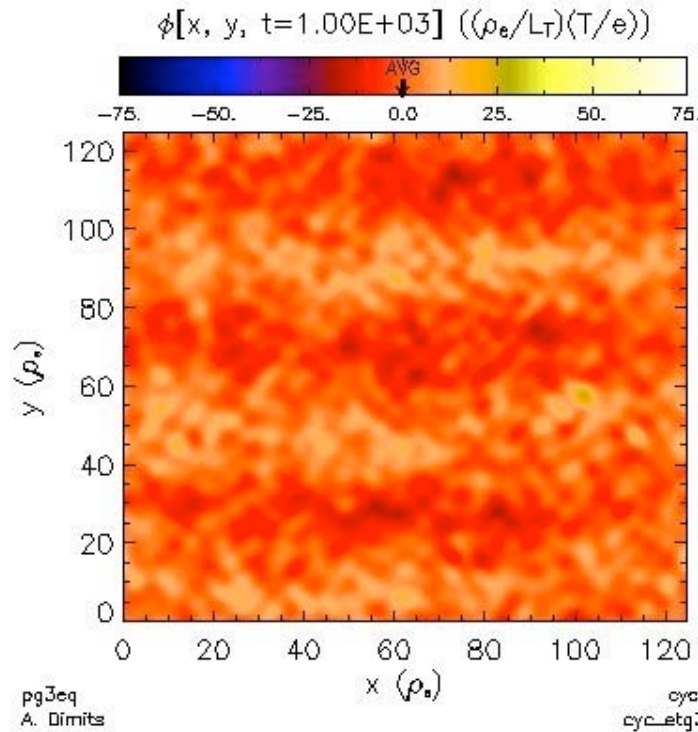


pg3eq  
A. Dimits

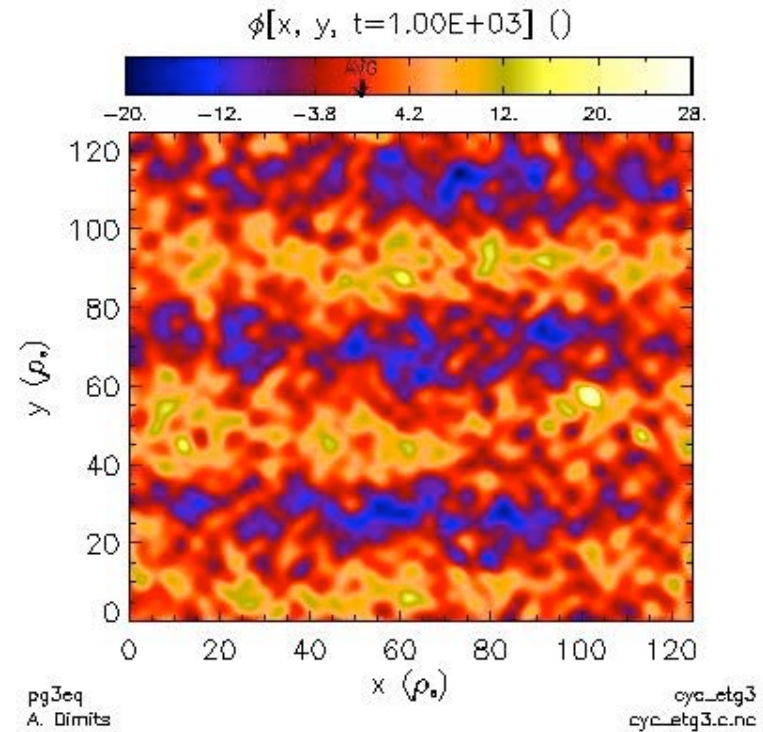
cyc\_etg3  
cyc\_etg3.c.nc

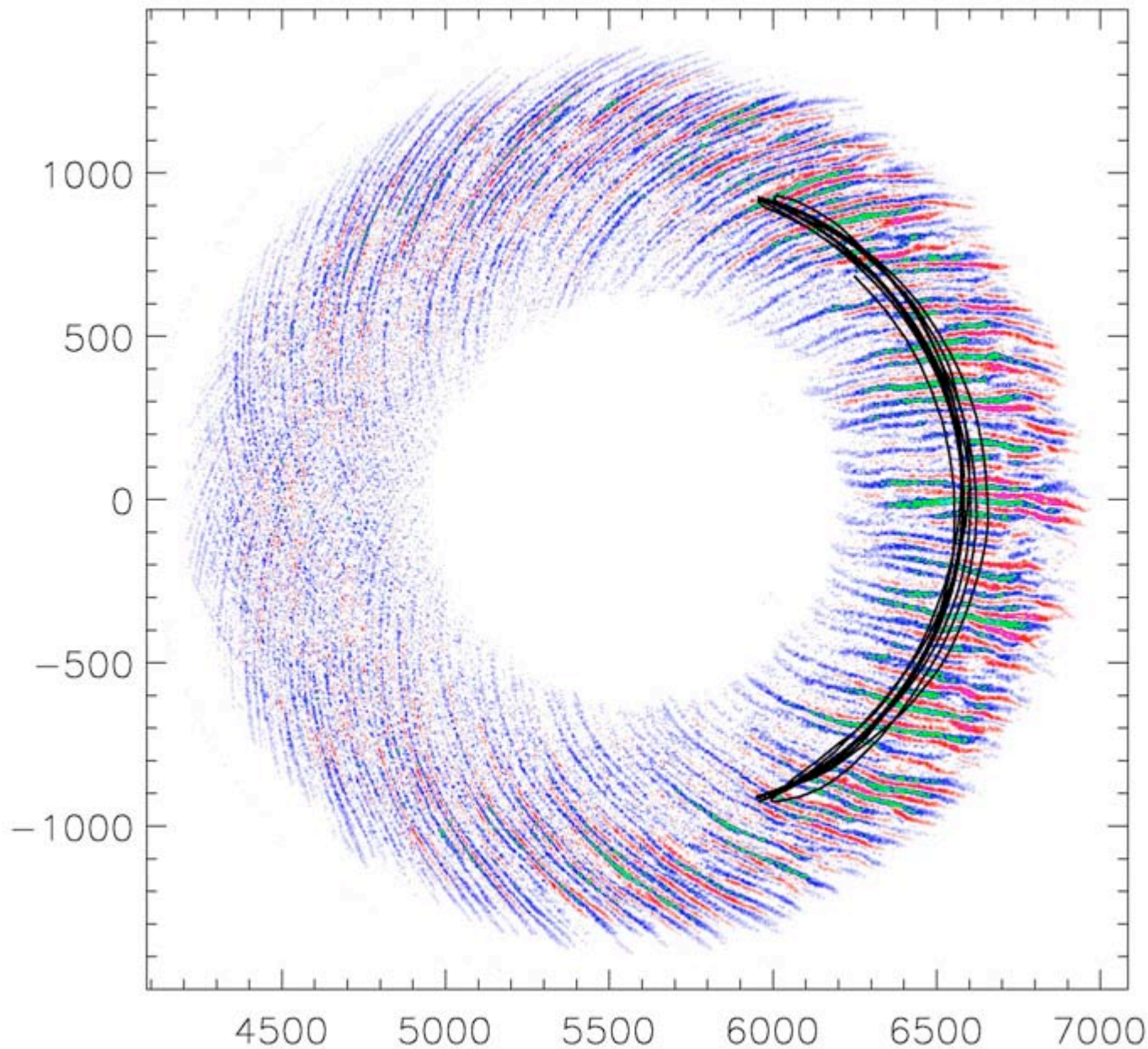
# Is the "eyeball" test an accurate measure of the noise level?

Streamers are nearly gone



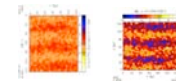
or, are they?  
(same data, new color bar)





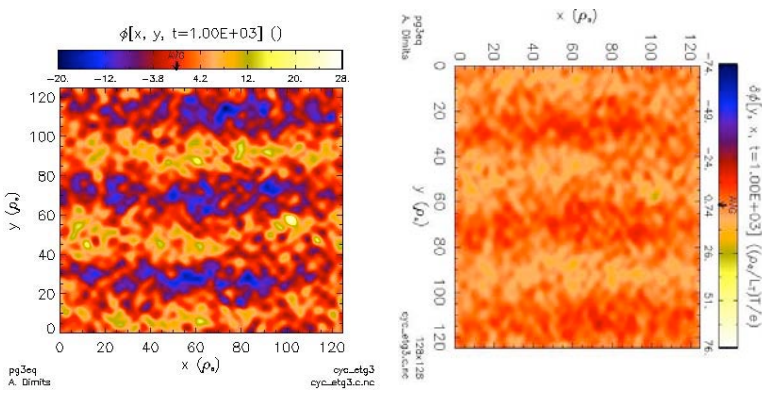
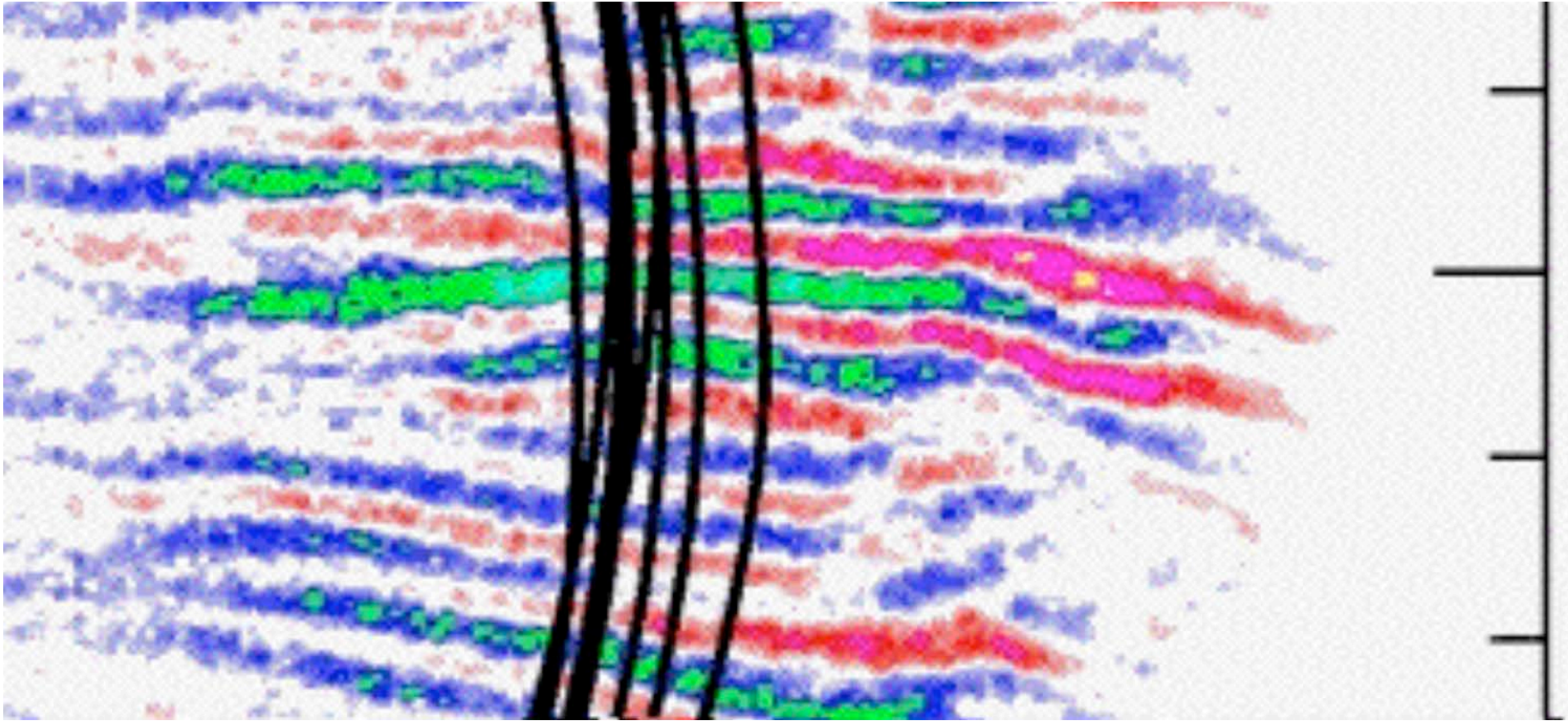
Dimits contour plots at  
Same scale as Z. Lin's

Dimits contour plot with  
Re-scaled color bar



Dimits contour plot at  $t=1000$ ,  
when  $\chi_e \sim 2 \times \text{final } \chi_{\text{noise}}$ . This is  
when noise effects are strong  
enough to reduce  $\chi_e$  to  $\sim 1/4^{\text{th}}$  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  $\chi_e \sim 2 \times \text{final } \chi_{\text{noise}} \sim 1/4^{\text{th}} \chi_{\text{Jenko-Dorland}}$ ).

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?

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

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

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

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

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

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