Discrete Particle Noise in PIC Simulations of Plasma Microturbulence

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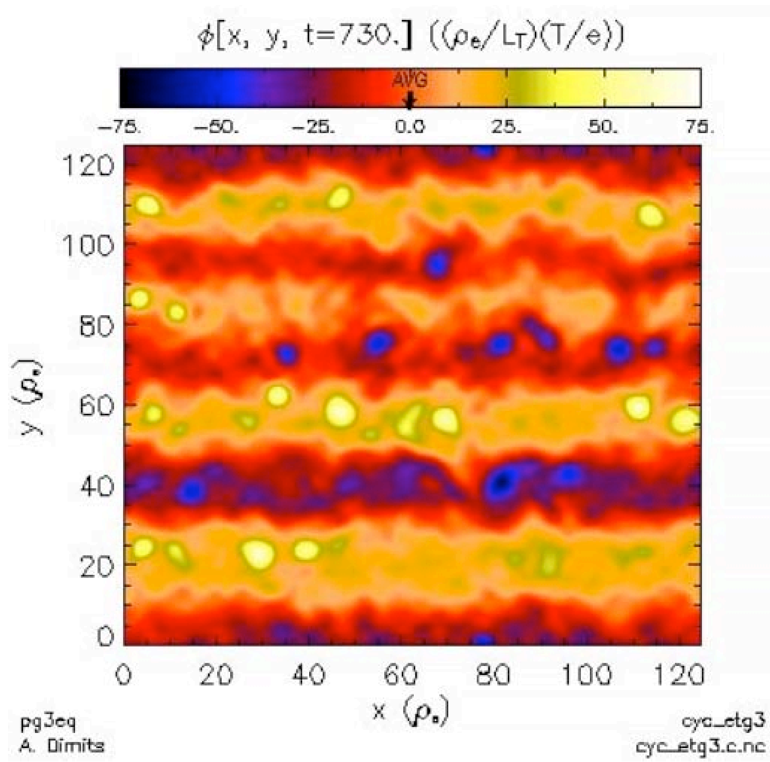
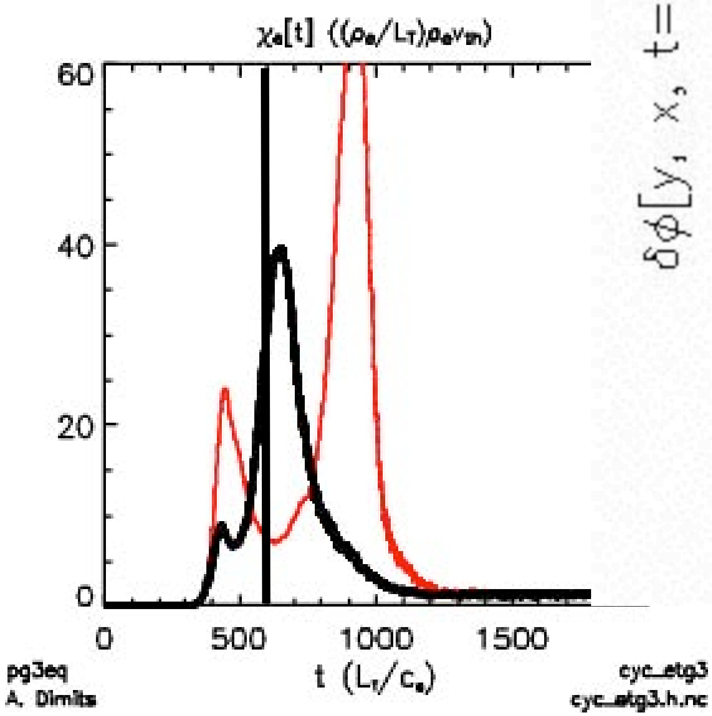
Discrete Particle Noise is a code verification issue

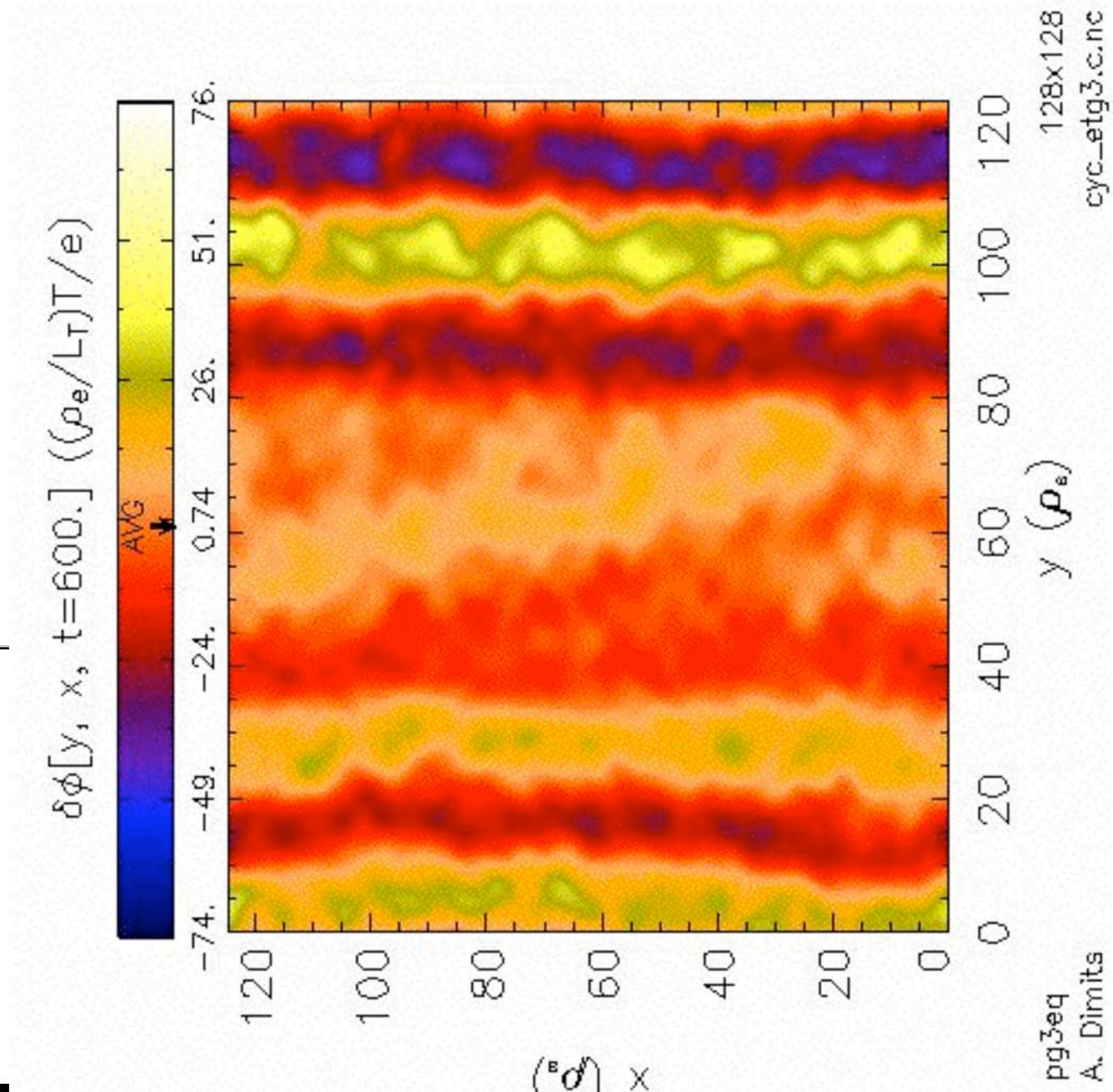
- An important issue because:
  - Particle discreteness in PIC codes does not correctly represent underlying GK-Maxwell system
  - A major source of controversy between PIC and Continuum GK-simulation communities
- Can be a problem for:
  - Cyclone base-case-like ETG
  - Cyclone base-case ITG
- It's quantifiable — a literature on particle discreteness in PIC codes:
  - Langdon '79 – Birdsall&Langdon '85
  - Krommes '93 – Hammett '05

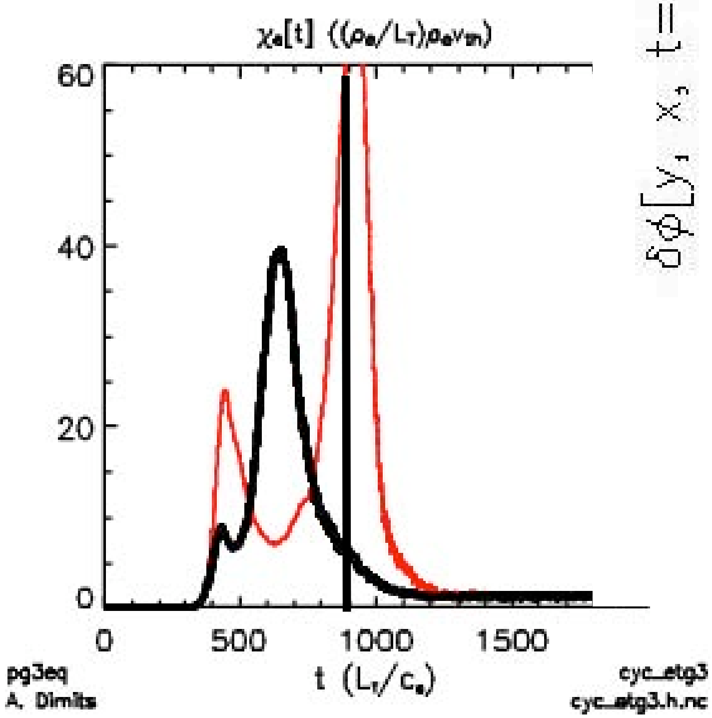
⇒ We can develop objective criteria to determining when discrete particle noise is a problem

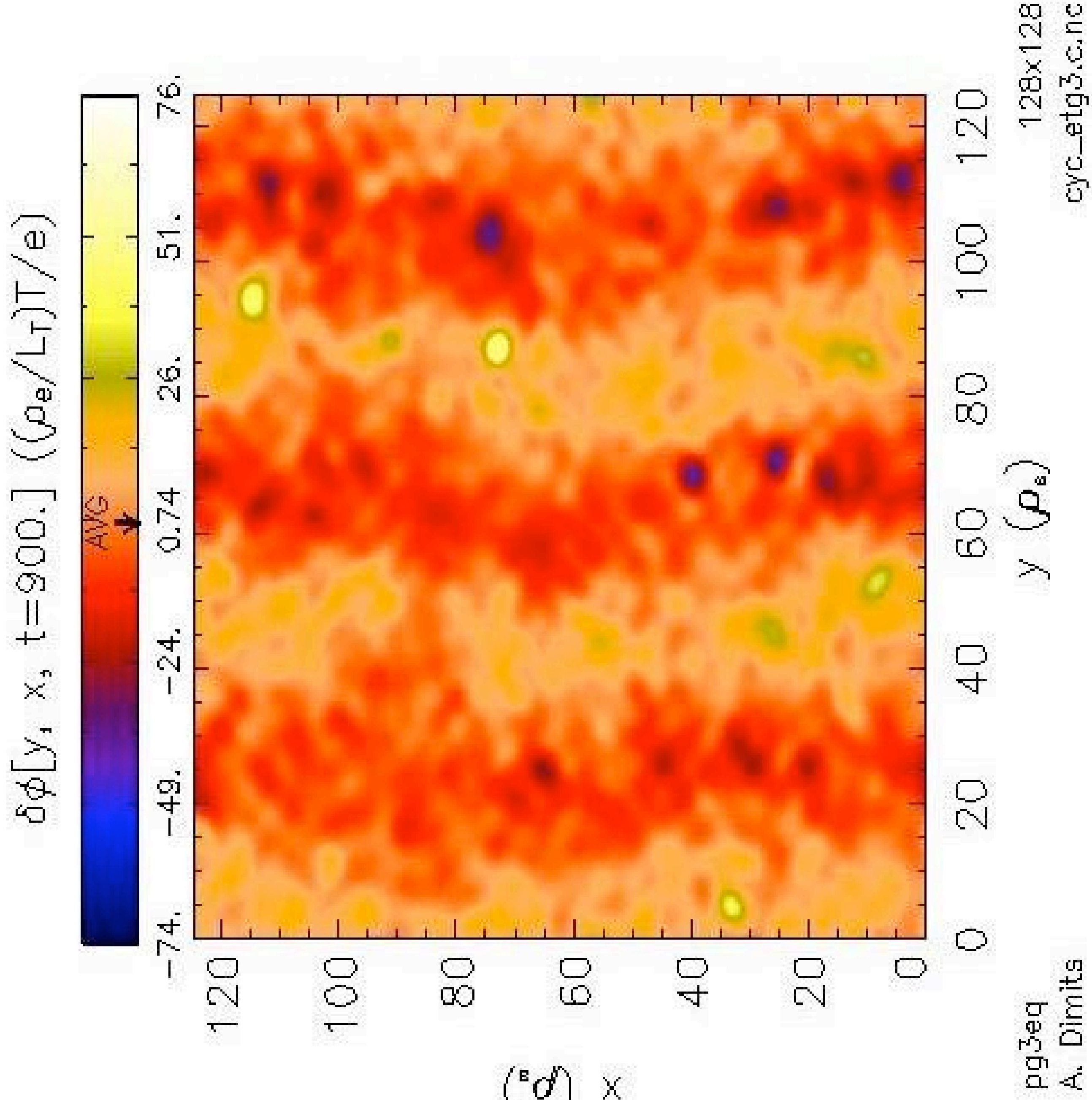
Cyclone base-case-like ETG
Mid-plane potential

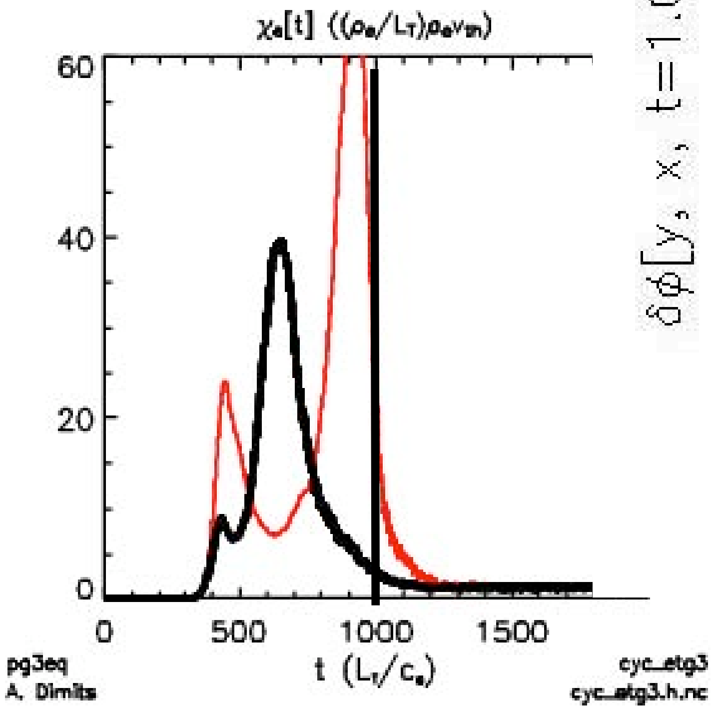


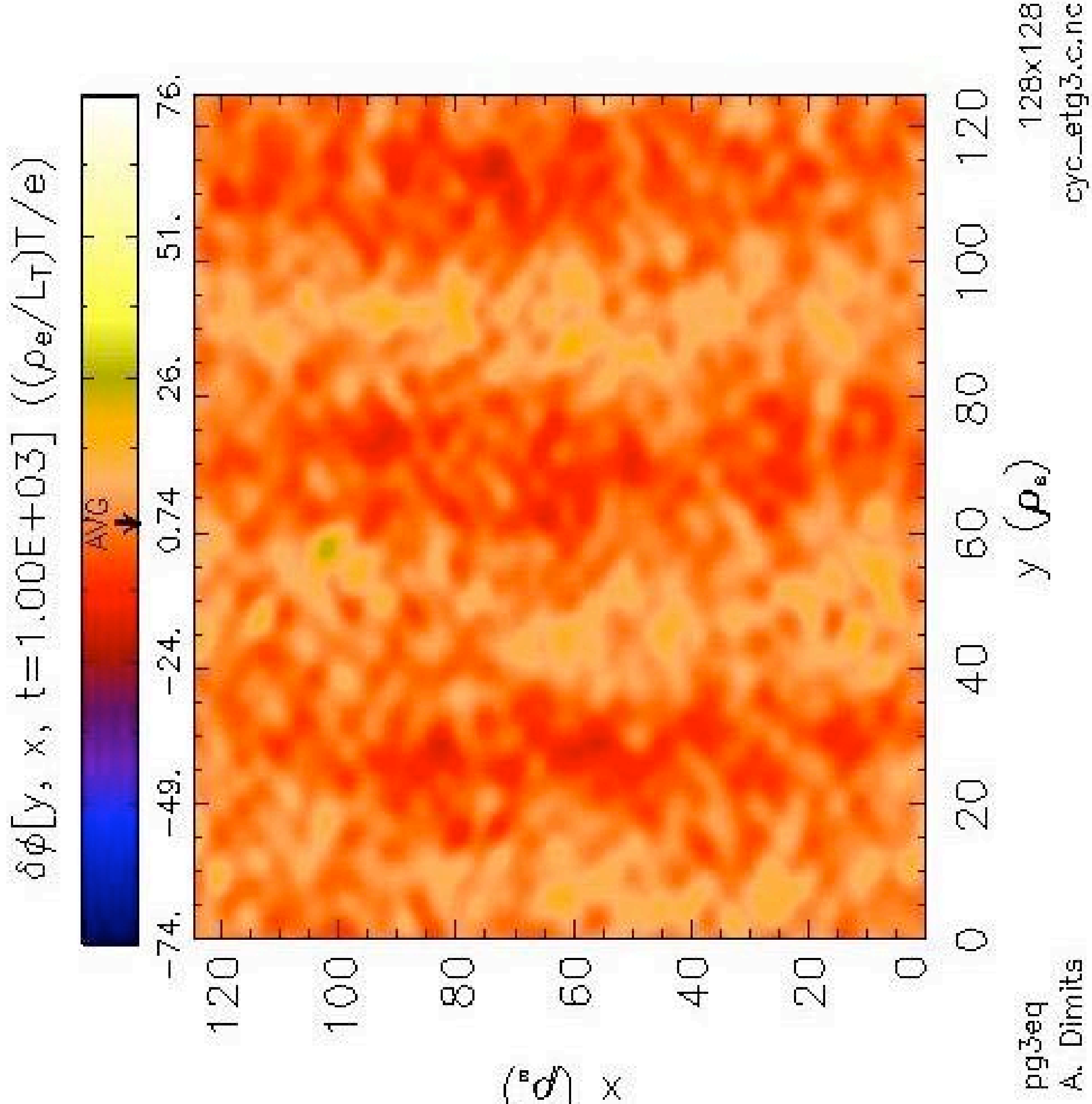

$\chi_e[t]$ $((\rho_e/L_T)\rho_e v_{th})$
60
40
20
0
0
500
1000
1500
t (L_T/c_s)
pg3eq
A. Dimits
cyc_etg3
cyc_etg3.h.nc

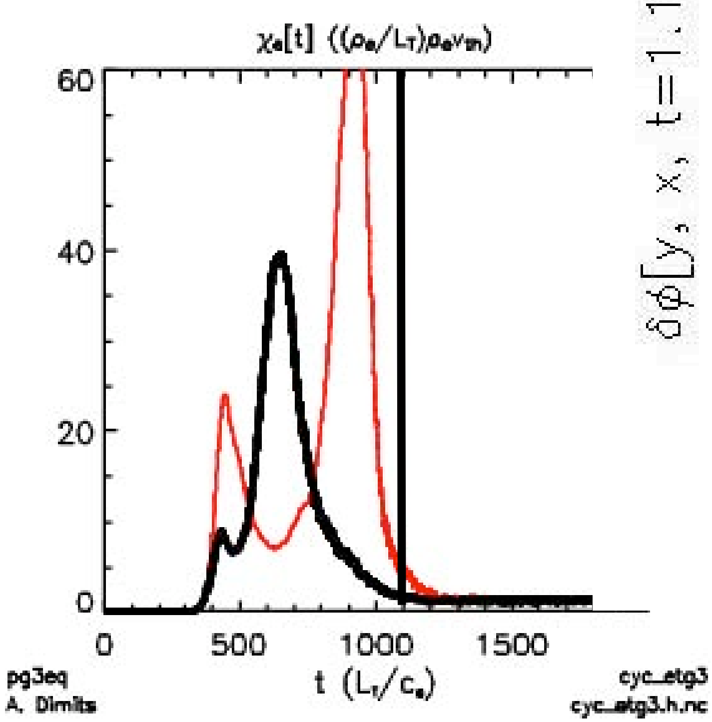

$\delta\phi[y, x, t=600.]$ $((\rho_e/L_T)T/e)$
AVG
76.
51.
26.
0.74
−24.
−49.
−74.
x (ρ_s)
y (ρ_s)
128x128
cyc_etg3.c.nc
pg3eq
A. Dimits


χe[t] ((ρe/LT)ρeVth)
60
40
20
0
0
500
1000
1500
t (LT/ce)
pg3eq
A. Dimits
cyc_etg3
cyc_etg3.h.nc

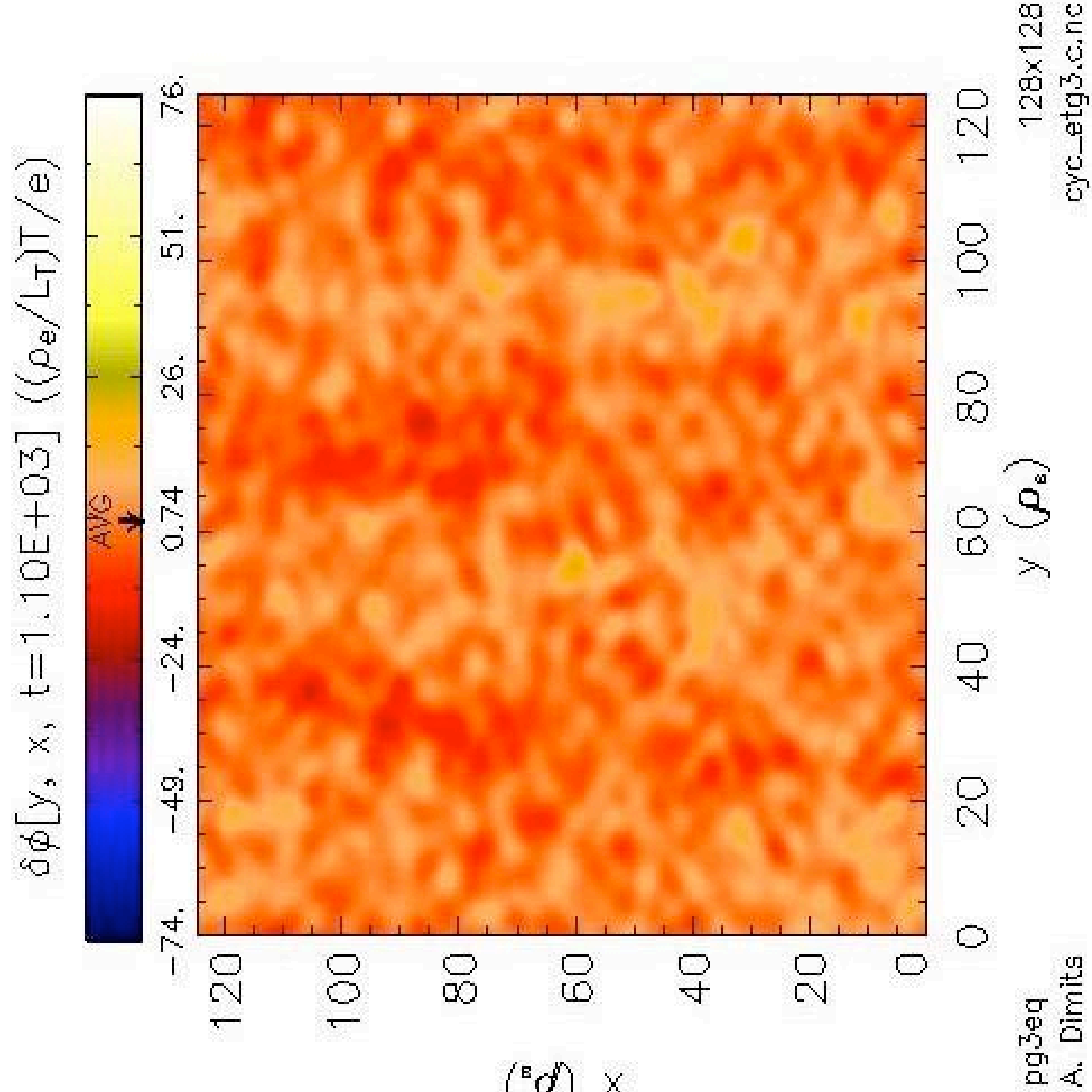

δφ[y, x, t=900.] ((ρe/LT)T/e)
AVG
76.
51.
26.
0.74
−24.
−49.
−74.
y (ρe)
x (ρe)
128x128
cyc_etg3.c.nc
pg3eq
A. Dimits


$\chi_e[t]$ $((\rho_e/L_T)\rho_e v_{te})$
t (L_T/c_s)
pg3eq
A. Dimits
cyc_etg3
cyc_etg3.h.nc

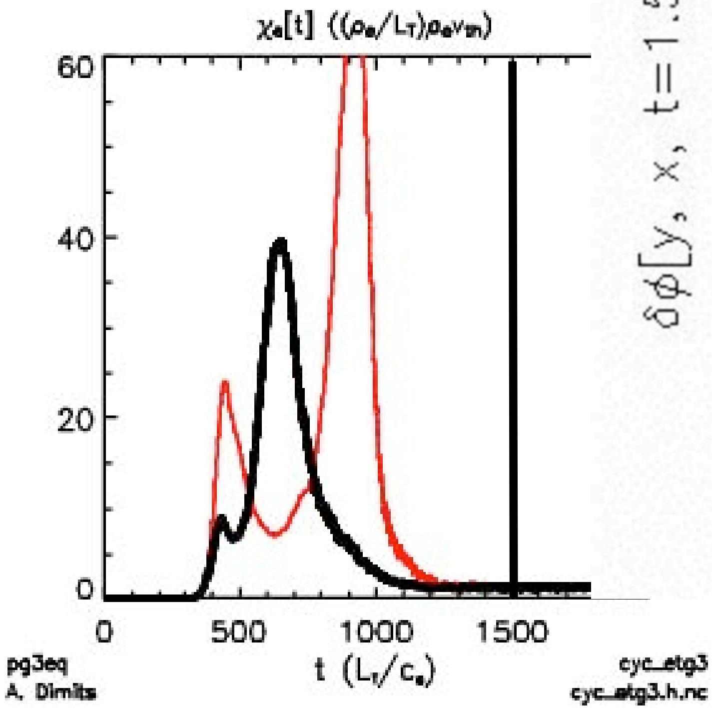

$\delta\phi[y, x, t=1.00E+03]$ $((\rho_e/L_T)T/e)$
AVG
y (ρ_s)
x (ρ_s)
128x128
cyc_etg3.c.nc
pg3eq
A. Dimits

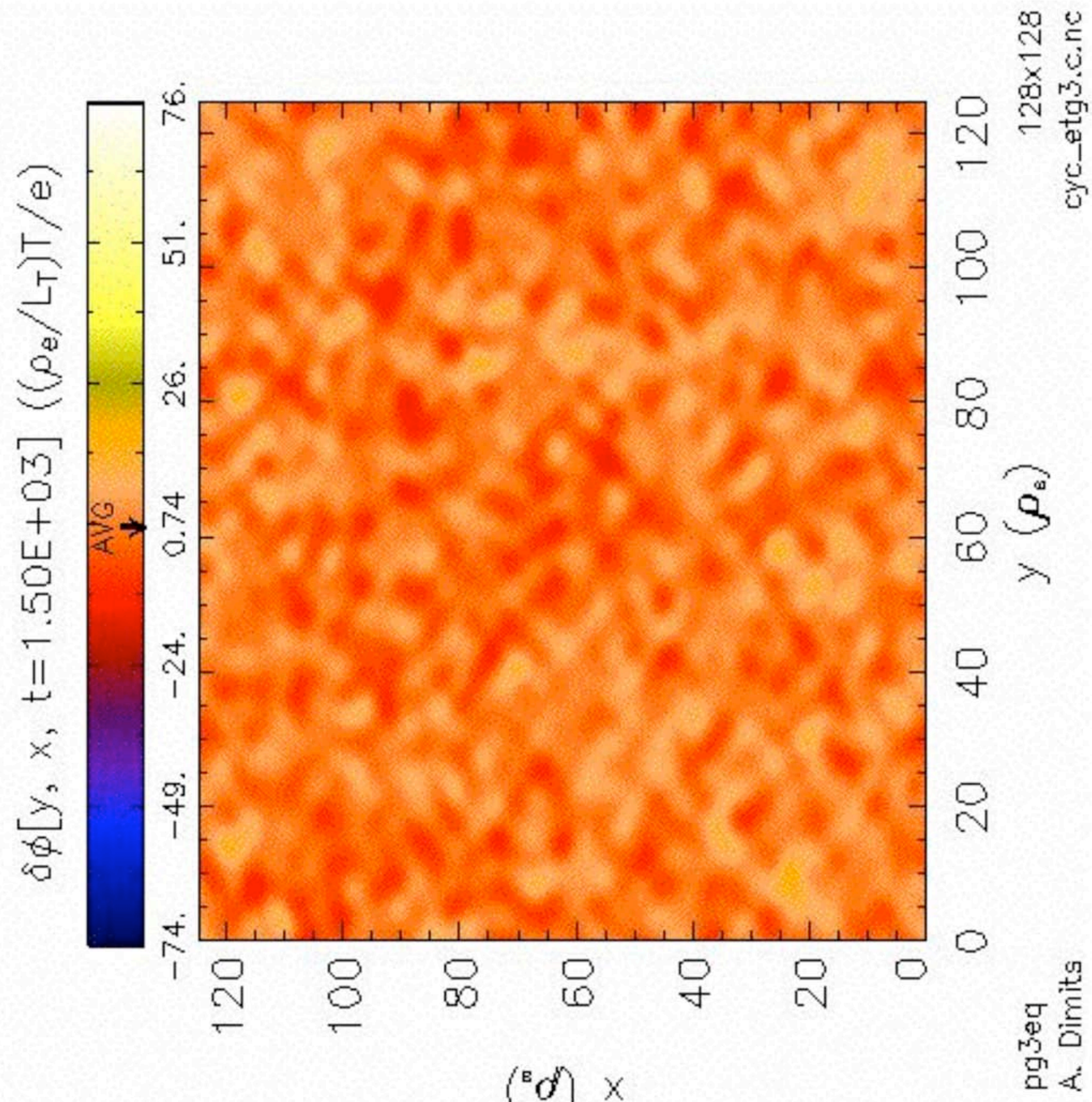


$\chi_e[t]$ $((\rho_e/L_T)\rho_e v_{th})$
t (L_T/c_e)
pg3eq
A. Dimits
cyc_etg3
cyc_etg3.h.nc



$\delta\phi[y, x, t=1.10E+03]$ $((\rho_e/L_T)T/e)$
AVG
y (ρ_s)
x (ρ_s)
128x128
cyc_etg3.c.nc
pg3eq
A. Dimits


χe[t] ((ρe/LT)ρevth)
t (LT/cs)
pg3eq
A. Dimits
cyc_etg3
cyc_etg3.h.nc


δφ[y, x, t=1.50E+03] ((ρe/LT)T/e)
AVG
y (ρs)
x (ρs)
128x128
cyc_etg3.c.nc
pg3eq
A. Dimits

Quantifying Particle Discreteness (1)

The fully uncorrelated fluctuation spectrum

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

Debye shielding

Polarization

“bare” gyro-center charge density

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

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

- The fluctuation spectrum

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

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

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)

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

- The fully uncorrelated spectrum (for comparison)

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

Krommes' Calculation of Noise Spectrum

Krommes' 1993 calculation of the gyrokinetic noise spectrum uses the fluctuation-dissipation theorem, and shows equivalent results from the test-particle superposition principle. (see also W.W. Lee 1987, and classic paper by A.B. Langdon, 1979)

Krommes' calculation used shielding by linear dielectric from gyrokinetic equation in a slab, uniform plasma. Hu & Krommes 94 extended to δf.

Hammett et al extended Krommes' test-particle superposition calculation to:

- Treat one species as adiabatic instead of with particles.

- Include factors for finite-size particle shape S (accounts for interpolation of particle charge to grid, and forces from grid to particles) & S_{filter} factor for explicit filtering of Φ. Important for quantitative comparisons.

- Use a renormalized dielectric, including a $k_\perp^2 D_{NL}$ term on the non-adiabatic part of the shielding cloud, and including random walks in the test particle trajectories instead of assuming straight-line trajectories. Affects frequency spectrum of fluctuations, but not the frequency-integrated k spectrum.

Renormalized Dielectric Shielding

Nonlinear gyrokinetic Eq. (uniform slab, electrostatic):

$$\frac{\partial \delta f}{\partial t} + \mathrm{v}_{\|}\hat{b}\cdot\nabla\delta f + \frac{c}{B}\hat{b}\times\nabla J_0\Phi\cdot\nabla\delta f = -\mathrm{v}_{\|}\left(\hat{b}\cdot\nabla J_0\frac{q\Phi}{T}\right)F_{Max,0}$$

If ExB velocity is small-scale random fluctuations, treat as random walk diffusion:

$$\frac{\partial \delta f}{\partial t} + \mathrm{v}_{\|}\hat{b}\cdot\nabla\delta f - D_{NL}\nabla_{\perp}^{2}\delta f = -\mathrm{v}_{\|}\left(\hat{b}\cdot\nabla J_0\frac{q\Phi}{T}\right)F_{Max,0}$$

Better renormalization (Catto 78): nonlinearity affects only non-adiabatic part of δf:

$$\frac{\partial \delta f}{\partial t} + \mathrm{v}_{\|}\hat{b}\cdot\nabla\delta f - D_{NL}\nabla_{\perp}^{2}\left(\delta f - F_{Max.0}J_0\frac{q\Phi}{T}\right) = -\mathrm{v}_{\|}\left(\hat{b}\cdot\nabla J_0\frac{q\Phi}{T}\right)F_{Max,0}$$

Preserves the form of the Fluctuation-Dissipation Theorem, insures no nonlinear damping of a thermal equilibrium solution (the adiabatic solution) (Catto78, Krommes81, Krommes02).

Detailed Calculation of Noise-Spectrum Incl. Self-Shielding

Potential induced by shielded test particle density ρ_{ext}: $\Phi = \dfrac{4\pi\rho_{ext}}{k^2 \varepsilon(\vec{k},\omega)}$

$$\varepsilon(\vec{k},\omega) = \frac{k_D^2}{k^2}\left[\frac{T}{T_a}\left(1-\delta_{k_\parallel}\right) + 1 - \Gamma_0 + S_{filt} d_\parallel S^2 \left\langle J_0^2 \right\rangle \left(1 + \zeta Z(\zeta + i\zeta_D)\right)\right]$$

Gyrokinetic dielectric shielding including simple renormalized D_{NL} model of nonlinear effects on shielding cloud and test-particle random walk trajectory, $\zeta_D = k_\perp^2 D_{NL} / (|k_\parallel|\, v_t\, 2^{1/2})$. Integrating $\langle|\Phi_k|^2\rangle(\omega)$ over all ω gives a result independent of D_{NL}. To preserve this feature of the Fluctuation-Dissipation Theorem, important to apply renormalized $k_\perp^2 D_{NL}$ only to the non-adiabatic part of δf (Catto78, Krommes81, Krommes02). Resulting k spectrum:

$$\left\langle \left| \frac{e\tilde{\Phi}_{noise,k}}{T} \right|^2 \right\rangle = \frac{V^2 \left\langle w^2 \right\rangle}{N} \frac{S_{filt}^2 S^2 \left\langle J_0^2 \right\rangle}{\left[\frac{T}{T_a}\left(1-\delta_{k_\parallel}\right) + 1 - \Gamma_0 + \underbrace{S_{filt} d_\parallel S^2 \left\langle J_0^2 \right\rangle}\right]\left[\frac{T}{T_a}\left(1-\delta_{k_\parallel}\right) + 1 - \Gamma_0\right]}$$

Only difference from simple random-particle spectrum.
$\langle \Phi_k^2 \rangle$ only 50% lower at low $k_\perp$, equal at high $k_\perp$

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

Requires:

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

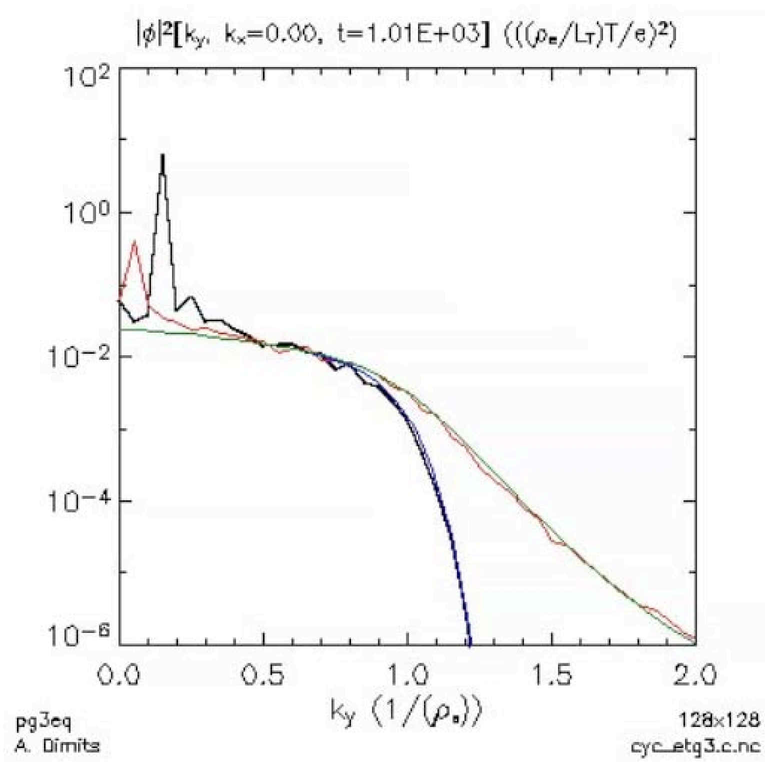
$$\left\langle \left| \frac{e\phi_{k_x,k_y}(z)}{T} \right|^2 \right\rangle = \sum_{k_z} \left\langle \left| \frac{e\phi_{k_x,k_y,k_z}}{T} \right|^2 \right\rangle =$$

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

⇒ Predicted noise spectrum fits the data

⇒ This simulation has a noise problem!

Cyclone base-case-like ETG
Mid-plane potential

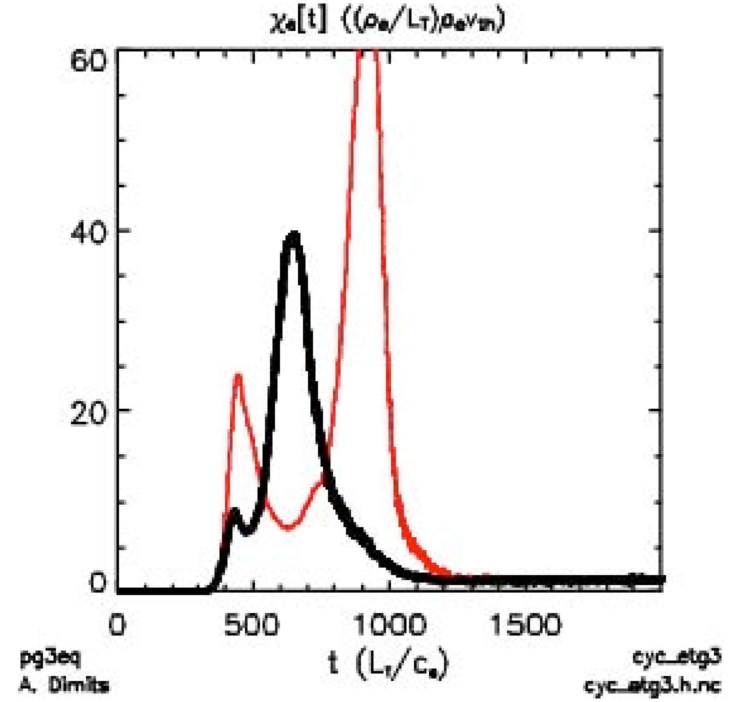


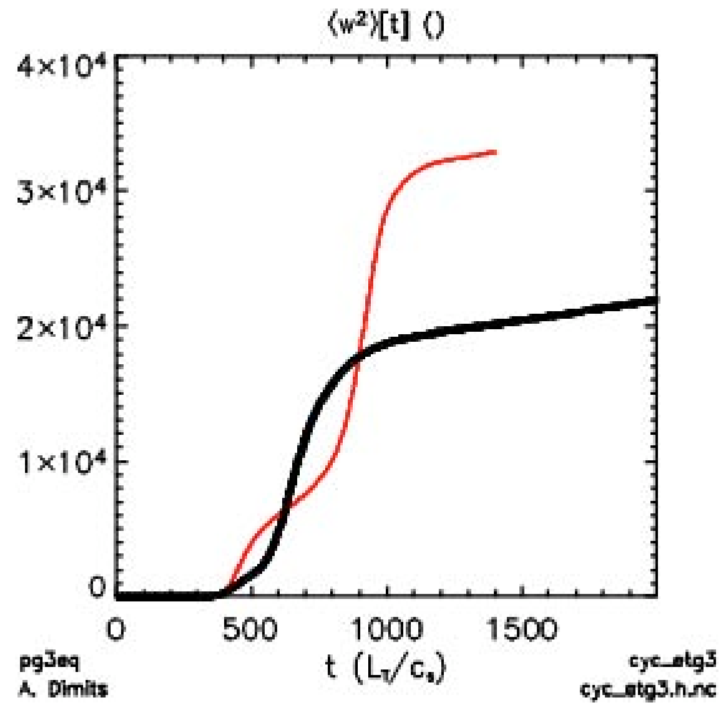
Discrete Particle Noise can sometimes be an issue for Particle-in-cell simulations

- Red curve: 16 particles/cell, 256 x 64 x 32
- Black curve: 8 particles/cell 128 x 128 x 64
- The mean square particle weight $<w^2>(t)$ measures discrete particle noise
- Entropy Theorem of Lee & Tang:

$$\frac{dw_{rms}^2}{dt} \approx \frac{2\chi_e}{L_T^2}$$

- χ_e is larger (in GK-units, $\rho^2 v_{th}/L_T$) Discrete particle noise a greater issue for ETG that ITG?
- Discrete particle noise looks important for $t > 700\ L_T/v_{th}$ in PG3EQ simulations





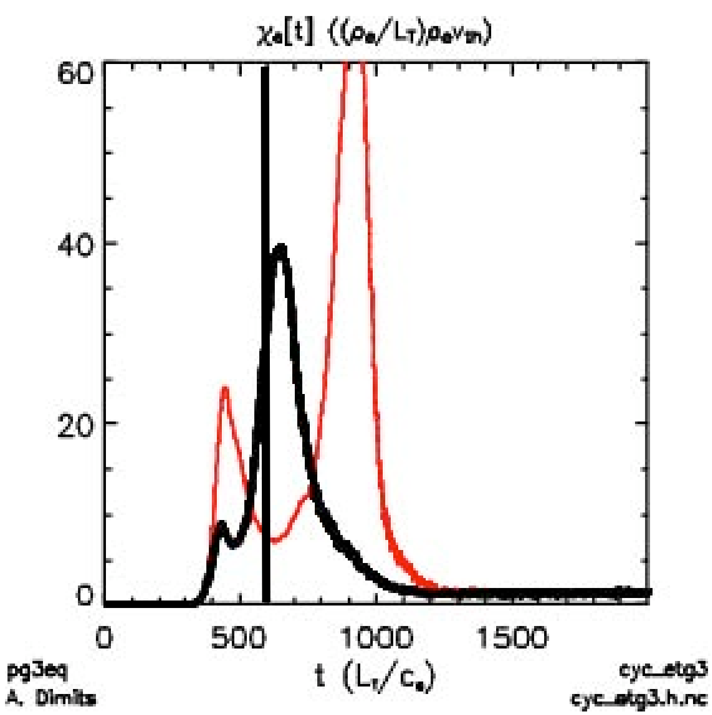
Total & Noise part of ϕ spectrum $S_\phi(k)$ at t=

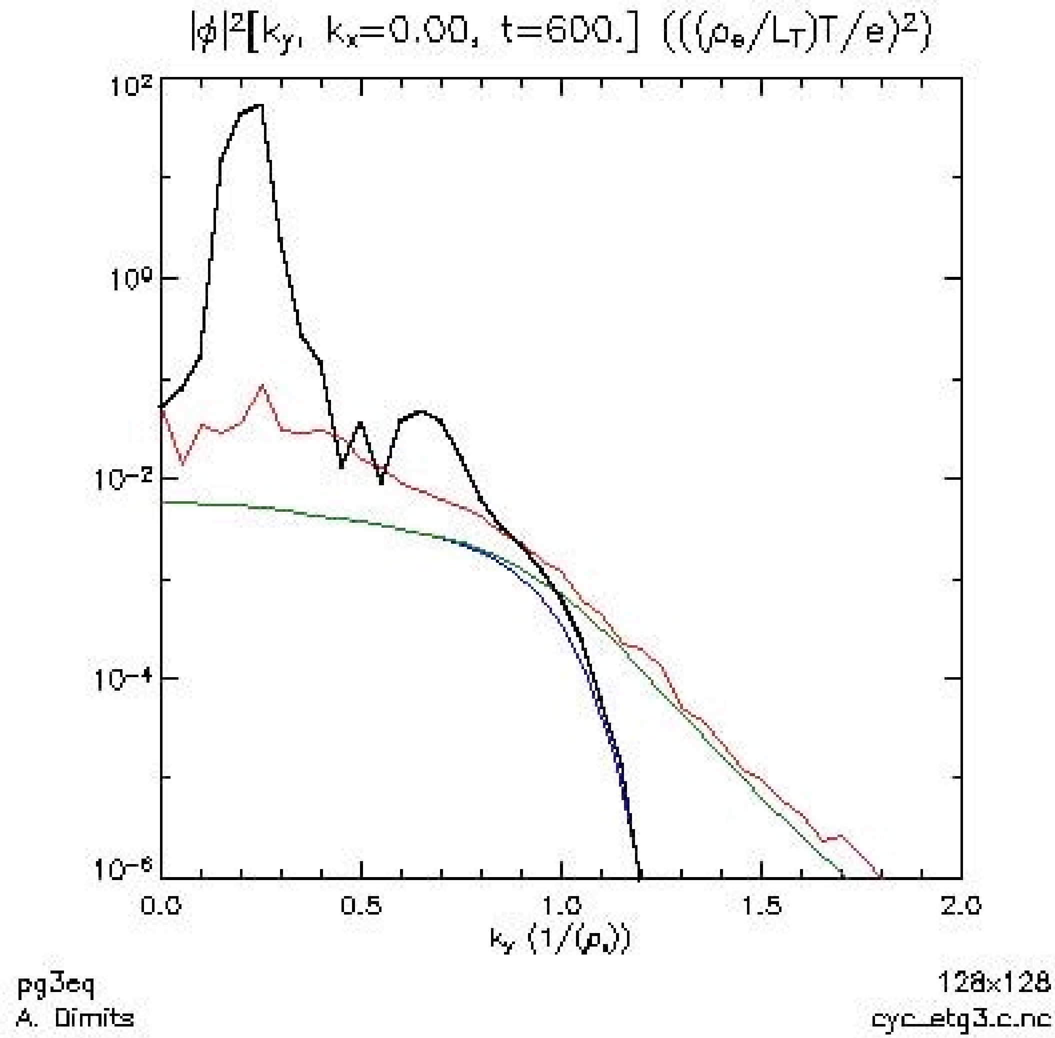
$S_\phi(k)$ from simulation:

- $S_\phi(k_x=0, k_y\ \ )$ — black
- $S_\phi(k_x\ \ , k_y=0)$ — red/brown

$S_\phi(k)$ from noise:

- $S_{noise}(k_x=0, k_y\ \ )$ — blue
- $S_{noise}(k_x\ \ , k_y=0)$ — green





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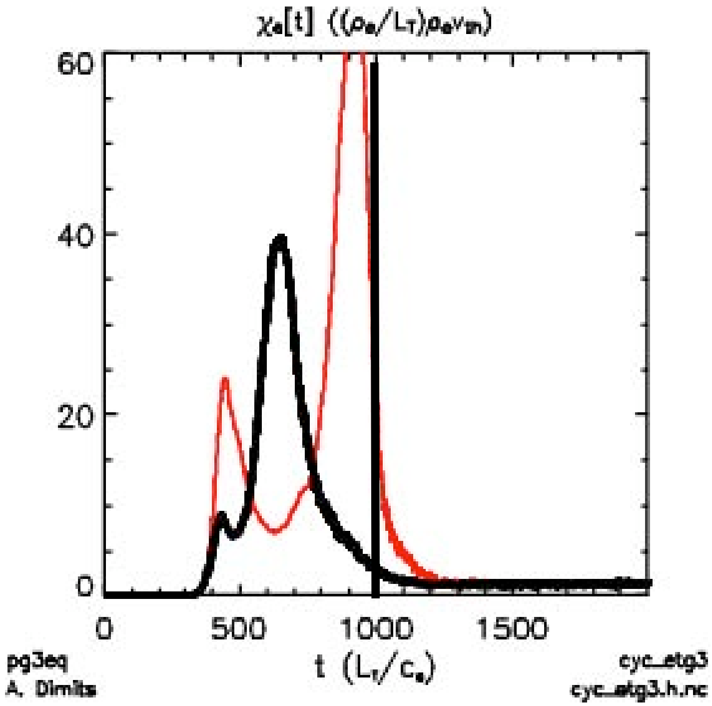
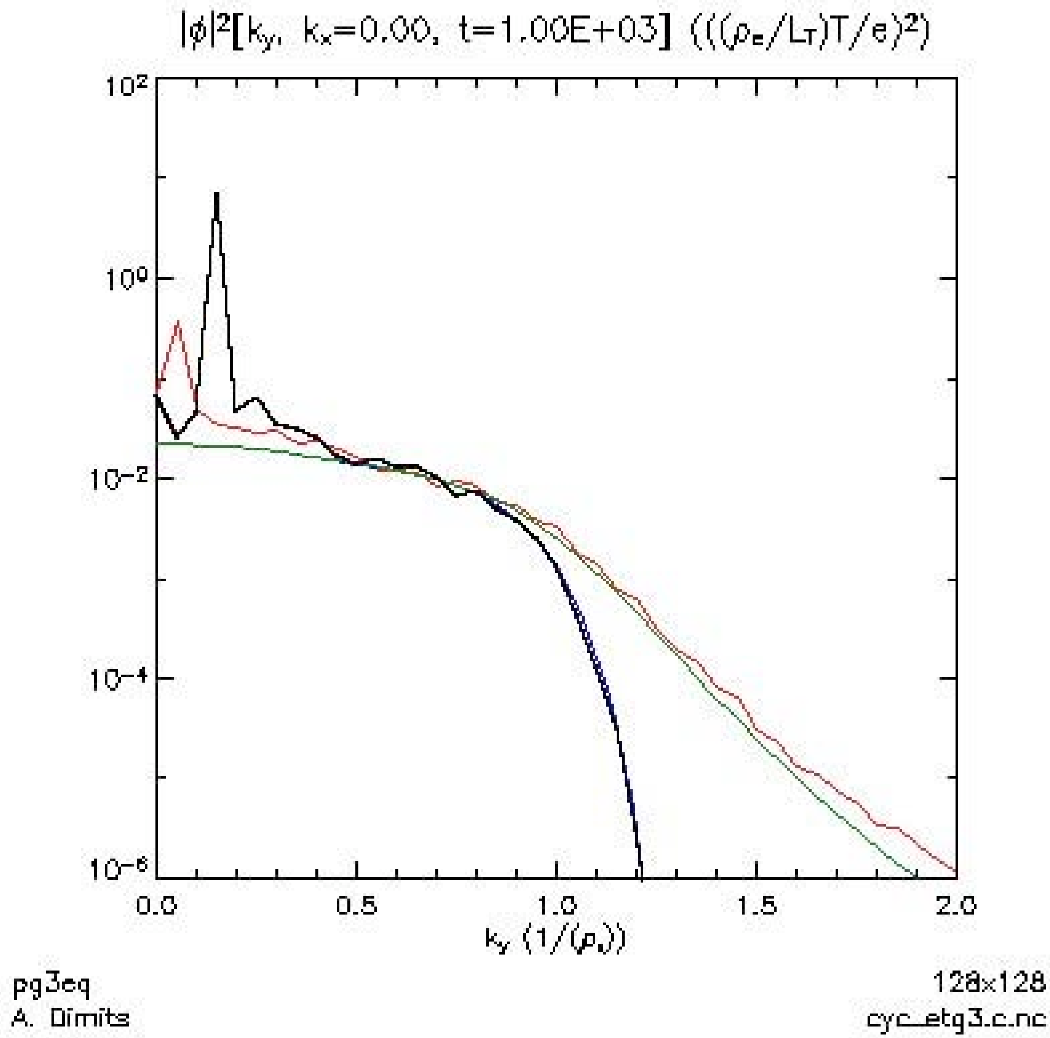
$S_\phi(k)$ from noise:

- $S_{noise}(k_x=0, k_y\quad)$ — blue
- $S_{noise}(k_x\quad, k_y=0)$ — green





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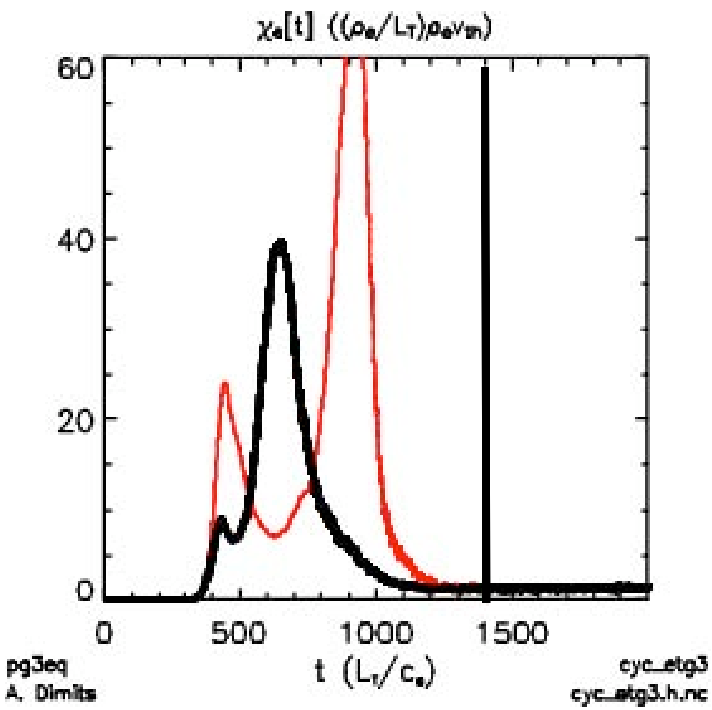
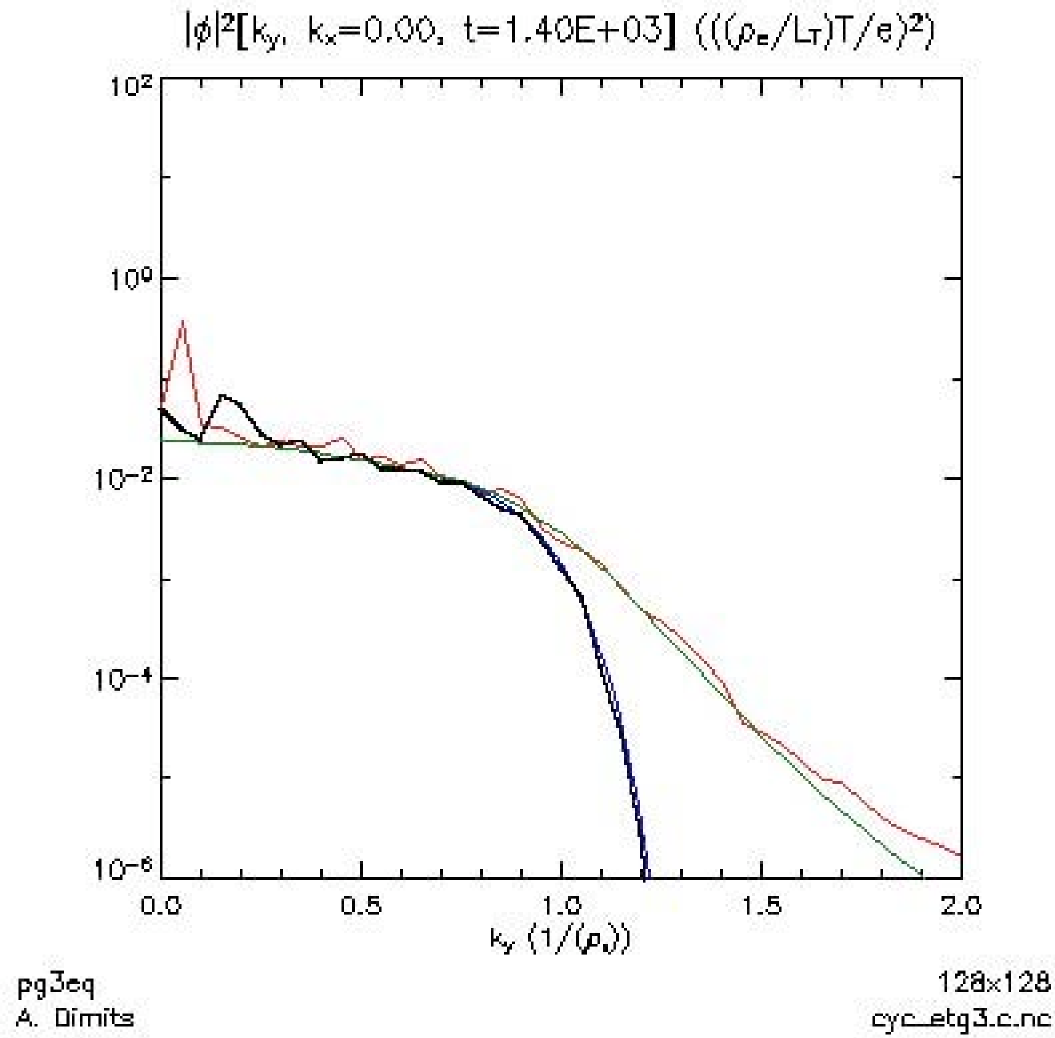
- $S_{noise}(k_x=0, k_y\quad)$ — blue
- $S_{noise}(k_x\quad, k_y=0)$ — green





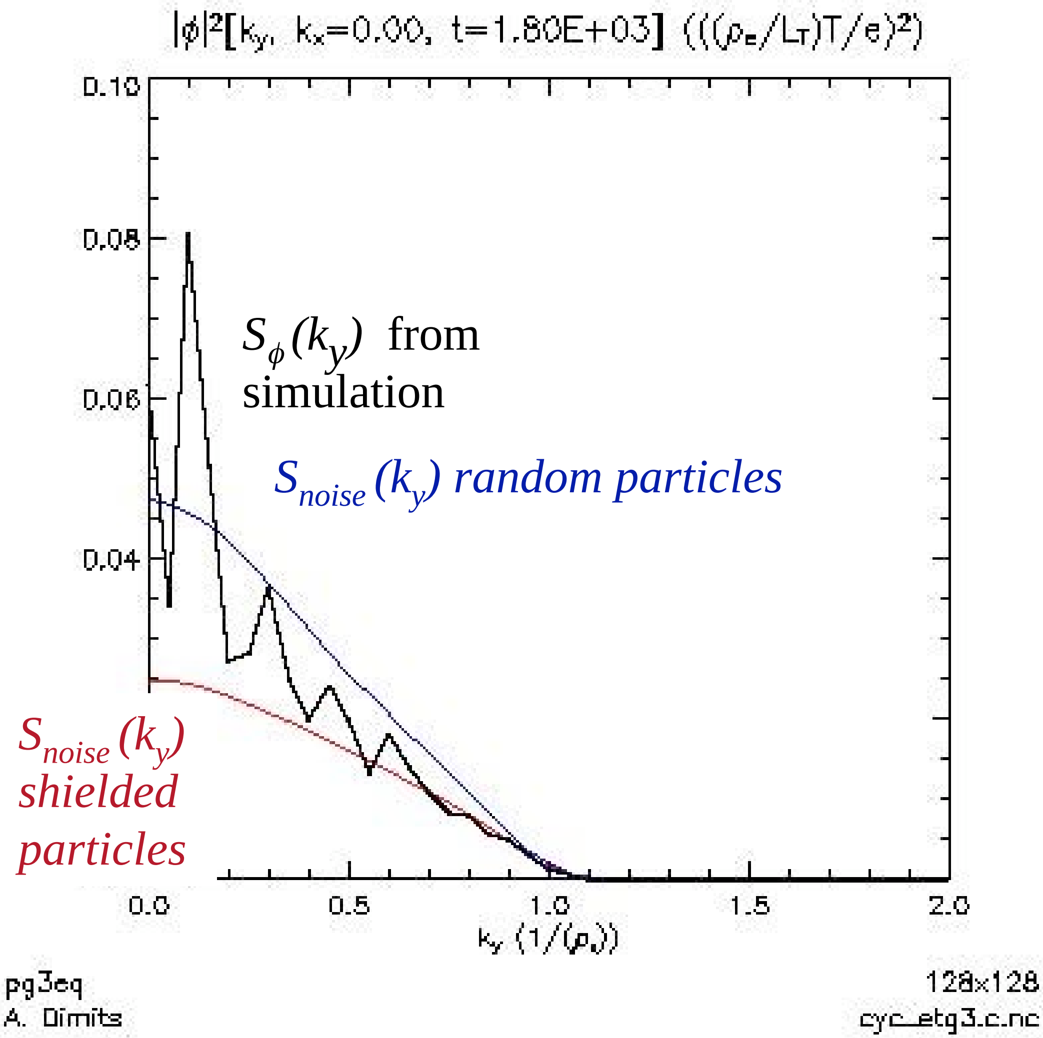
Noise calculation including shielding more accurate.

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.

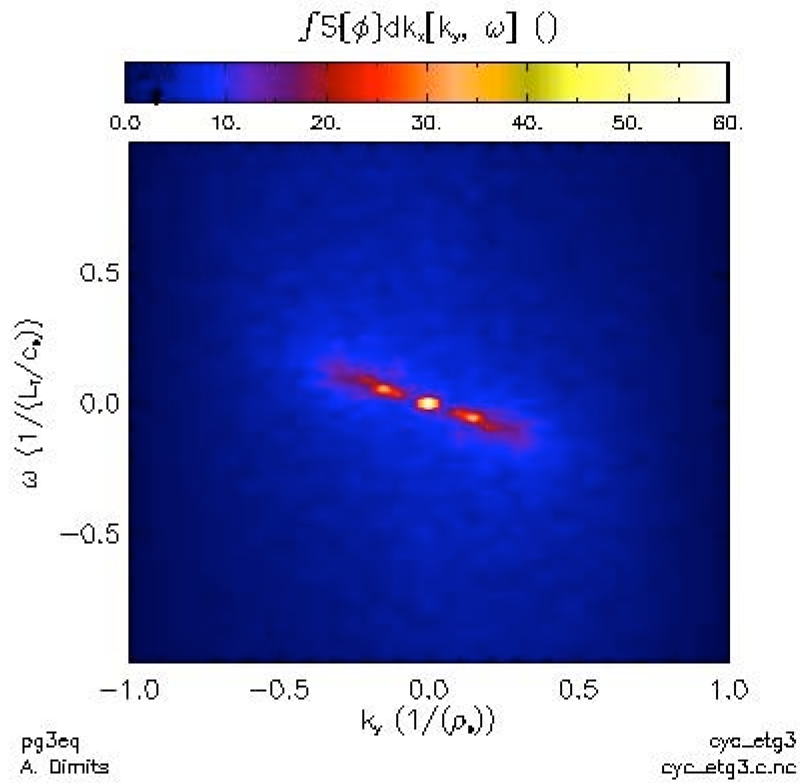
Simple noise from random particles slightly overpredicts observed spectrum.

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

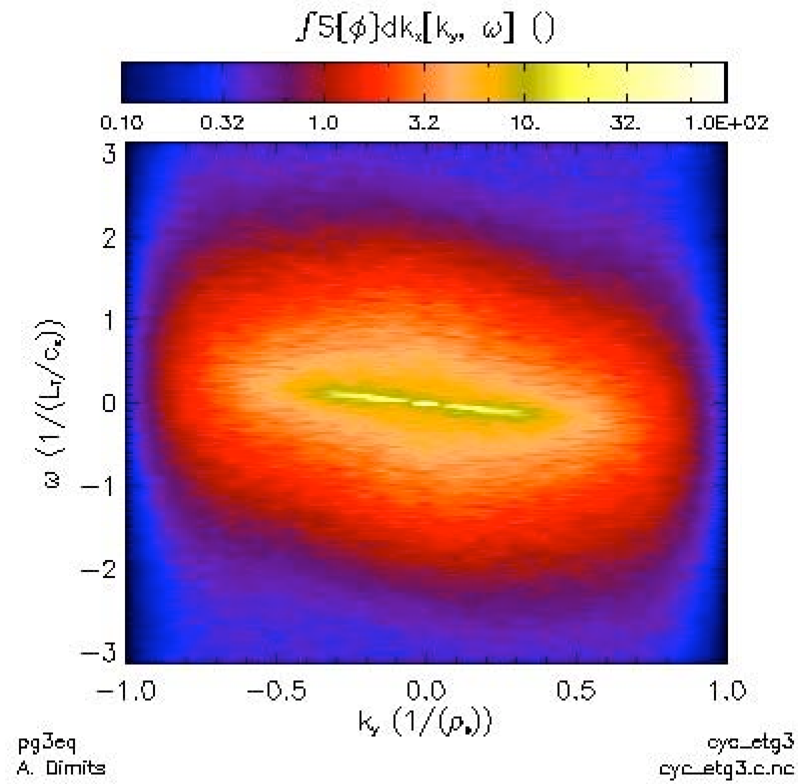


Frequency Spectrum

Drift waves at low-$k_\perp$



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



Simulation Verification (2)
The Fluctuation Intensity

A less computationally intensive diagnostic

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

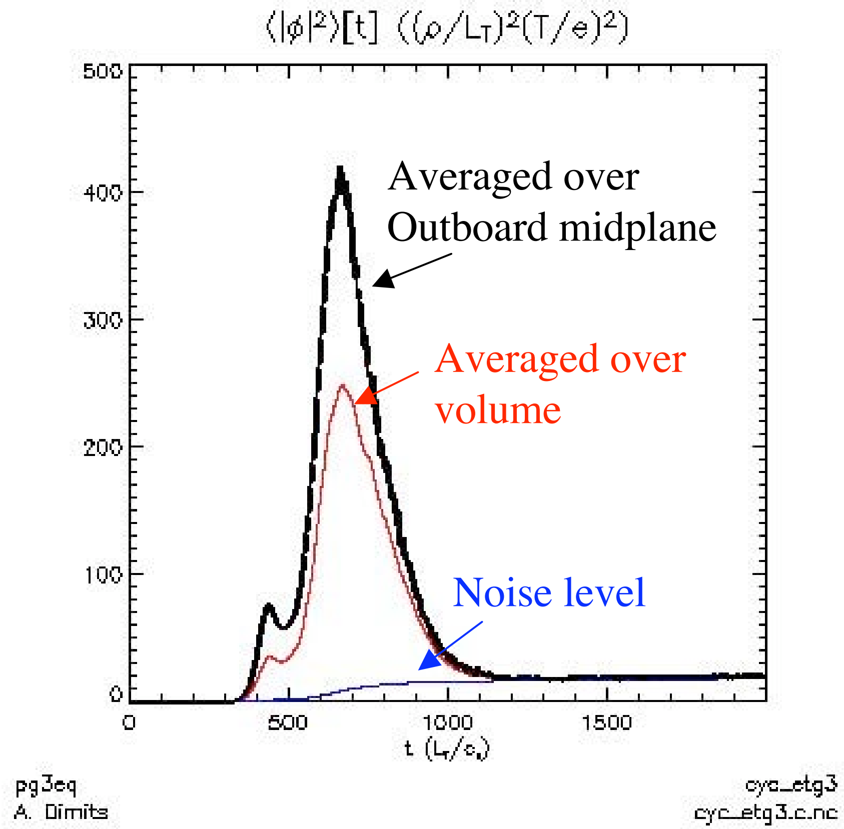
where

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

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

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

Cyclone base-case-like ETG Fluctuation Intensity



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

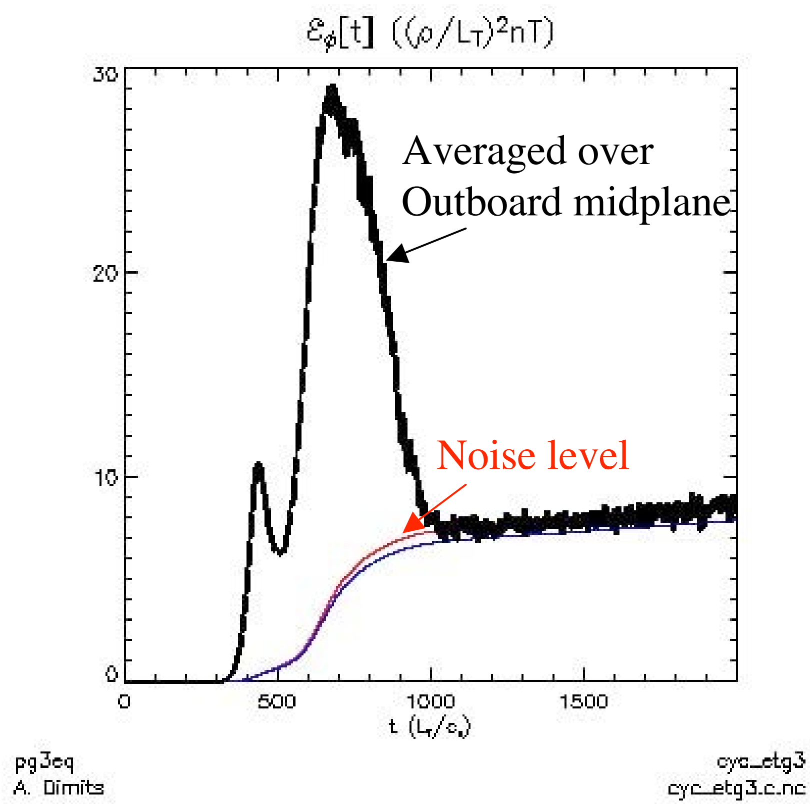
$$-\frac{\omega_p^2}{\Omega_c^2}\left\langle \frac{\phi \nabla_\perp^2 \phi}{4\pi} \right\rangle_H = nT \frac{\langle w^2 \rangle}{n_p V_{shield}} \left\langle K_\perp^2 \rho^2 \right\rangle_{noise}$$

where

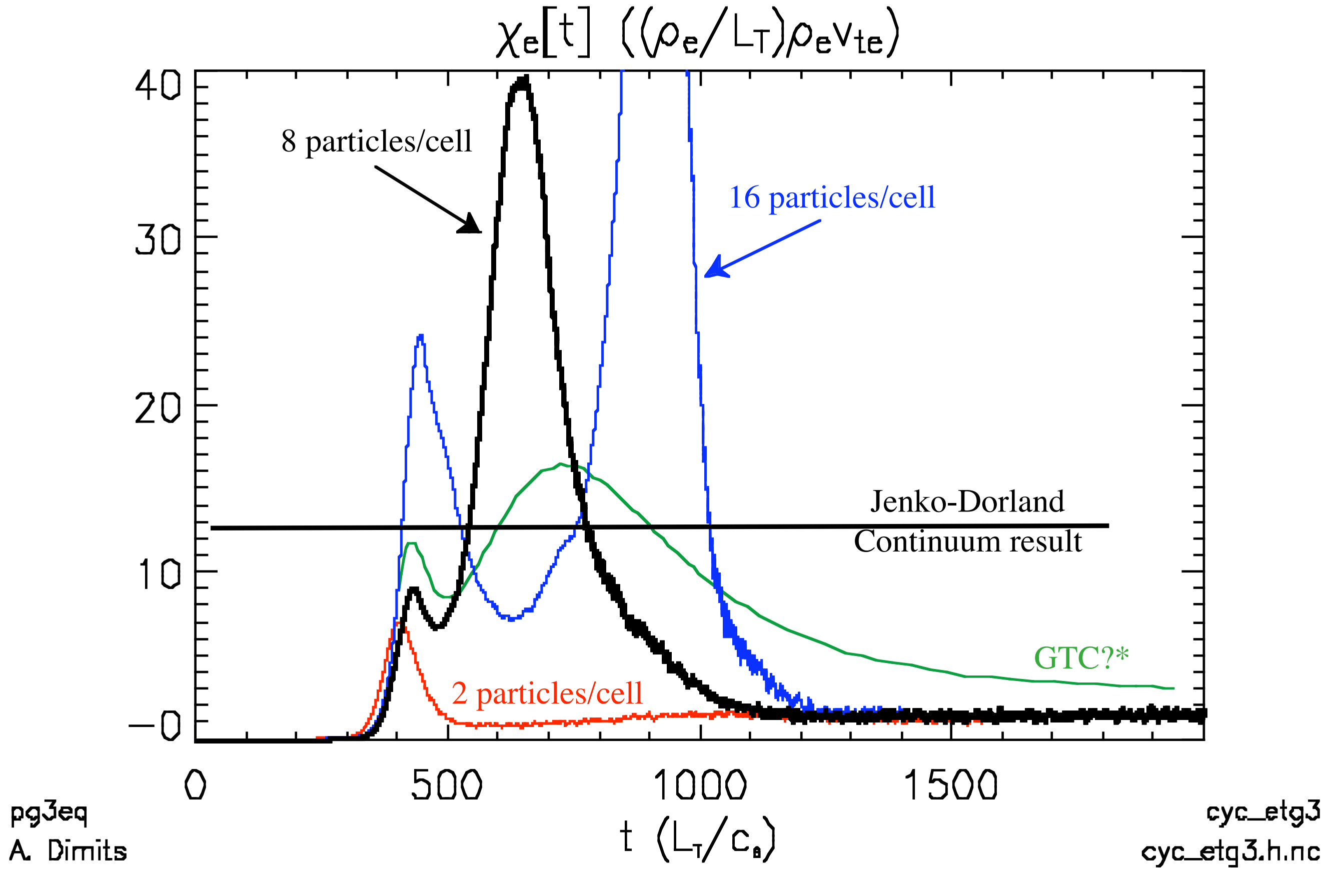
$$\left\langle K_\perp^2 \rho^2 \right\rangle_{noise}^{(H)} \equiv \left\{ \frac{V_{shield}}{(2\pi)^3} \int d^3k \frac{K_\perp^2(k)\rho^2 S_{filter}^2(k)\Gamma_0(k_\perp^2 \rho_{th}^2)}{\left[2-\Gamma_0\right]\left[2-\left(1-S_{filter}d_\parallel\right)\Gamma_0\right]} \right\}$$

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

Cyclone base-case-like ETG
Fluctuation Energy



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



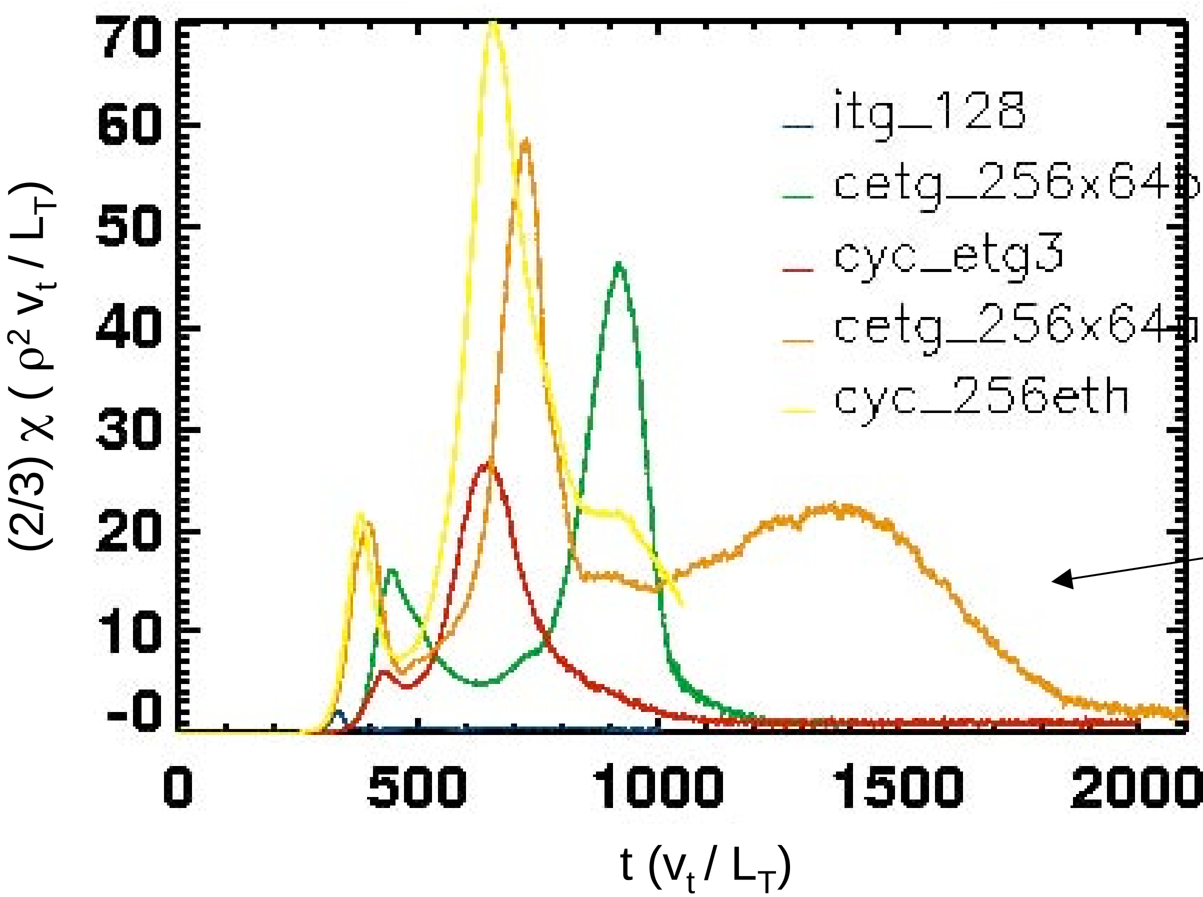
*GTC curve from Slide #13 of Z. Lin's IAEA presentation, which can be found at:
http://www.cfn.ist.utl.pt/20IAEAConf/presentations/T5/2T/5_H_8_4/Talk_TH_8_4.pdf

Particle Number Scan (above)

- Particle number scan used to decide between two hypothesis:
  - ETG turbulence vanishes for reasons unrelated to noise (leaving only discrete particle noise)
    - Above some threshold we would expect the time-evolution of the ETG turbulence to be largely independent of number of simulation particles.
  - ETG turbulence is suppressed by the noise
    - Increasing the number of particles will reduce the rate at which the noise increases. Hence, the time-duration of the burst of ETG turbulence should increase with increasing particle number.
    - ETG Turbulence suppressed at some critical value of discrete particle noise. Hence, the noise level [and, hence, $\chi(t)$] should be the same when the ETG turbulence disappears independent of the number of simulation particles.

⇒ Particle number scan supports hypothesis that ETG turbulence is suppressed by discrete particle noise

Including trapped particles extends burst of ETG turbulence (but ETG still dies at late time)



256x 64x32 r/R=0

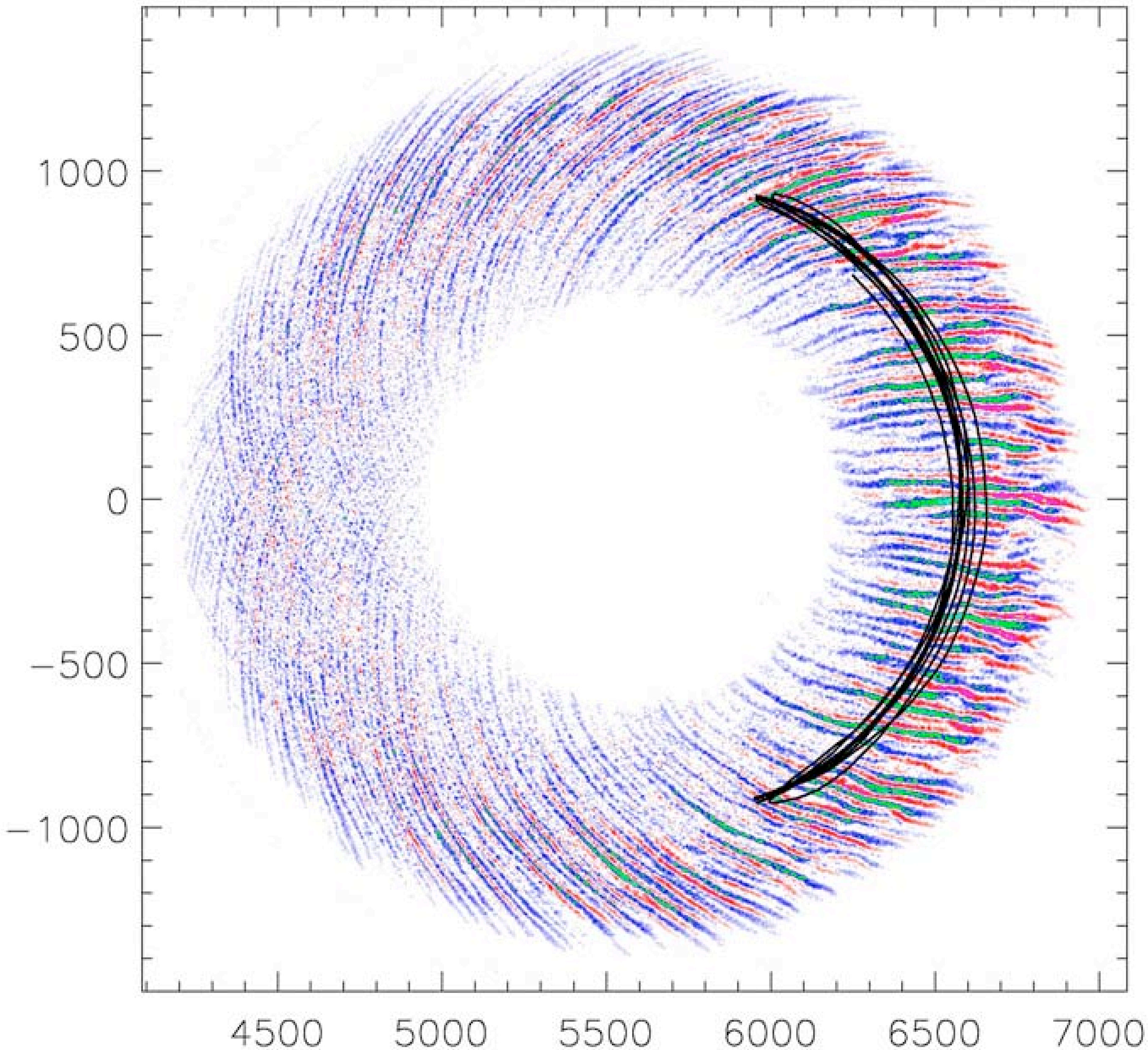
128x128x64 r/R=0

256x 64x32 r/R=0.18

256x256x32 r/R=0.18

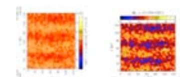
With trapped particles, spectrum shifts to lower k_θ, takes longer for noise to grow to larger level for $k_\perp{}^2 D_{noise} > \gamma_{lin}$

16 particles/cell



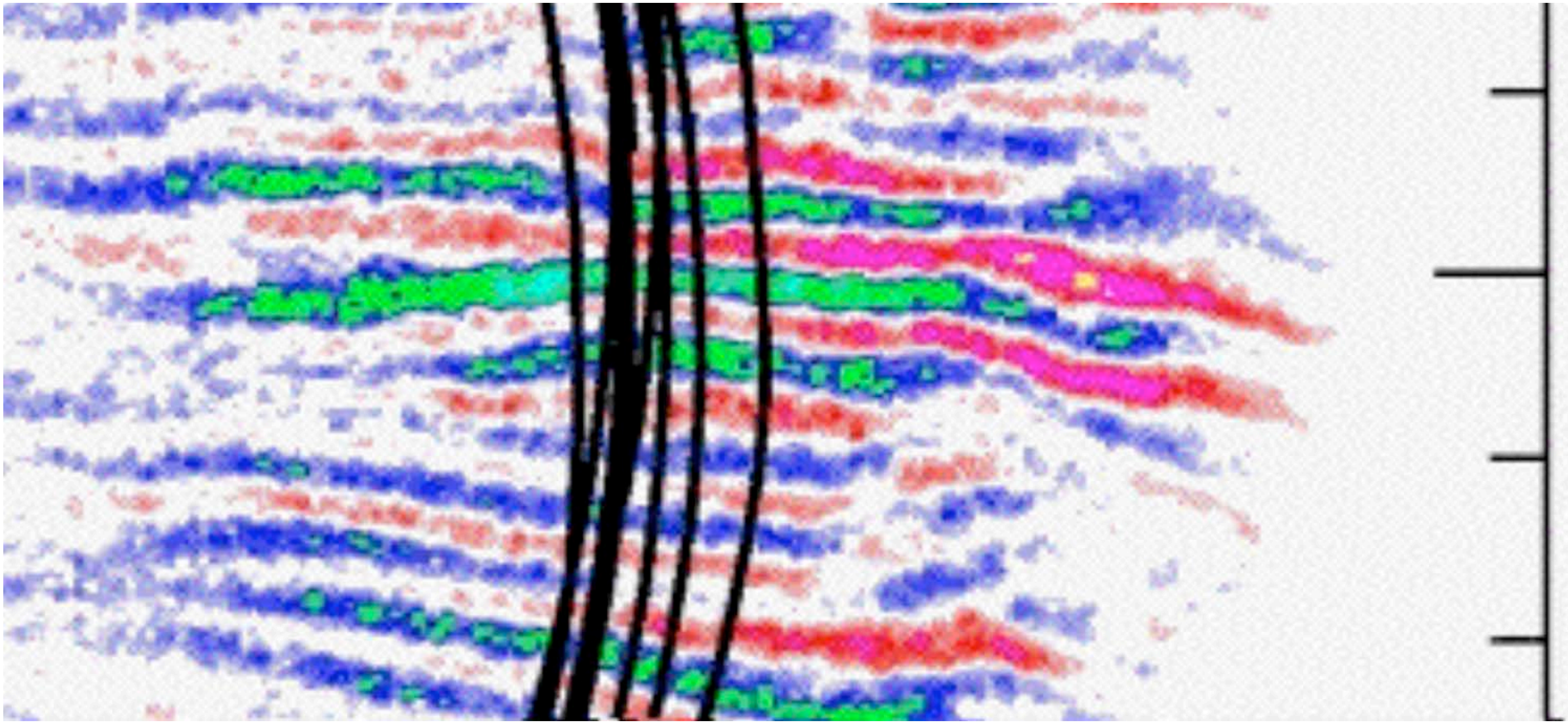
Dimits contour plots at
Same scale as Z. Lin's

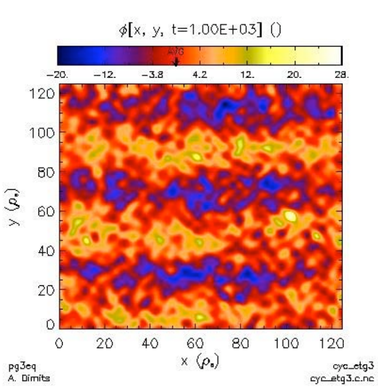
Dimits contour plot with
Re-scaled color bar

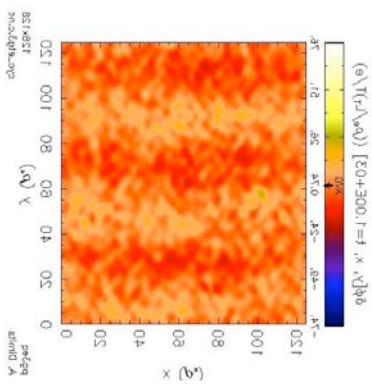


Dimits contour plot at t=1000, when χ_e ~2 x final χ_{noise}. This is when noise effects are strong enough to reduce χ_e to ~1/4th of Jenko-Dorland result, but ETG mode is still apparent.

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.



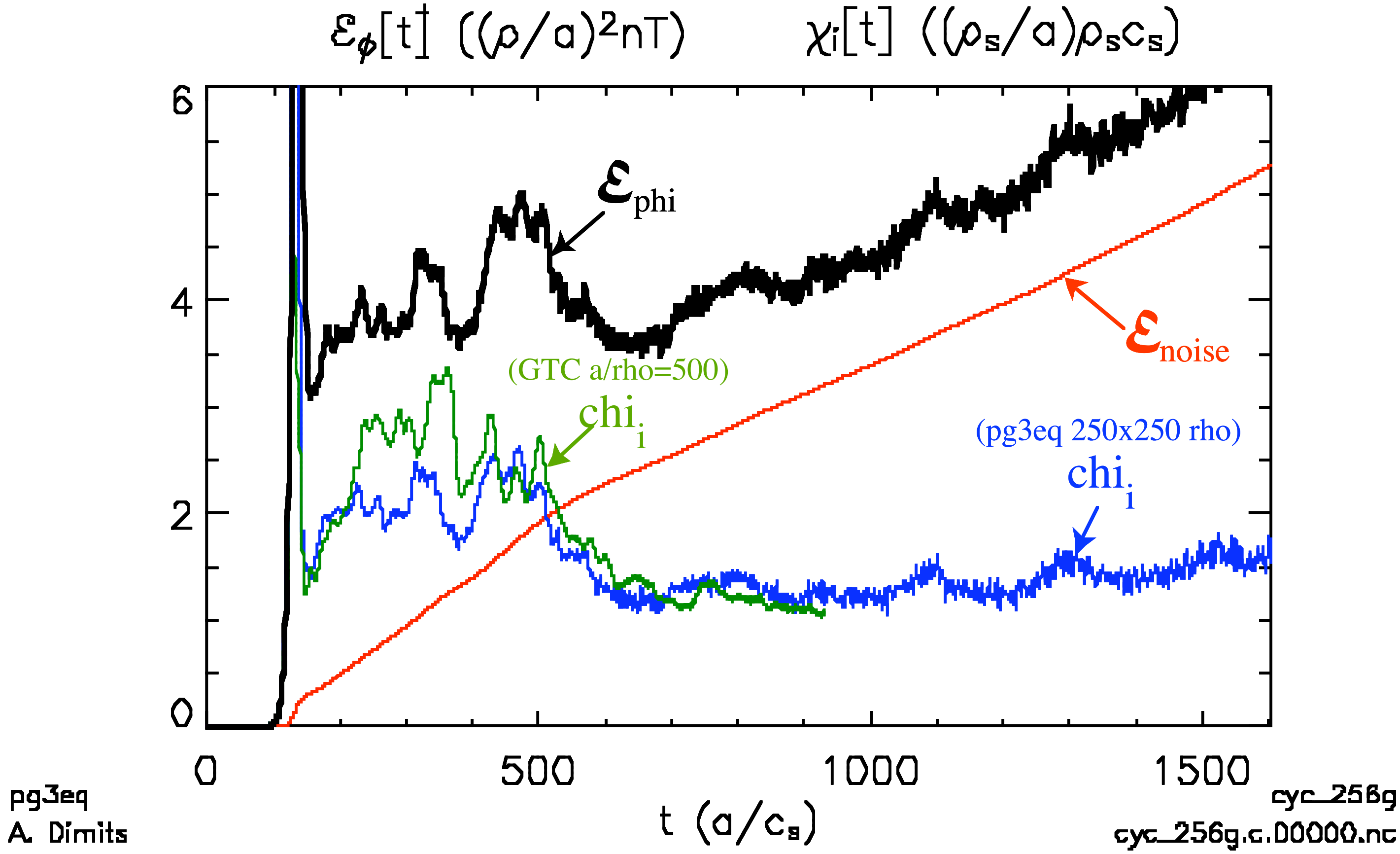




If we blow up Z. Lin's contour plot, then we can see the noise at small scales more easily. It looks roughly comparable to Dimits' contour plot at t=1000 (when χ_e ~ 2 x final χ_{noise} ~ 1/4th $\chi_{Jenko\text{-}Dorland}$.

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".

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



Summary

- Quantitative comparisons between simulation data and computed fluctuation level from discrete particles noise
  - Flux-tube simulations of ETG turbulence show:
    - ⇒ Late-time spectrum is well-predicted by noise level given measured $\langle w^2 \rangle(t)$
    - ⇒ Late-time fluctuation intensity, $\langle \phi^2 \rangle(t)$ is well predicted by expected noise level
    - ⇒ Late-time fluctuation energy is well-predicted by noise level
  - Strong similarity between flux-tube and global ETG simulations
    - ⇒ Global (GTC) simulations of ETG turbulence may be noise-dominated
    - ⇒ Verification possible with the noise-diagnostics presented above
    - ⇒ May explain discrepancy between PIC and continuum ETG simulations
  - Simulations of ITG turbulence
    - ⇒ Fluctuation energy dominated by discrete particle noise at late times
    - ⇒ May explain drop in $\chi_i(t)$ often observed at late times in PIC simulations (~50% of discrepancy between PIC and Continuum simulations of ITG)

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

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