Continuum and PIC approaches to Gyrokinetic Simulations

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with W.M. Nevins, A.M. Dimits, D.E. Shumaker (LLNL), W. Dorland (U. Maryland)
and many results borrowed from J. Candy and R.E. Waltz (General Atomics)

AST558: Graduate Seminar, May 8, 2006

http://w3.pppl.gov/~hammett/papers, Phys. Plasmas, Dec. 2005

http://w3.pppl.gov/~hammett/talks

Acknowledgments: S. Cowley, B. Cohen, F. Jenko, J. Krommes, M. Kotschenreuther

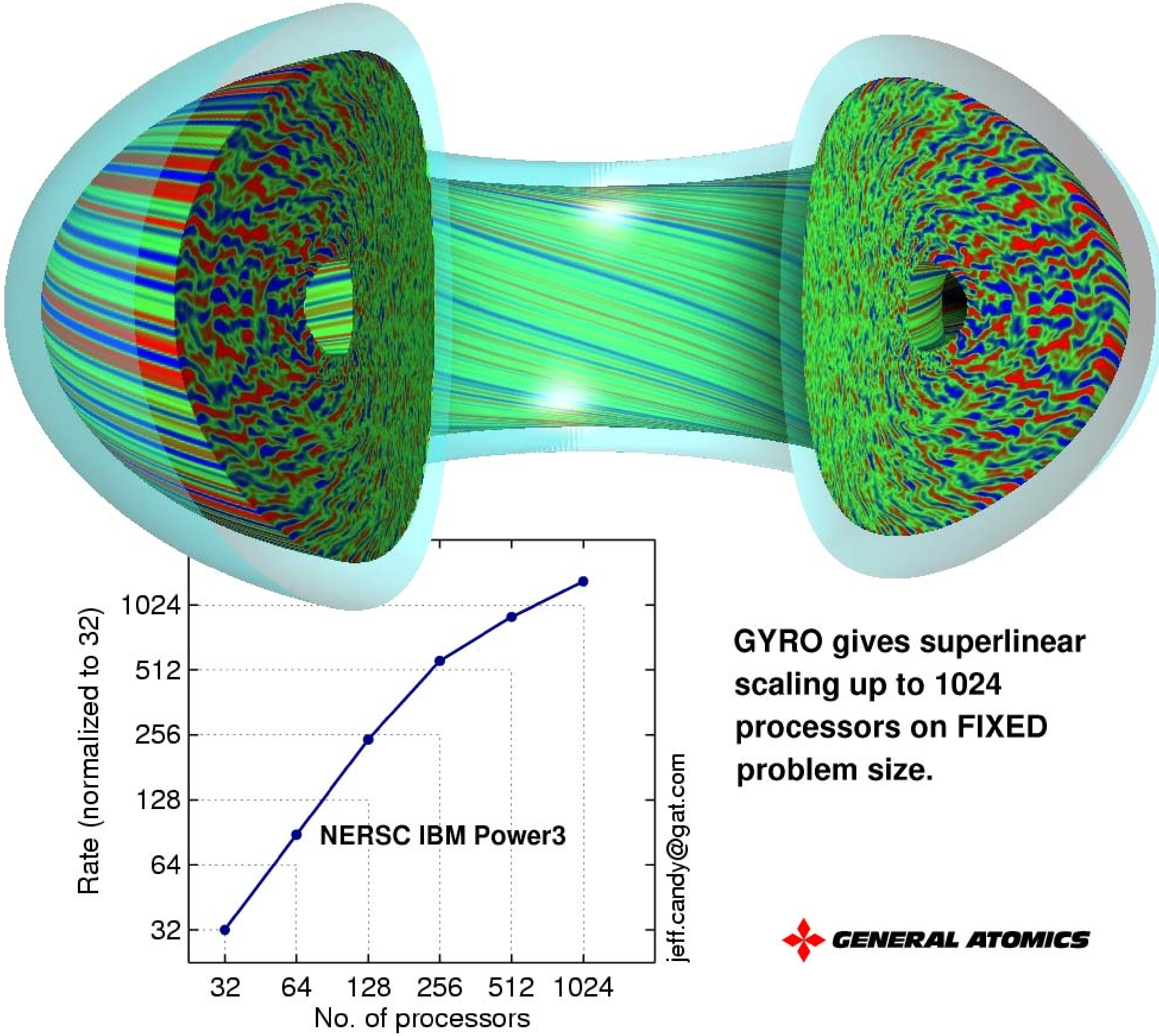
(w/ corrections on p.5)

Summary

1. Continuum/Eulerian approach to gyrokinetic simulations
   - Introduction to one class of modern advection algorithms:
     high-order upwind with limiters
   - GYRO, GS2, &GENE continuum codes
     - demonstrated that 5-D continuum approach to gyrokinetics is feasible by using the latest most powerful advanced computers and a number of clever advanced algorithms.
     - These are the most comprehensive 5-D gyrokinetic turbulence codes in existence & the most widely used in the fusion program.
   - Interesting potential grad student projects!

2. Noise issues in PIC simulations of ETG turbulence
   - A very simple 2-page derivation of noise spectrum
   - Full noise theory agrees very well with Dimits PIC simulations, resolves previous PIC/continuum differences

Note: this talk focusses on the continuum approach to gyrokinetic simulations (except for part 2). The PIC approach to gyrokinetic simulations was covered in several previous graduate student seminar talks by W.W. Lee.



Comprehensive 5-D computer simulations of core plasma turbulence developed by Plasma Microturbulence Project. Candy & Waltz (GA) movies shown: d3d.n16.2x_0.6_fly.mpg & supercyclone.mpg, from http://fusion.gat.com/comp/parallel/gyro_gallery.html (also at http://w3.pppl.gov/~hammett/refs/2004).

Basic Eulerian/Continuum Advection Algorithms

$$\frac{\partial f}{\partial t} + \frac{\partial (\mathrm{v} f)}{\partial z} = 0$$

Discrete grid, $f(z_j) = f_j$ Conservative differencing:

$$\frac{\partial f_j}{\partial t} = -\frac{\mathrm{v}_{\mathrm{j+1/2}} f_{j+1/2} - \mathrm{v}_{\mathrm{j-1/2}} f_{j-1/2}}{\Delta z}$$

Std 2cd order centered differencing (okay for smooth regions, phase errors too large for sharp-gradient regions, gives unphysical oscillations):

$$f_{j+1/2} = \frac{1}{2}\left(f_j + f_{j+1}\right)$$

1st order upwind (eliminates unphysical oscillations, but too dissipative):

$$f_{j+1/2} = f_j$$

Higher-order upwind Methods with clever monotonicity-preserving slope limiters

Reconstruct f(z) in each cell, extrapolate to bdys: $f(z) = f_j + s_j(z - z_j)$

Piecewise constant = 1st order upwind : $s_j = 0$

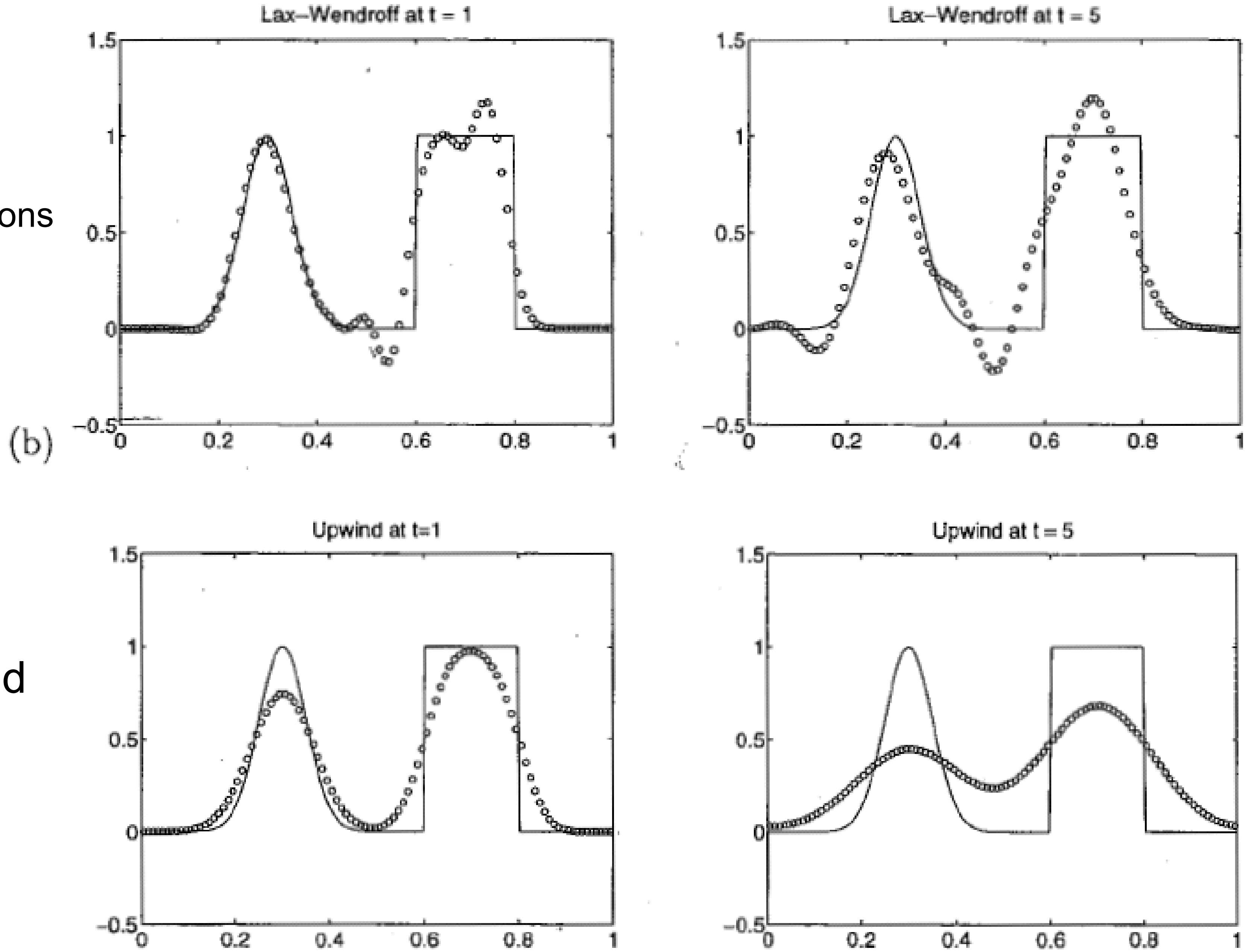
Van Leer's (MC) limiter:
"Monotonized Central"

$$s_j = \mathrm{minmod}\left(\frac{f_{j+1} - f_{j-1}}{2\Delta z}, 2\frac{f_{j+1} - f_j}{\Delta z}, 2\frac{f_j - f_{j-1}}{\Delta z} \right)$$

Advection tests

2cd order Centered
Algorithm
okay in smooth regions
Phase errors large
for sharp gradients

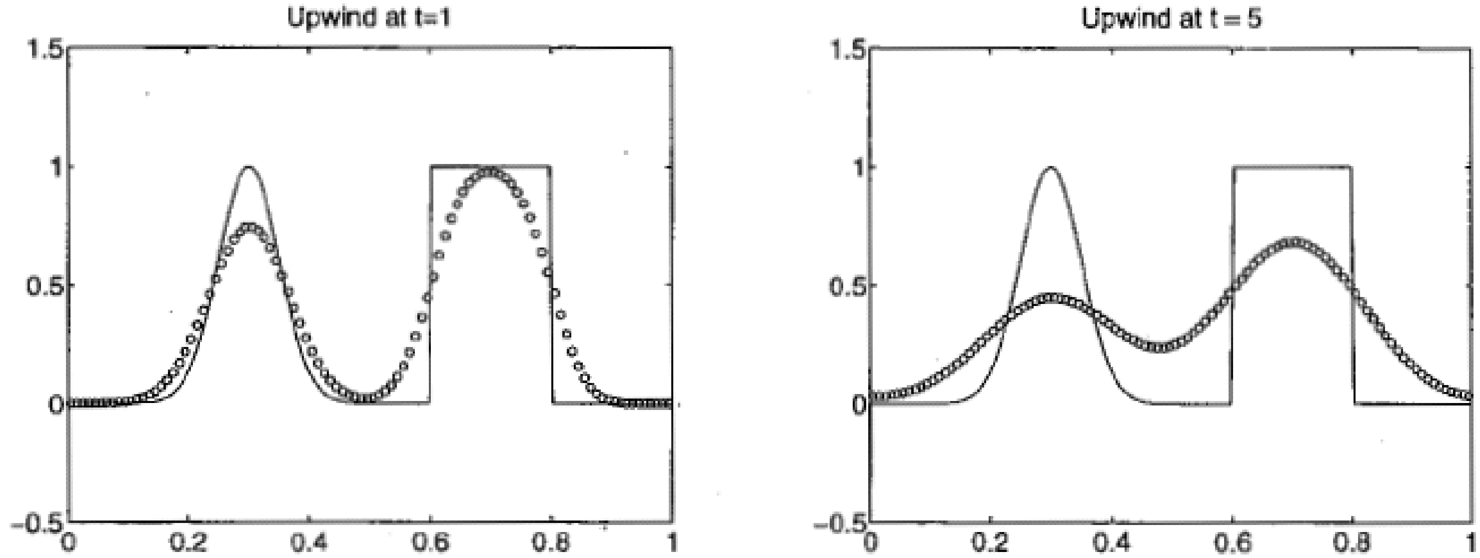
1st Order upwind
Too dissipative



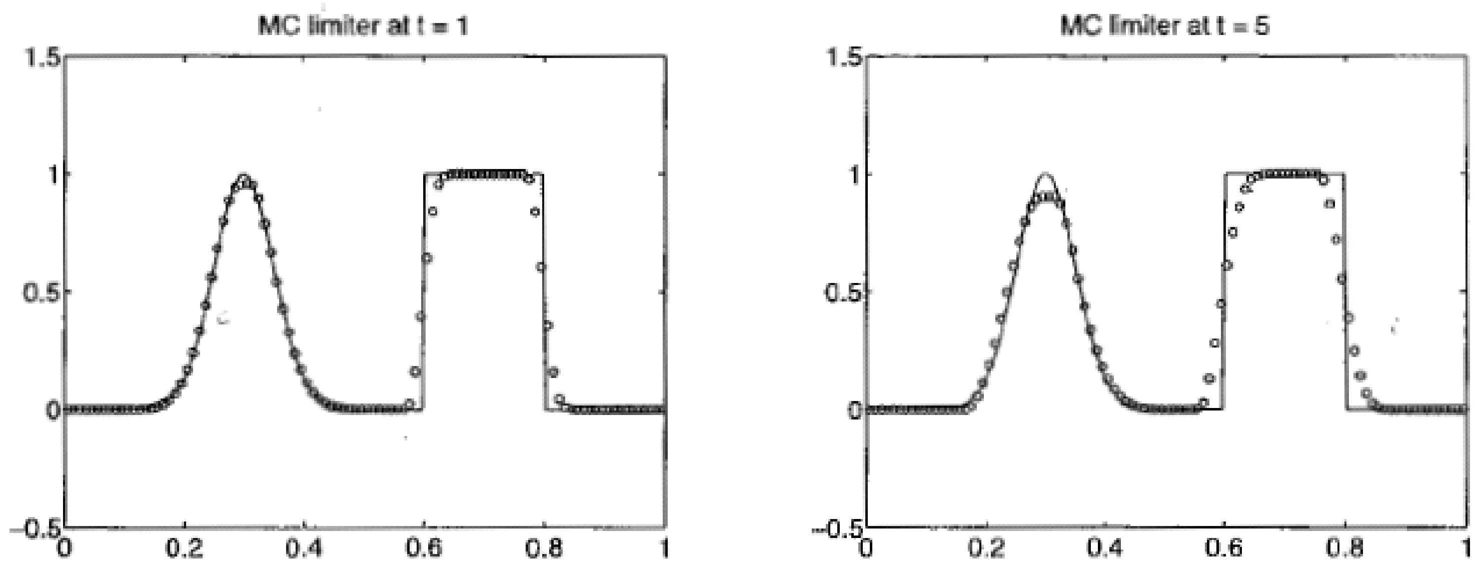
From R.J. Leveque, Finite Volume Methods for Hyperbolic Problems, Cambridge Univ. Press (2002).

Advection tests: Higher order upwind w/ limiters

1st Order upwind
Too dissipative



2cd order upwind
With MC limiter
Much better



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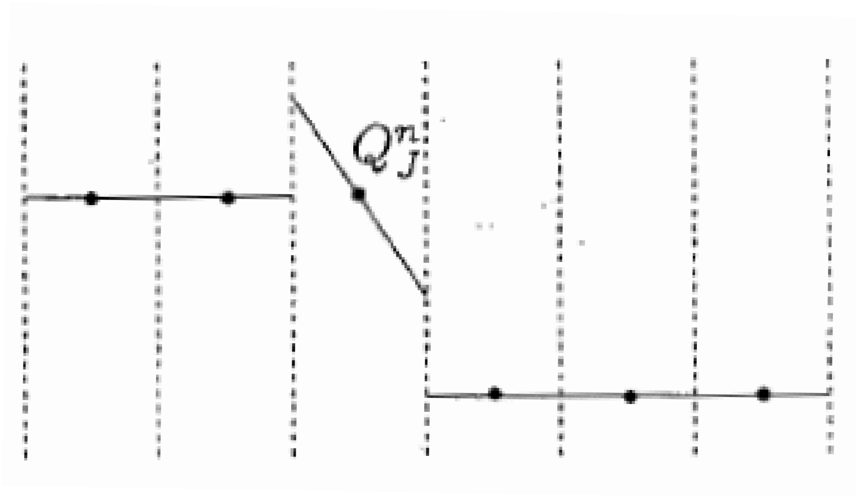


Central differencing to determine slopes can lead to overshoots in reconstruction

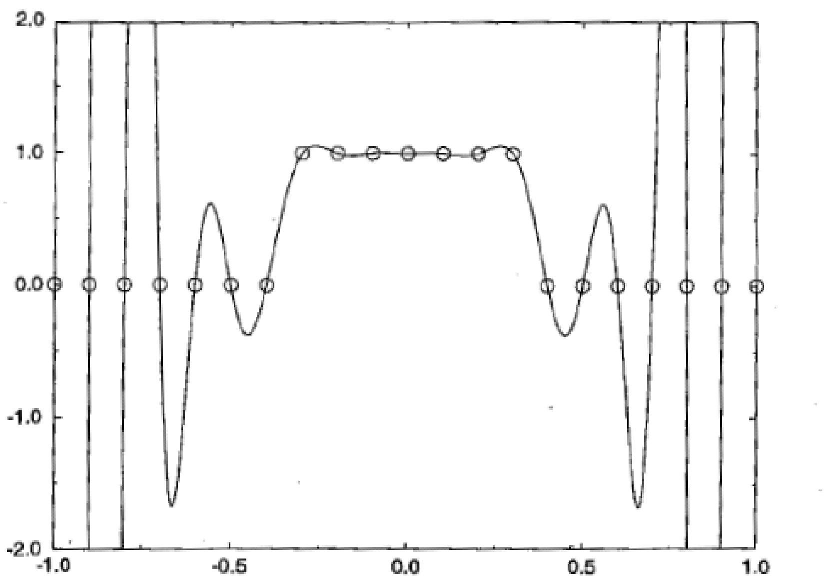
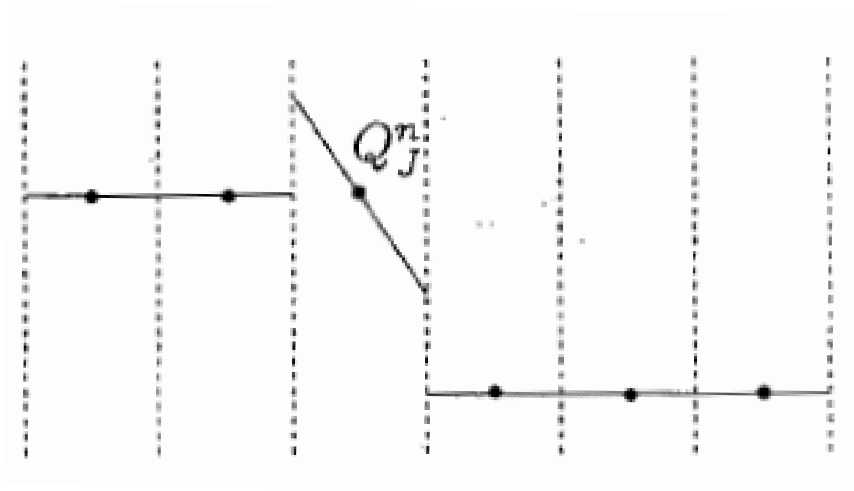


Figure 8.5 Twentieth-order polynomial interpolation for a square wave.

Just going to higher order doesn't help near sharp gradient regions (Gibb's phenomena)

Top Fig. From R.J. Leveque, Finite Volume Methods for Hyperbolic Problems, Cambridge Univ. Press (2002).
2cd Fig. From C.B. Laney, Computational Gasdynamics, Cambridge Univ. Press (1998).



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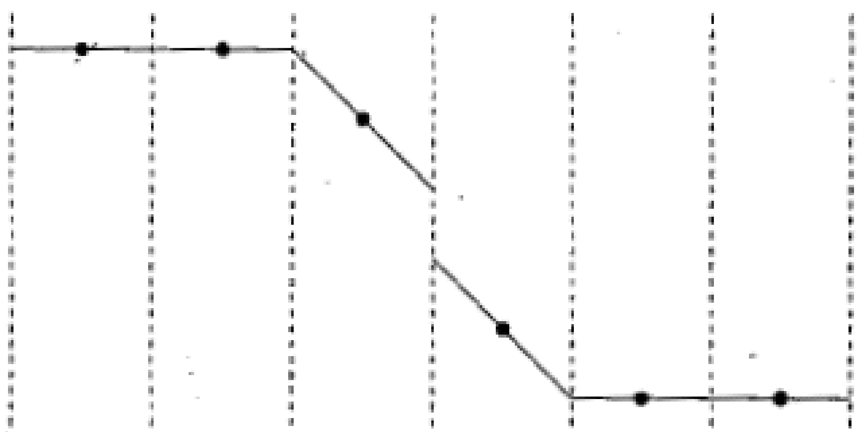


MC limiter gives much more robust result.

From R.J. Leveque, Finite Volume Methods for Hyperbolic Problems, Cambridge Univ. Press (2002).

State of the Art in CFD Codes for airplanes, etc., and astrophysical MHD where shocks can be important

- PPM Piecewise Parabolic Method (Colella & Woodward 1980's) (extension of previous high-order upwind limited method from 2cd to 3rd order)
- WENO Weighted Essentially Non-Oscillatory methods (1990's)
  - 3rd to 5th to nth order
  - Interpreted as minimizing error in a Sobolev norm ?

$$\| f \|^2 = \int dx \left(f^2 + \left(\frac{d^n f}{dx^n} \right)^2 \right)$$

  - or minimizing information entropy in the functional reconstruction?

- Higher-order Flux-Corrected Transport (Zalesak, Boris, Book) also used
- (Many other algorithms also in use for Eulerian fluid codes w/o shocks.)

Continuum/Eulerian Approach to Electromagnetic Gyrokinetic Turbulence

GS2 (Dorland & Kotschenreuther), GENE (Jenko), and GYRO (Candy & Waltz) have demonstrated that direct Eulerian simulations of microturbulence using the 5-D electromagnetic gyrokinetic equations can be effective, by

(1) Using modern massively parallel supercomputers and clusters, and

(2) Using modern advanced algorithms, including

- implicit / semi-implicit methods (or carefully designed explicit methods)

- pseudo-spectral and/or Arakawa treatment of nonlinearities (preserves all 3 conservation properties of Poisson bracket nonlinearities)

- pseudo-spectral and/or high-order upwind advection algorithms: very low dissipation at long wavelengths, effective sink at small scales.

- high-order velocity-space integration algorithms,

- efficient field-aligned coordinate systems, …

Continuum/Eulerian Approach to Electromagnetic Gyrokinetic Turbulence

GS2 (Dorland & Kotschenreuther) http://gs2.sourceforge.net
GENE (Jenko) http://www.ipp.mpg.de/~fsj/
GYRO (Candy & Waltz) http://fusion.gat.com/comp/parallel/

These codes widely used by many to study plasma turbulence in fusion devices. GYRO is currently the most comprehensive gyrokinetic code available:

- Gyrokinetic ions (multiple species) & adiabatic/drift-kinetic/gyrokinetic electrons
- Trapped and passing electrons (and ions) for Trapped Electron Mode
- Pitch-angle scattering collision operator (TEM / neoclassical effects)
- Finite beta magnetic fluctuations as well as electrostatic fluctuations (important for kinetic-ballooning modes, magnetic flutter contribution to transport)
- General shaped tokamak geometry
- Equilibrium ExB and parallel velocity shear
- Finite-ρ_* effects (profile shear stabization, nonlocal transport)…

Nevertheless, a lot of interesting work remains to be done: more tests against experiments, particle transport, transport barrier formation, shaping effects, understand scalings, couple to transport codes for complete predictive ability, &:

edge simulations (new codes needed to do gyrokinetics in the edge, challenging…)

Typical Resolution for Continuum Gyrokinetics

Typical moderate-resolution parameters for GYRO:

$$f\,(\,r,\quad n_\phi,\quad \tau_{||},\quad E,\quad \lambda\,)$$
$$140 \times 32 \times 12 \times 8 \times 16 \qquad \times\ 2 \text{ species}$$

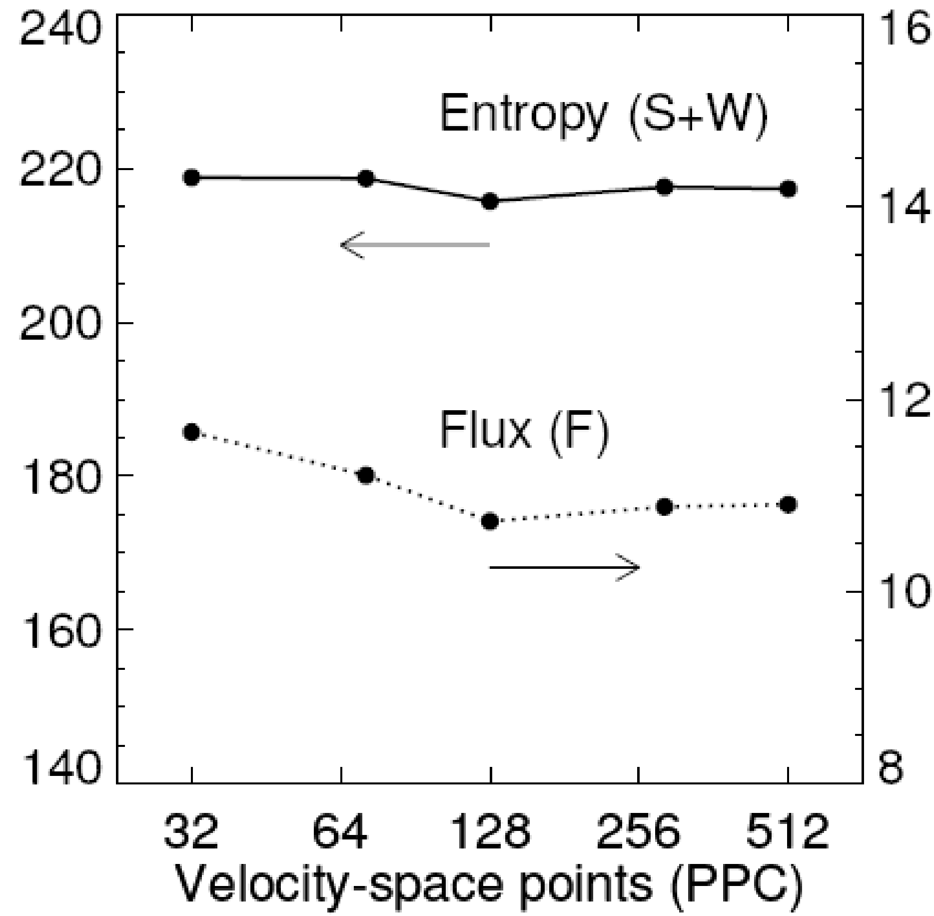
Much larger simulations also done.

GYRO well-converged w/ velocity resolution

Fluctuations in *f* cascade to small spatial scales where dissipation needed for steady state is provided by hyperdiffusion from high-order upwind algorithms.

Fluctuations in *f* also cascade to small velocity scales where collisions (or hypercollisions) are also a sink.

(Hyperdiffusion was more important in this low ν case.)



Note suppressed zeros!

Candy & Waltz, PoP 2006, “Velocity-space resolution, entropy production & upwind dissipation in Eulerian gyrokinetic simulations”
http://fusion.gat.com/comp/parallel/gyro_publications.html

A Simple Phase-Mixing Paradigm

(Carl Oberman reminded me of this view of Landau damping)

Consider simple 1-D kinetic Eq. for $f(z,v_{||},t)$

$$\frac{\partial f}{\partial t} + \mathrm{v}_{||}\frac{\partial f}{\partial z} = 0$$

(solutions of this simple equation are Green's functions for more complicated problems that could include E fields etc. on RHS)

Exact solution: $f\left(z, \mathrm{v}_{||}, t\right) = f_0\left(z - \mathrm{v}_{||}t, \mathrm{v}_{||}\right)$

Start with Maxwellian with spatial density perturbation:

$$f_0 = e^{ik_{||}z} f_M(\mathrm{v}_{||})$$

$$f \propto e^{ik_{||}(z-\mathrm{v}_{||}t)} n_0 e^{-\mathrm{v}_{||}^2/(2\mathrm{v}_t^2)}$$

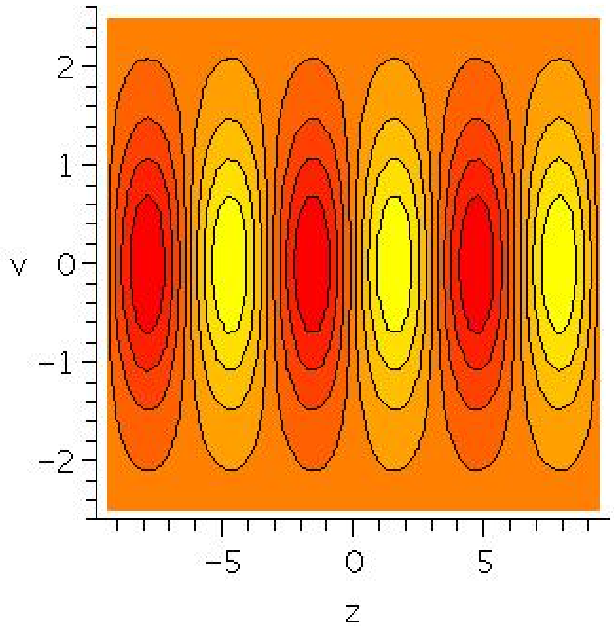
At any fixed $\mathrm{v}_{||}$, f oscillates in time with $\omega = k\,\mathrm{v}_{||}$ and no damping. However, any v-integral of f will exponentially decay in time:

$$n(z,t) = \int d\mathrm{v}_{||} f \quad \propto n_0 e^{ik_{||}z} \underbrace{\int d\mathrm{v}_{||}}_{mixing} \underbrace{e^{-ik_{||}\mathrm{v}_{||}t}}_{phases} e^{-\mathrm{v}_{||}^2/(2\mathrm{v}_t^2)}$$

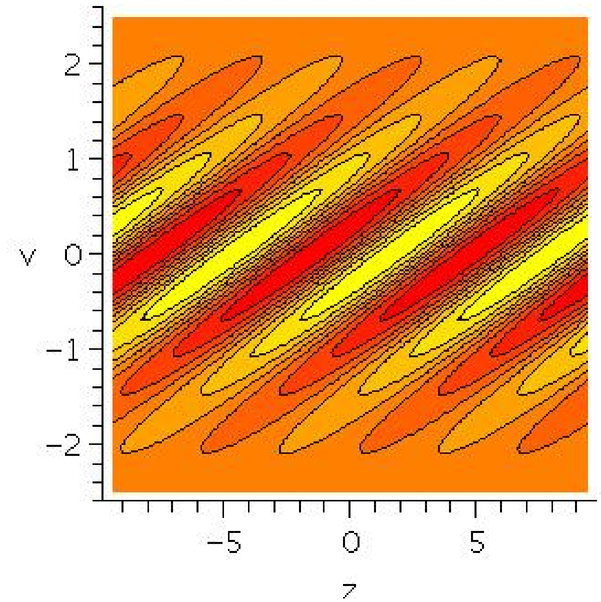
$$\boxed{n(z,t) = n_0 e^{ik_{||}z} e^{-k_{||}^2 \mathrm{v}_t^2 t^2/2}}$$

Phase-mixing -> fluid moments of *f* decay in time

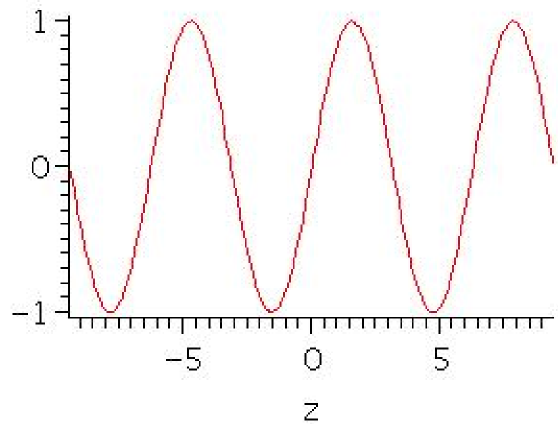
f(z,v)
t=0



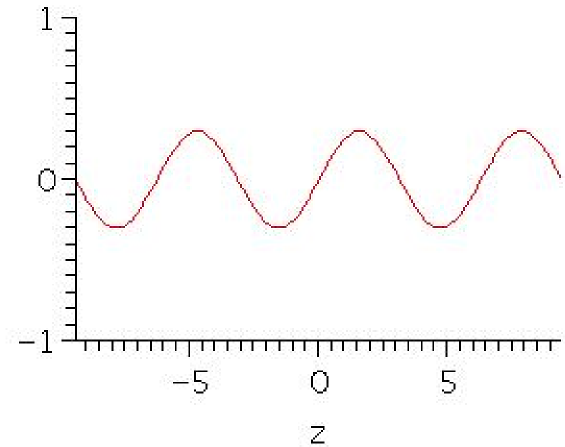
f(z,v)
t=5



n(z)
t=0



n(z)
t=1.5

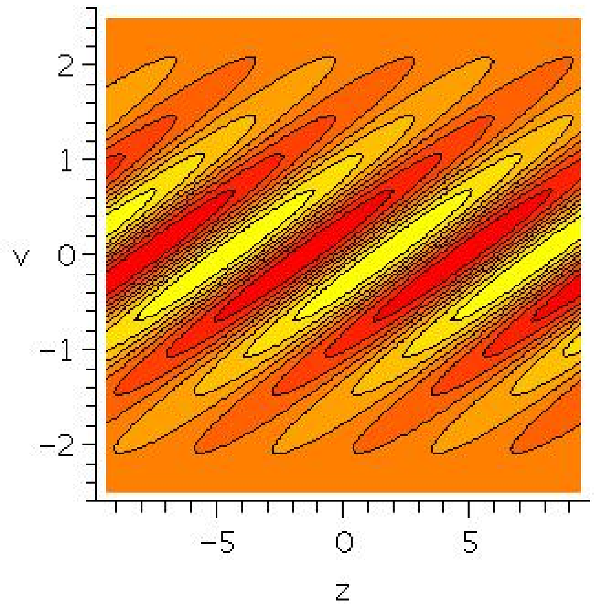


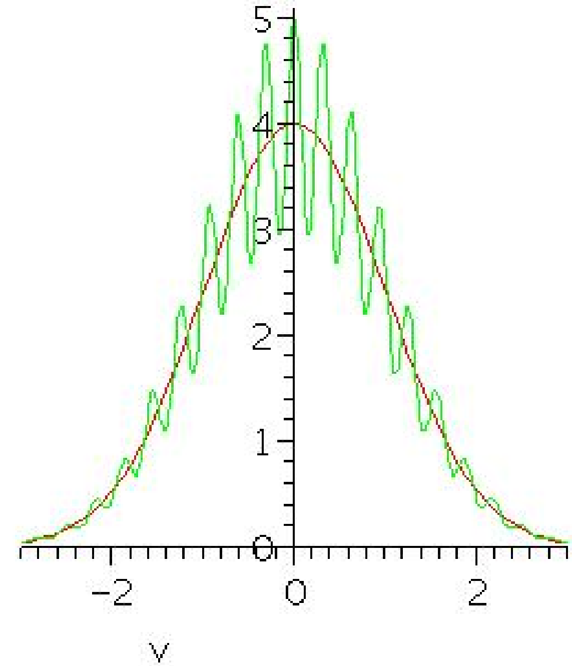
Fluid closure approximations need to introduce damping at rate ~ $|k_{||}|\ v_t$

$$\boxed{n(z,t) = n_0 e^{ik_{||}z} e^{-k_{||}^2 v_t^2 t^2/2}}$$

Phase-mixing -> very fine scales in velocity easily wiped out by a small amount of collisions

f(z,v)
t=5





At late times, $f = exp(- i\, k_{||}\, v\, t\,)\, f_M(v)$ is very oscillatory in v

Collisions dominate at time $\tau \sim (\, 3 \,/\, \nu\, v_t^2\, k_{||}^2)^{1/3}$

$$C(f) \approx \nu\, \mathrm{v}_t^2 \frac{\partial^2 f}{\partial \mathrm{v}^2} \approx -\nu\, \mathrm{v}_t^2 k_{||}^2 t^2 f$$

Full resolution in velocity requires:

$$\Delta \mathrm{v}_{||} / \mathrm{v}_t \sim \left(\nu / 3 k_{||} \mathrm{v}_t\right)^{1/3}$$
$$\sim \left(\nu_* / 3\right)^{1/3} (a/R)^{1/2} \sim 0.08$$

($k_{||} \sim 1/(qR)$ ITER $\nu_* \sim 0.008$)

Low collisionality dynamics can be simulated on an even coarser velocity grid using hypercollisions & hyperdiffusion, to damp small velocity and spatial scales

Possible Graduate Student Projects

- Numerical analysis of iterative implicit gyrokinetic algorithms and physics-based preconditioners
  - kinetic theory with discrete analog of Z-function
  - use insight into physics to try to develop fast approximations…

- Development of a continuum kinetic-MHD version of Stone's ATHENA astrophysical MHD code (start with 1-D + 2-V) drift-kinetic f…

- Work with new edge gyrokinetic turbulence simulation code being developed in collaboration with LLNL, LBNL (Colella), GA, …
  - Goal to eventually be very comprehensive: real geometry of open and closed field lines, kinetic w/ collisions, neutral fuelling, wall losses,…
  - Test w/ analytic/simple limits: GAMs, Alfven-waves, ITG growth rates, SOL
  - Investigate improved iterative implicit solvers
  - Compare with other existing core and edge codes

- Analytic analysis of nonlinear ETG dynamics

Part II: Noise issues

Outline

- Motivation: Jenko and Dorland continuum gyrokinetic simulations found that ETG turbulence could be large in some regimes. Recent PIC simulations by Z. Lin (IAEA 2004, APS 2004) claimed much lower ETG turbulence. Investigate particle noise as possible explanation of differences between the two simulations.

- Simple estimate of the spectrum of potential fluctuations due to a discrete number of gyrokinetic particles, shielded by an adiabatic species. Within a factor of 2 of the more detailed calculation based on an extension of Krommes' 1993 using the classic fluctuation-dissipation theorem or test-particle superposition principle.

- Noise spectrum agrees very well with Dimit's gyrokinetic PIC ETG simulations (with no free parameters!)

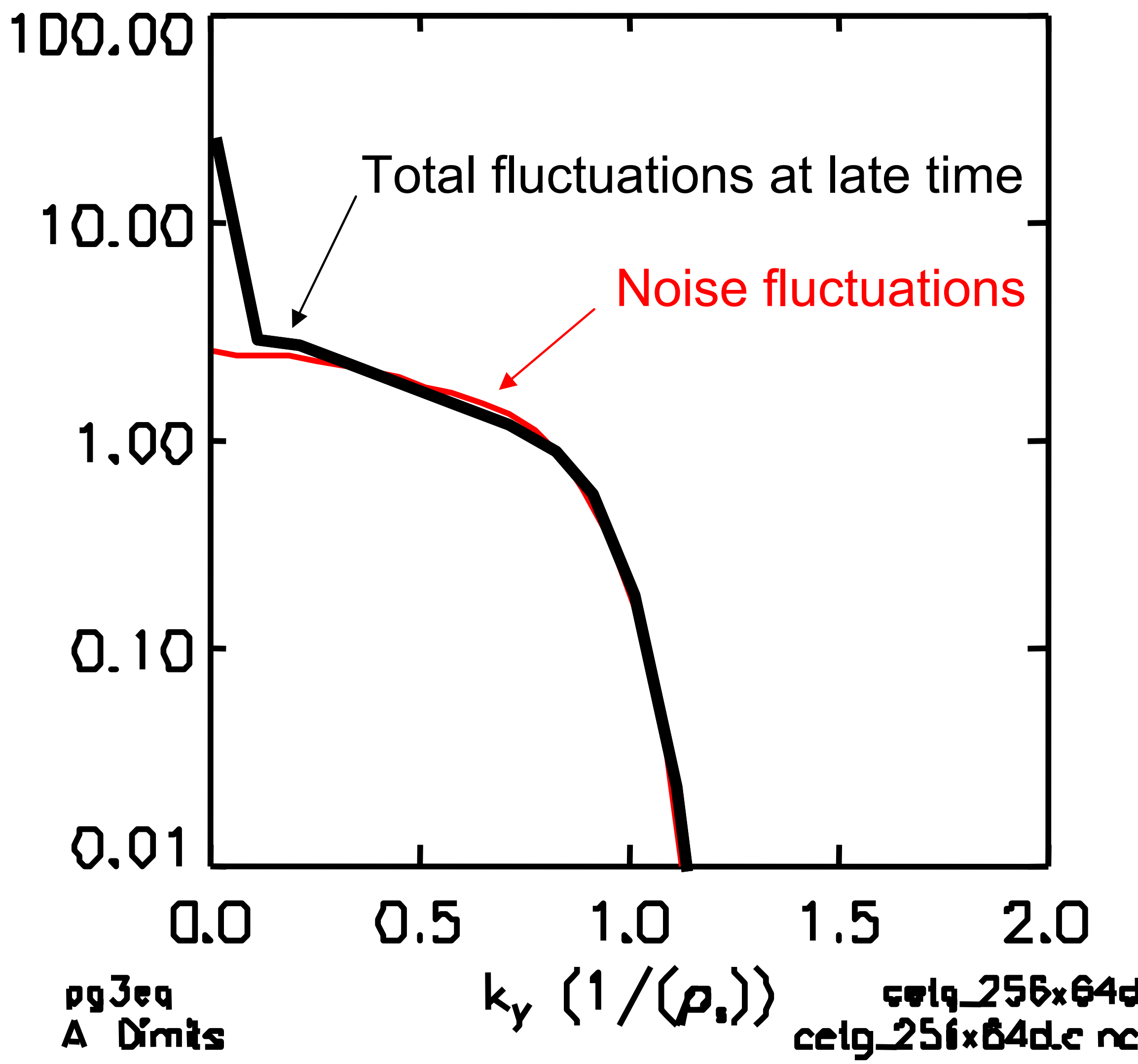
- Renormalized calculation of noise-induced ExB diffusion, D_{noise}, for a test-particle in this spectrum of random potential fluctuations. Agrees very well with observed χ at late times when noise dominates (again with no free parameters).

Predicted Noise Spectrum Agrees Well with Dimits PIC ETG Simulation at Late Times

- No Free Parameters in Theory!

- Discrete particle noise in PIC codes is quantifiable — well studied in past:
  - Langdon '79 – Birdsall&Langdon '83, Krommes '93

⇒ Useful code verification tool. We can develop objective criteria to determining when discrete particle noise is a problem



Isn't Electron Temperature Gradient (ETG) Turbulence Too Weak?

- ETG modes with $k_\perp \rho_e \sim 1$ with adiabatic ion response
  are (nearly) isomorphic to
  ITG modes with $k_\perp \rho_i \sim 1$ with adiabatic electron response
  therefore 60× smaller ?

$$\chi_i = \chi_{i0}\left(\frac{v_{ti}}{L_T}\right)\rho_i^2$$

$$\chi_e = \chi_{e0}\left(\frac{v_{te}}{L_T}\right)\rho_e^2 = \sqrt{\frac{m_e}{M_i}}\chi_i$$

- But Jenko & Dorland (PRL 2002, PoP 2000) found that isomorphism broken by
  nonlinearly by difference in ion/electron adiabatic response:
  zonal flows reduced in ETG -->

  In some regimes ETG turbulence increases: $\chi_{e0} >> \chi_{i0}$ so that $\chi_e \sim \chi_i$

Stiff critical gradients can cause $\chi_e \sim \chi_i$ even if χ_{e0} isn't as big as 60 χ_{i0}.

$$\chi_i = \chi_{i0}\left(\frac{v_{ti}}{R}\right)\rho_i^2\left(\frac{R}{L_{Ti}} - \frac{R}{L_{Ti,crit}}\right)$$

$$\chi_e = \chi_{e0}\left(\frac{v_{te}}{R}\right)\rho_e^2\left(\frac{R}{L_{Te}} - \frac{R}{L_{Te,crit}}\right)$$

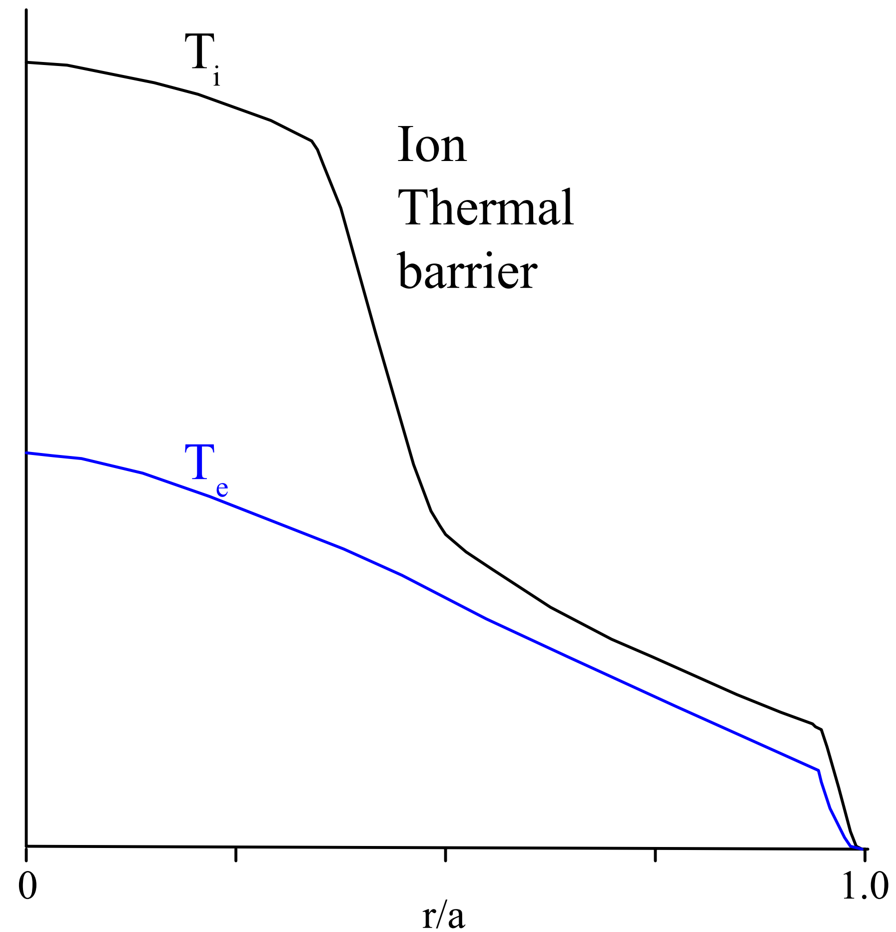
ITG threshold improved by high Ti/Te, impurity dilution
Ions may be close to critical gradient,
Electrons may be further above critical gradient

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

  ⇒Instabilities with $\lambda \sim \rho_e$



Jenko & Dorland found ETG turbulence >> ITG turbulence (in Gyro-Bohm units)

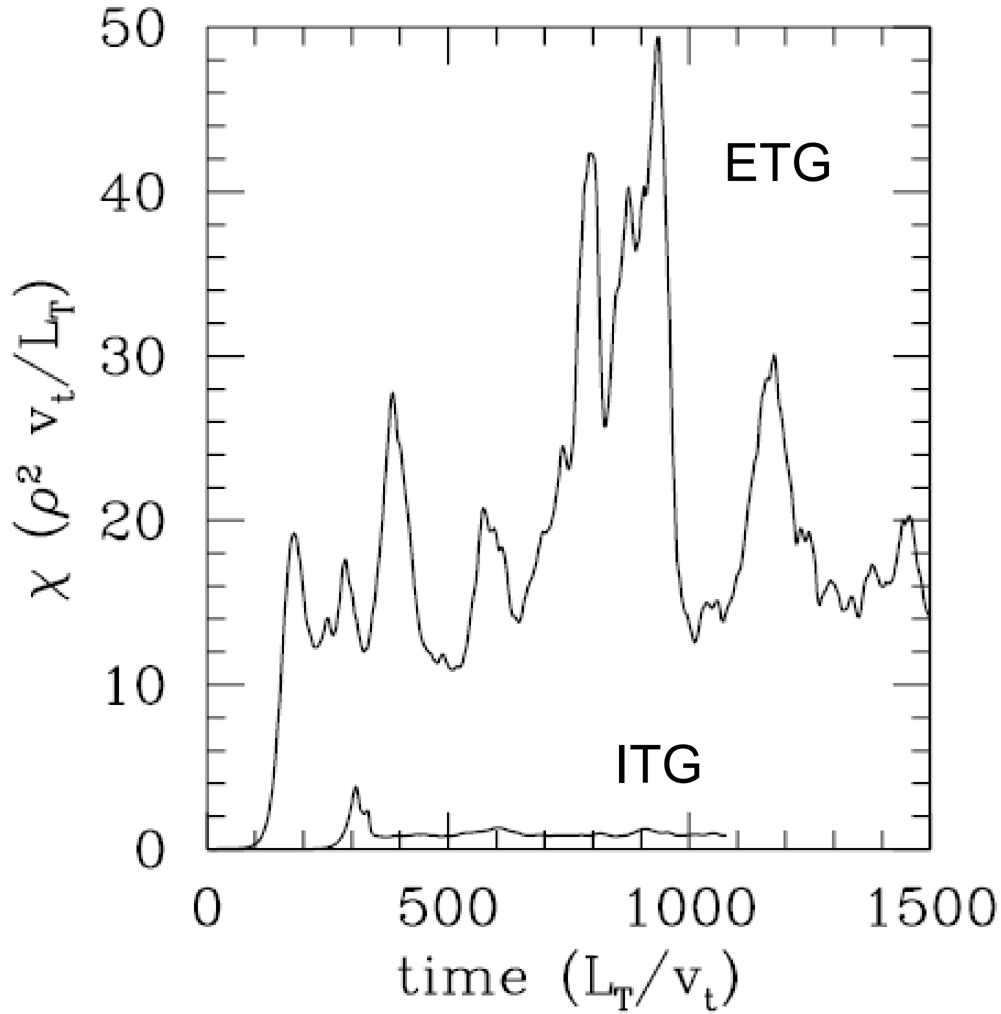


FIG. 1. χ_e^{ETG} (upper curve) and χ_i^{ITG} (lower curve) for similar parameters.

(Dorland & Jenko 2000, see also Jenko & Dorland 2002: with larger box, Lx=512 ρ, report χ_e = 13)

ETG eddies are radially extended streamers

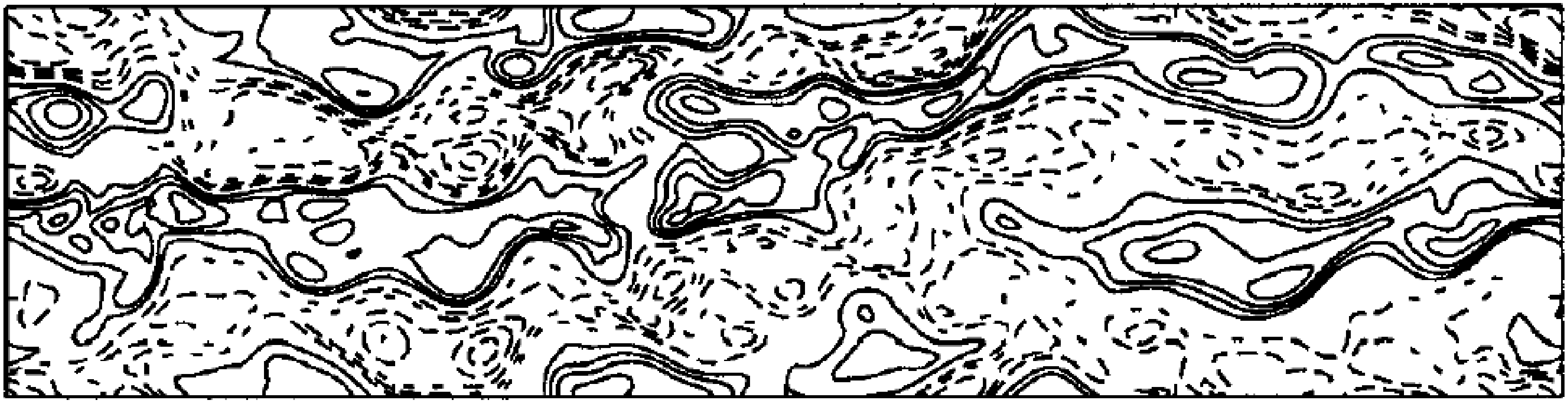


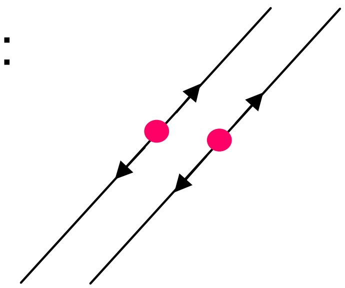
FIG. 2. Characteristic ϕ contours in the outboard x-y plane. This snapshot was taken at the end of the ETG run shown in Fig. 1. The figure is $256\rho_e \times 64\rho_e$.

High ETG transport relative to ITG transport theoretically understood as due to difference in adiabatic response for ions vs. electrons ==> reduces ETG zonal flows ==> ETG streamers get to higher velocity and are more elongated. (Rogers & Dorland, Jenko & Dorland 2000, 2002, etc.)

(Jenko & Dorland 2000)

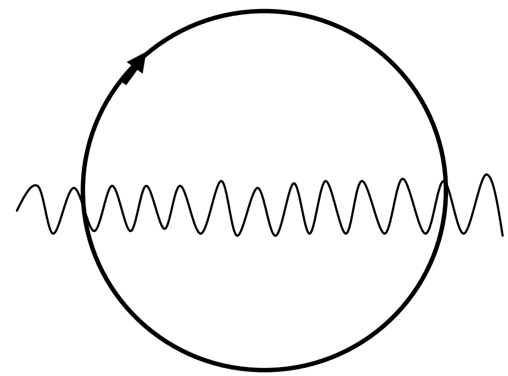
Key ITG/ETG Difference: different adiabatic response to zonal flows

ITG turbulence, adiabatic electron response:



electrons ***don't*** respond to zonal flows ($k_{||}$=0, pure E_r).
since electrons are adiabatic because $k_{||}v_{te} >> \omega$

ETG turbulence, adiabatic ion response:



Ions do shield zonal flows for ETG
Since ions are adiabiatic because $k_{\perp}\rho_i >> 1$.
↓ zonal flows --> streamers elongate --> transport ↑

Detailed secondary/tertiary instability analysis includes this, explains ITG/ETG saturation level differences, scalings (Rogers, Dorland, Jenko papers)

Key ITG/ETG Difference: different adiabatic response to zonal flows

ITG turbulence, adiabatic electron response:

$$n_e = n_i$$

$$n_{e0}\frac{e}{T}\left(\Phi - \left\langle \Phi \right\rangle\right) = \int d^3v\, J_0 f_i - n_{i0}\left(1 - \Gamma_0(k_\perp \rho_i)\right)\frac{e}{T}\Phi$$

Flux-surface averaged potential, electrons adiabatic because $k_{||}$=v_{te} >> ω don't respond to zonal flows ($k_{||}$=0, pure E_r).

ETG turbulence, adiabatic ion response:

$$n_i = n_e$$

$$n_{i0}\frac{e}{T}\Phi = \int d^3v\, J_0 f_e + n_{ei0}\left(1 - \Gamma_0(k_\perp \rho e)\right)\frac{e}{T}\Phi$$

Ions adiabiatic because $k_\perp \rho_i$ >> 1. Ions CAN shield zonal flows.
↓ zonal flows --> streamers elongate --> transport ↑

Detailed secondary/tertiary instability analysis includes this, explains ITG/ETG saturation level differences, scalings (Rogers, Dorland, Jenko papers)

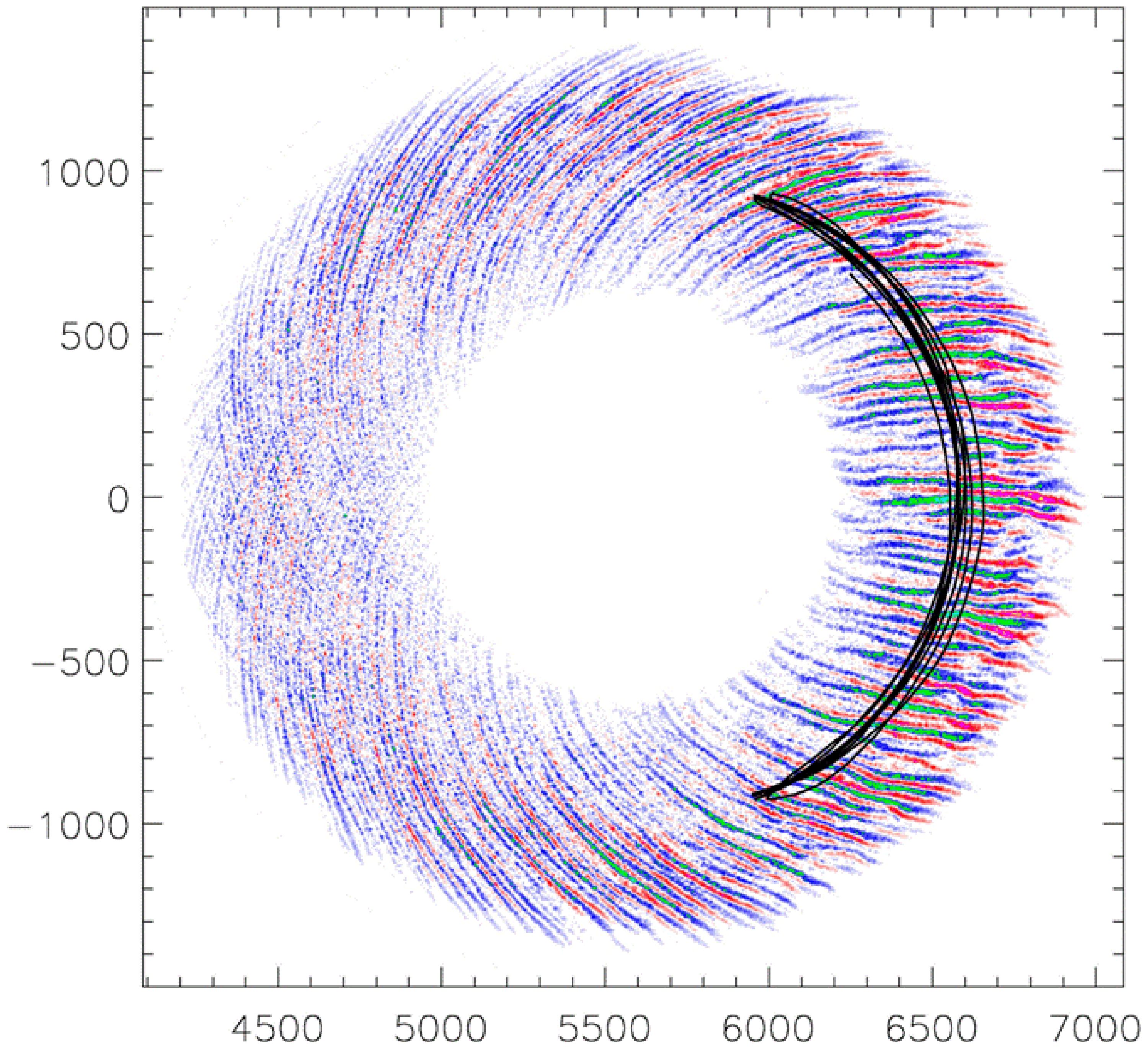
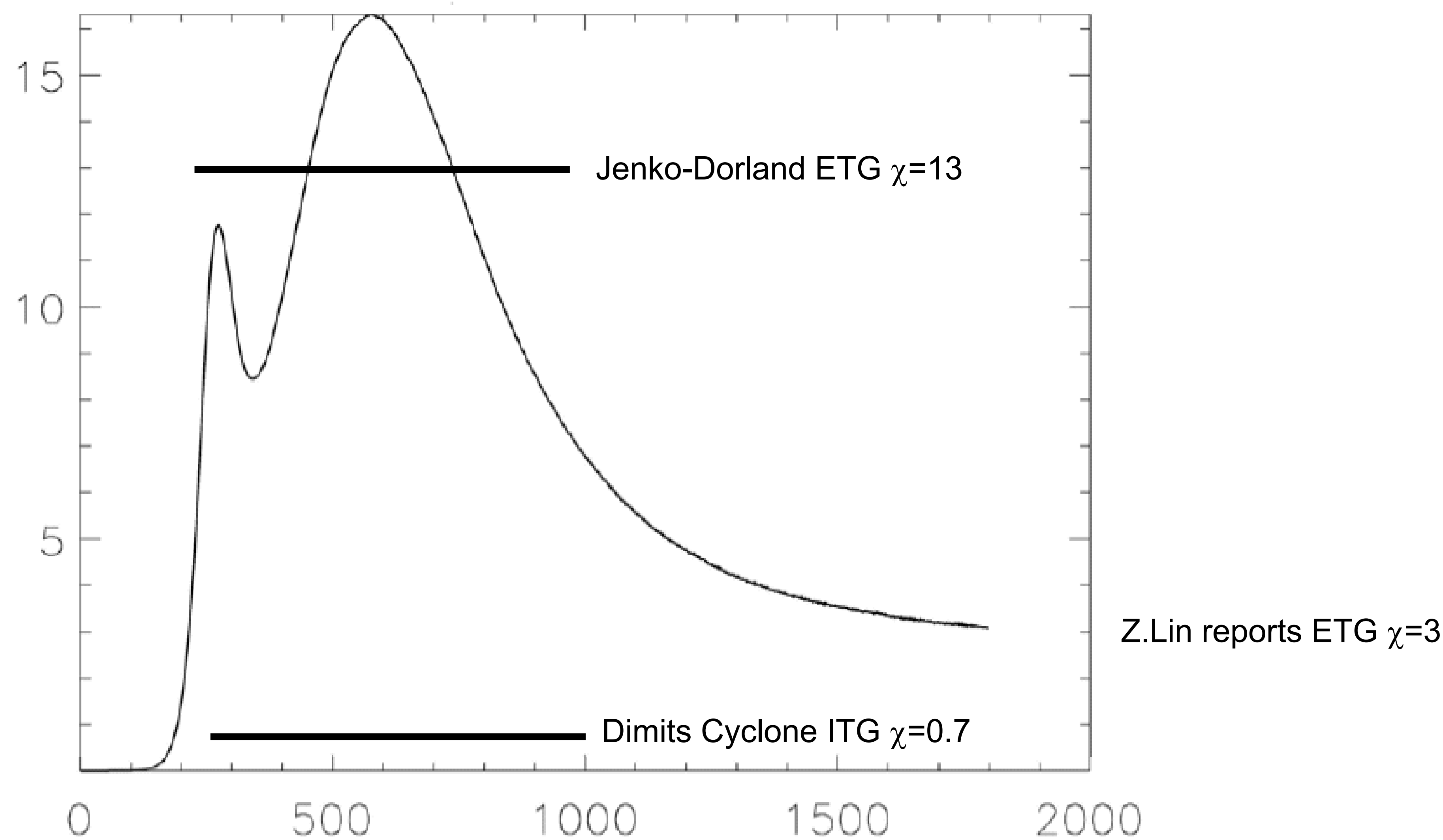


Fig. of etg streamers
from Z. Lin global PIC
simulations IAEA 2004



From Z.Lin's IAEA 2004 slides (at URL below). Believed to be χ_{etg}(t). Initial large values of χ_{etg} comparable to Jenko-Dorland 2002 χ_{etg} ~ 13. Ignoring initial "transient", reported result is χ_{etg} ~ 3. Scanned 5 to 20 particles/cell.

http://www.cfn.ist.utl.pt/20IAEAConf/presentations/T5/2T/5_H_8_4/Talk_TH_8_4.pdf

Standard approach to discrete particle noise

Particle discreteness ==> Fluctuations ==> Collision operator

Klimontovich Eq. ==> Vlasov Eq. + Collisions C(f)

diffusion in velocity
from $<\delta E^2>$ fluctuations
$\propto 1/(n\lambda_D^3)$

Gyrokinetic Klimontovich Eq. ==> Gyrokinetic Eq. + $C_{GK}(f)$

diffusion in g.c. position
from $<(\delta E \mathrm{x} B)^2>$ fluctuations
$\propto 1/(nV_{smooth})$

Various standard approaches to calculating C(f): binary collision operator cut off at Debye shielding scale, BBGKY hierarchy, etc.

Krommes' Calculation of Gyrokinetic Noise Spectrum

Krommes' 1993 calculation of the gyrokinetic noise spectrum uses the classic fluctuation-dissipation theorem, and shows equivalent results from the test-particle superposition principle (shielded test particles can be treated as independent). (see also W.W. Lee 1987, 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.

We have 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_{filt} 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.

Applying thermal noise to non-equilibrum systems

Can't directly apply Fluctuation-Dissipation Theorem or Test-Particle Superposition Principle to a linearly unstable plasma, because they use the dielectric response to calculate particle correlations and shielding, and rely on all poles being in lower half ω plane. In an unstable plasma, the linear dielectric leads to amplification of noise, not shielding.

Standard approach is indirect: use FDT or TPSP to calculate spectrum of fluctuations and the resulting collision operator C(f) in thermal equilibrium, then use that C(f) to study collisional effects on non-equlibrium problems (e.g., effects of collisions on trapped particle modes or reconnection). Good approximation if sufficient separation of time/space scales.

Our calculation of $|\Phi_{noise}(k,\omega)|^2$ spectrum and D_{noise} follow similar approach. D_{noise} dominated by high $k_\perp$ & high $k_{||}$, so a self-consistent regime exists where

$$\nu_{noise} \sim |k_{||}|\, v_t + k_\perp^2\, D_{noise} >> \gamma,\ \omega_*\, \Gamma_0$$

Alternatively, as suggested in Hu & Krommes '94, etc., one could use a renormalized nonlinear dielectric to model nonlinearly saturated turbulent system. (All perturbations decay in nonlinearly saturated system. Future work…)

Simple Estimate of Noise: Randomly Positioned Particles

Fourier conventions:

$$\Phi(\vec{x}) = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} \widetilde{\Phi}_{\vec{k}}$$

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

Within a factor of 2 of more detailed theory because one species is adiabatic, which provides half of the shielding in thermal equilibrium.

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:

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

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

Averages to zero unless i=j

Simple Estimate of Noise: Randomly Positioned Particles (II)

Average over uncorrelated random particles:

$$\left\langle \left| \frac{e\tilde{\Phi}_k}{T} \right|^2 \right\rangle_N = \frac{S_{filt}^2}{n_0^2 V^2 (2-\Gamma_0)^2} \sum_i w_i^2 J_{0i}^2$$

$$= \frac{S_{filt}^2\left(\vec{k}\right)}{\left(n_0 V\right)^2 (2-\Gamma_0)^2} n_0 V \left\langle w_i^2 \right\rangle \Gamma_0$$

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

$$= \frac{\left\langle w_i^2 \right\rangle}{n_0 V} \sum_k \frac{S_{filt}^2}{(2-\Gamma_0)^2} \Gamma_0 = \frac{\left\langle w_i^2 \right\rangle}{n_0 V_{smooth,N}}$$

Noise power 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:

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

- The fully uncorrelated spectrum (for comparison), equivalent at high k, only a factor of 2 larger at small k:

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

Test Particle Superposition with Renormalized Trajectories

Test Particle Superposition Principle: Trajectories of “dressed” test particles can be treated as statistically independent. Dominant correlations included by a shielding cloud (calculated using the plasma dielectric response) that follows each moving test particle.

Intuitive approach, usually agrees with the rigorous Fluctuation-Dissipation Theorem in thermal equilibium (Krommes’93, Rostoker, …).

Include resonance-broadening type of renormalization of test particle trajectory:

$$\left\langle \exp(-i\mathbf{k}\cdot\left(\mathbf{x}_i(t)-\mathbf{x}_i(t_2)\right))\right\rangle = \exp(-ik_{\parallel}\mathrm{v}_{\parallel,i}(t-t_2) - D_{t.p.}k_{\perp}^2\left|t-t_2\right|)$$

Renormalization important for consistently handling both
weak noise limit, where $D_{noise} \propto \Phi^2_{noise}$, and
strong noise limit, where $D_{noise} \propto \Phi_{noise}$.

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:

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

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

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

Insures no nonlinear damping of a thermal equilibrium solution (the adiabatic solution) (Catto78, Krommes81, Krommes02). Combined with using the same D_{NL} for the shielding cloud as the $D_{t.p.}$ for the test-particle trajectory, preserves the form of the Fluctuation-Dissipation Theorem.

Detailed Calculation of Noise-Spectrum Incl. Self-Shielding

Potential induced by shielded test particle density ρ_{ext}:

$$\Phi = \frac{4\pi q \rho_{ext}}{k^2 \varepsilon(\vec{k},\omega)}$$

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

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} (but D_{nl} important for getting frequency spectrum right to calculate test-particle diffusion). Resulting k spectrum:

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

Only difference from simple random-particle spectrum. $\langle \Phi_k^2 \rangle$ only 50% lower at low $k_\perp$ (adiabatic electrons already got half of shielding), equal at high $k_\perp$ (ion shielding vanishes)

Why Particle Weights Grow in Time

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

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

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

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

$$\frac{D}{Dt}\delta f = -\frac{Dx}{Dt}\frac{df_0}{dx}$$

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

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

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.

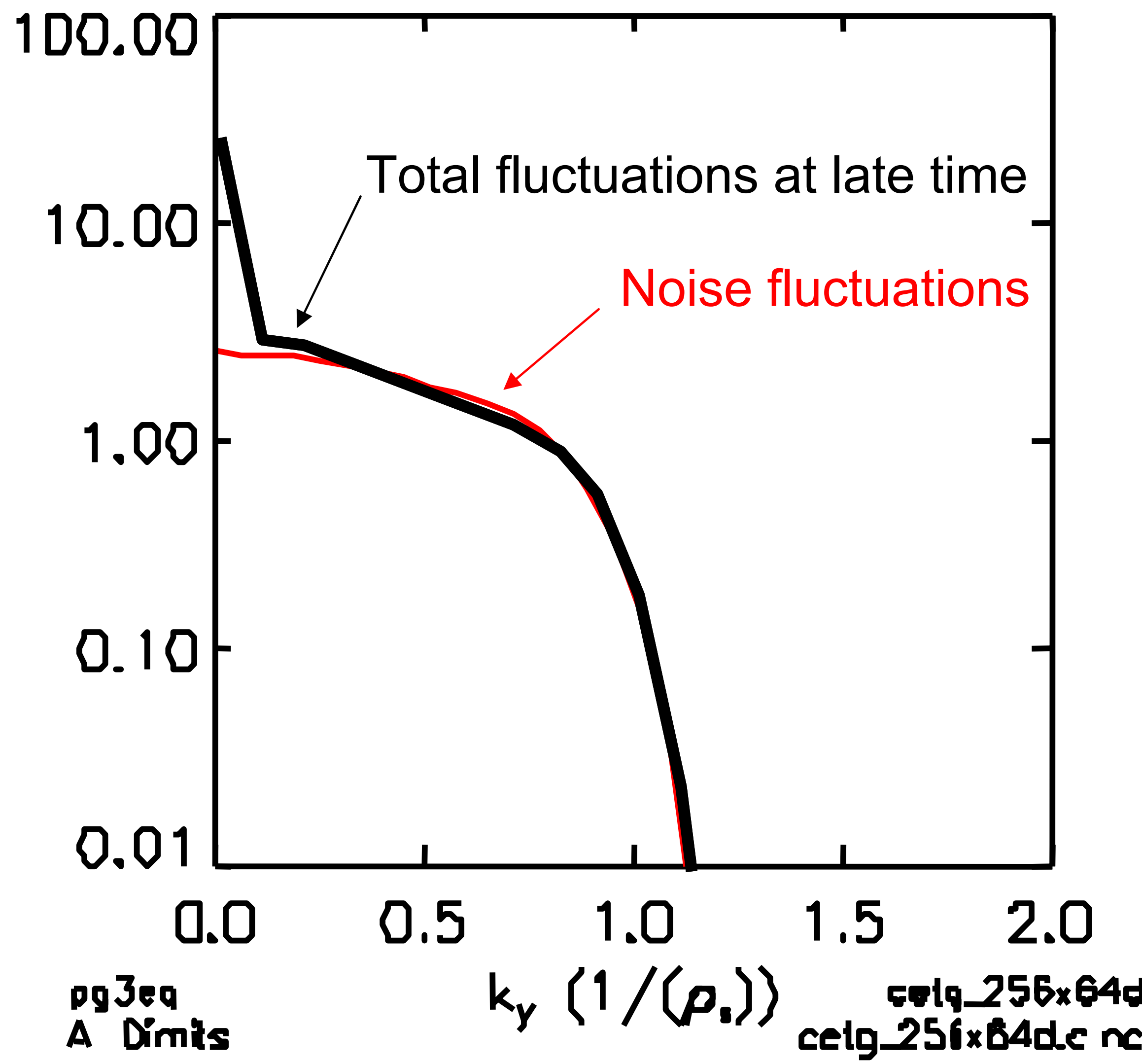
$$\frac{dw_{rms}^2}{dt} = \frac{d}{dt}\frac{\left\langle \left(\delta f\right)^2 \right\rangle}{f^2} \approx \frac{2\chi_{tot}}{L_T^2}$$

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

Predicted Noise Spectrum Agrees Well with Dimits PIC ETG Simulation at Late Times

- No Free Parameters in Theory!
- Discrete particle noise in PIC codes is quantifiable — well studied in past:
  - Langdon '79 – Birdsall&Langdon '83, Krommes '93

⇒ Useful code verification tool. We can develop objective criteria to determining when discrete particle noise is a problem



Renormalization of Noise-induced test-particle diffusion

$$D_{noise} = \int_{-\infty}^{t} dt' \left\langle \mathrm{v}(x(t),t)\,\mathrm{v}(x(t'),t') \right\rangle$$

$$= \left\langle \mathrm{v}_{ExB}^2 \right\rangle \tau_c \quad \propto \sum_{\vec{k}} k_y^2 J_0^2 \,|\, \phi_{noise,k} \,|^2 \frac{1}{|\,k_{\|}\,|\,\mathrm{v}_t}$$

(in simple limits)

$$\rightarrow \sum_{\vec{k}} k_y^2 J_0^2 \,|\, \phi_{noise,k} \,|^2 \frac{1}{|\,k_{\|}\,|\,\mathrm{v}_t + k_\perp^2 D_{noise} + \nu_{turb}}$$

$$\propto L_z \sum_{k_x,k_y} k_y^2 J_0^2 \,|\, \phi_{noise,k} \,|^2 \log\left(\frac{|\,k_{\|,\max}\,|\,\mathrm{v}_t + k_\perp^2 D_{noise} + \nu_{turb}}{k_\perp^2 D_{noise} + \nu_{turb}} \right)$$

Test-particle diffusion coefficient has a logarithmic divergence in the correlation time if integration is over straight-line trajectories. Use standard trick of treating trajectories as stochastic random walks consistent with diffusion. Include also model of effect of larger-scale turbulence on smaller scales as turbulent shearing rate ν_{turb} (but results insensitive to this at late times when turbulence is small).

Noise-induced test-particle diffusion

Integrate over properly weighted (ω,k) spectrum of noise fluctuations to find test-particle diffusion coefficient. Used a renormalized propagator to resolve a logarithmic divergence in the correlation time. (Have also included est. of turbulent shearing decorrelation, etc.)

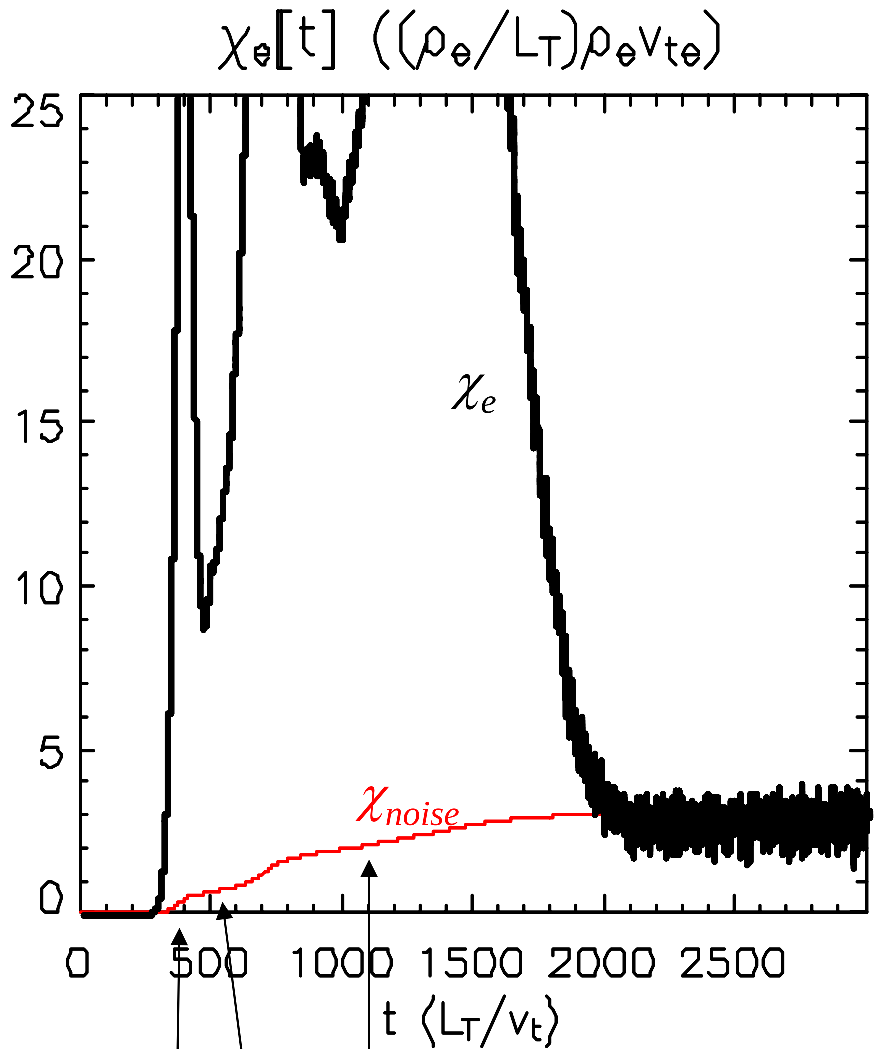
$$D_{noise} = \frac{1}{12}\frac{V_{Shield}^{(H)}}{V_{Sh,2}} \underbrace{k_{\perp N}^2\left(\frac{cT}{eB}\right)^2\left\langle\left|\frac{e\phi}{T}\right|^2\right\rangle_{noise}}_{V_{ExB}^2} \underbrace{\frac{3.05}{k_{\parallel\max} v_{te}\sqrt{2}}}_{\text{Decorrelation rate } \nu_\parallel} \underbrace{\log\left[1+\frac{k_{\parallel\max} v_{te}\sqrt{2}}{3.05\left(D_{noise}k_{\perp N}^2+\nu_*\right)}\right]}_{\text{Renormalized decorrelation rate depends on } D_{noise}}$$

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

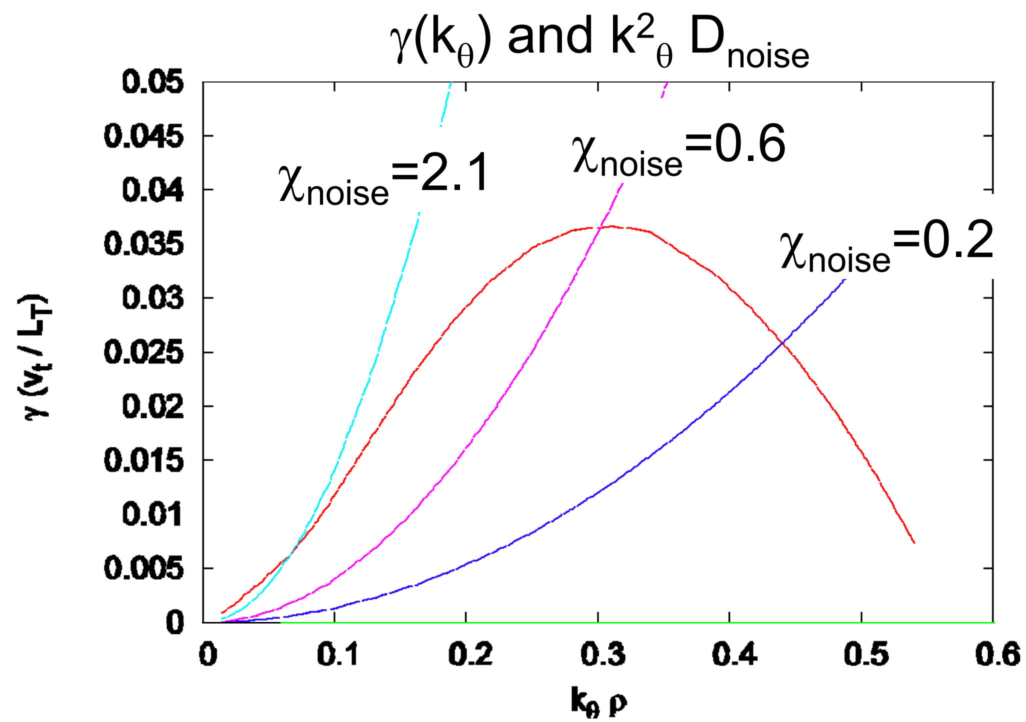
For details see
http://www.mfescience.org/mfedocs/ucrl-jrnl-212536.pdf

Dimits GK ETG simulations demonstrate χ_e falls to χ_{noise} by end of run, when $D_{noise}\, k_\perp^2 > \gamma$

Although χ_{noise} << max $\chi_{turbulence}$, this χ_{noise} is still large enough to give significant damping, $\chi_{noise}\, k_\perp^2 >> \gamma_{linear}$



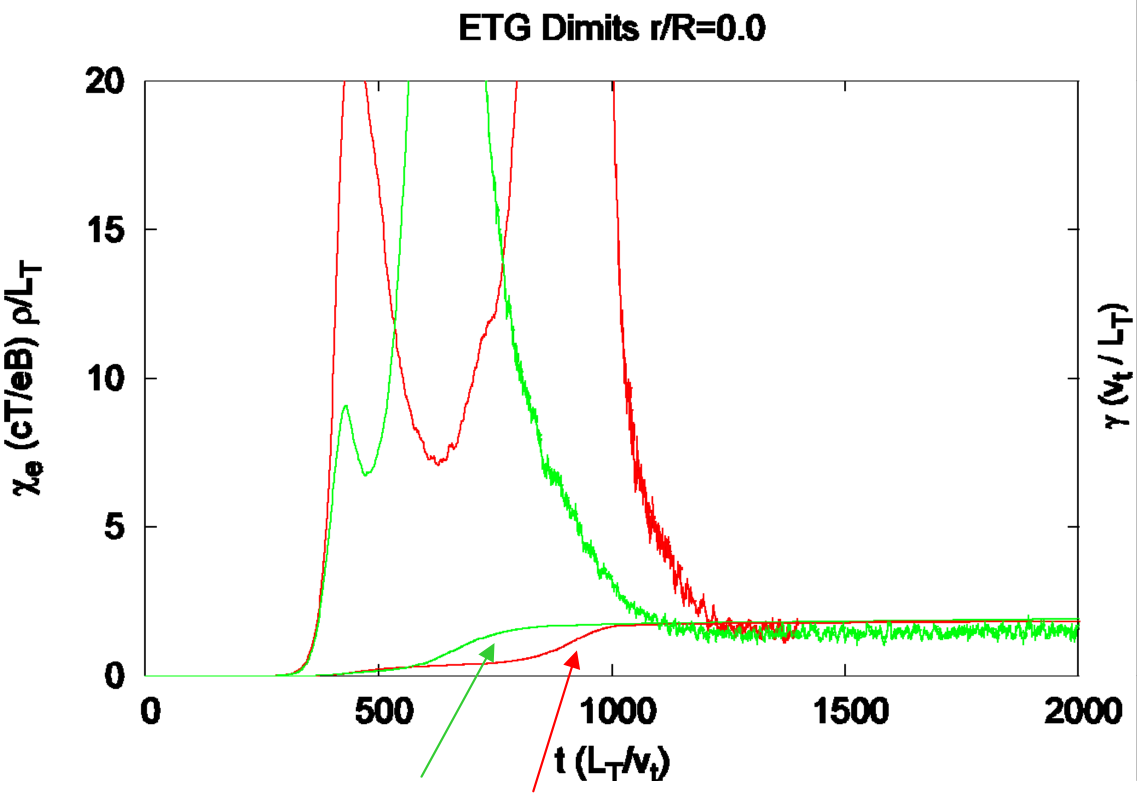
χ_{noise}=0.2, 0.6, 2.1

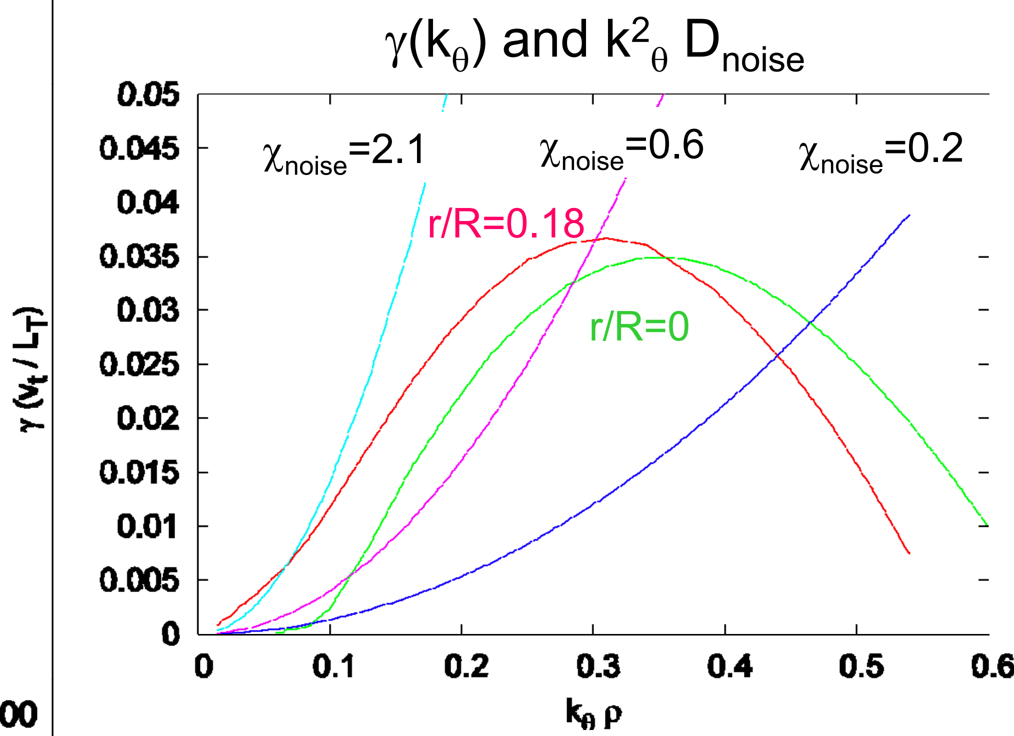


Growth rate for Cyclone base case with s-alpha geometry.

Final χ_{noise} (with no free parameters) agrees well with simulation at late times

Noise follows expected trends as particle number varied & trapping turned off





Turning off particle trapping (*r/R*=0) significantly reduces γ at low *k*

$$\chi_{noise} \propto \frac{w^2}{N} \propto \frac{\int^t dt' \chi(t)}{N}$$

Increasing # particles just leads to longer initial period of high χ_{tot}, so final χ_{noise} is not sensitive to N.

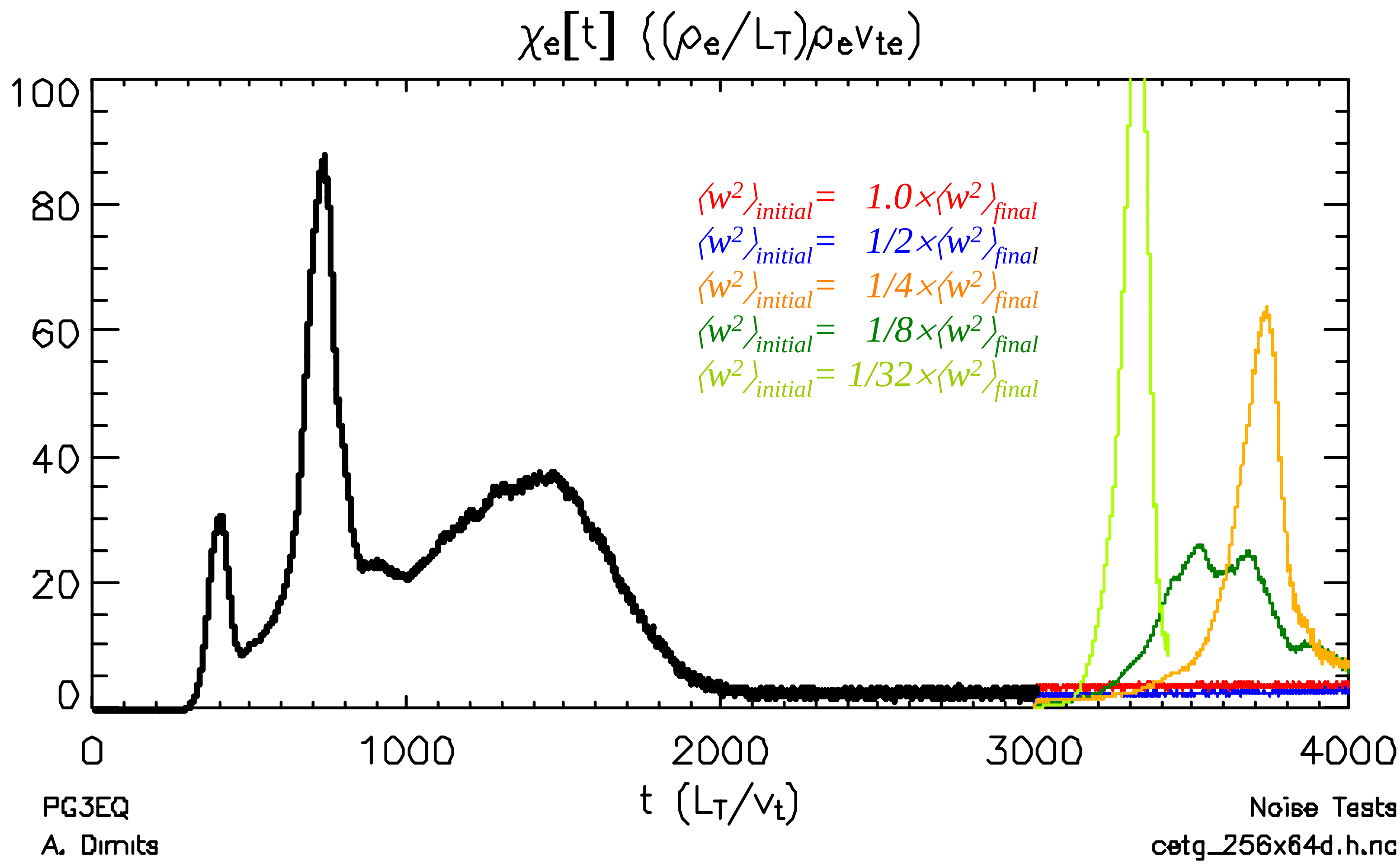
The Bolton/Lin "Noise Test"

- 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 $\langle w^2 \rangle_{final}$

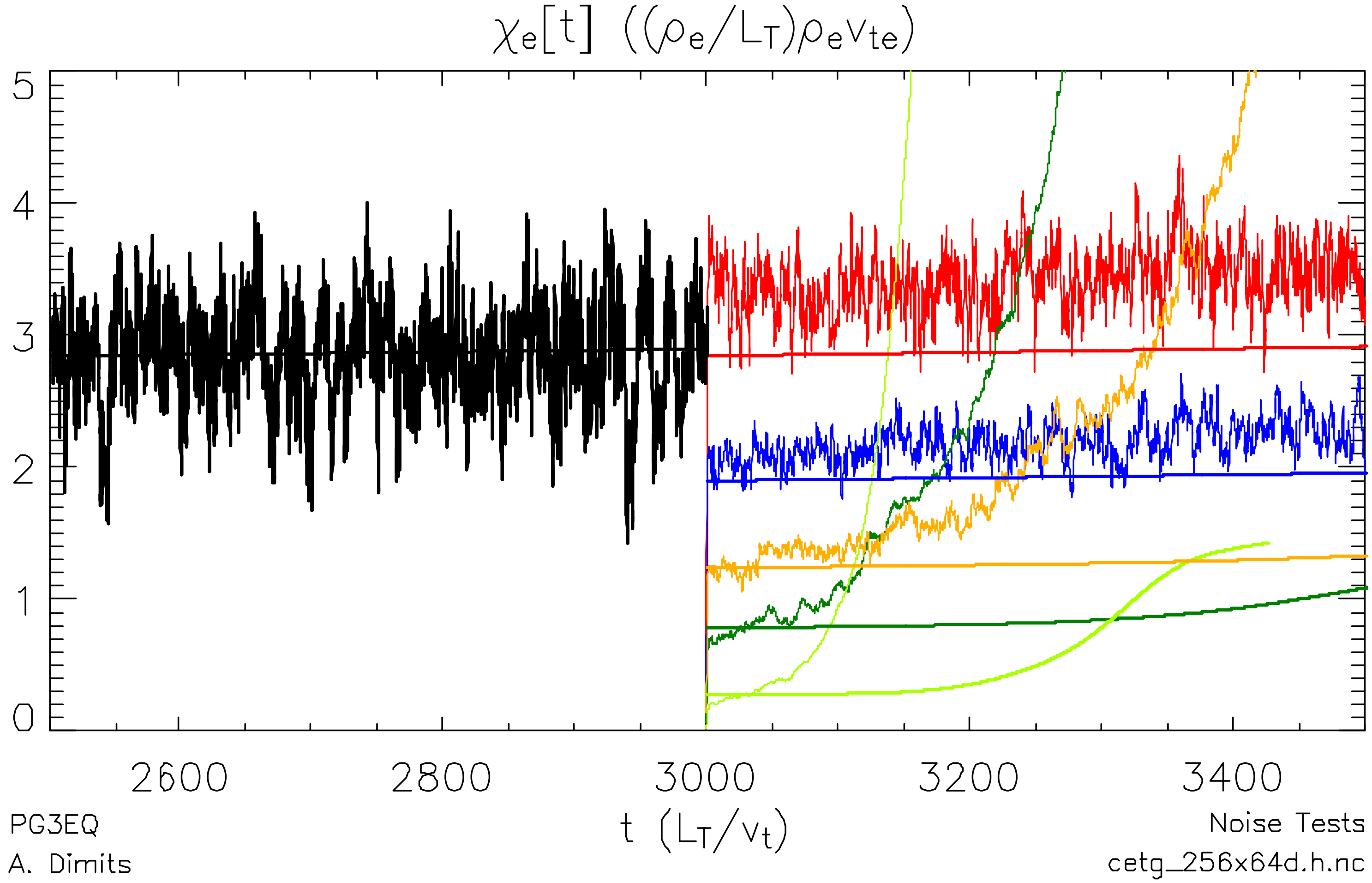
$\Rightarrow$ Only "memory" in GK simulations encoded in particle weights/positions

- 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 $\langle w^2 \rangle_{initial}$

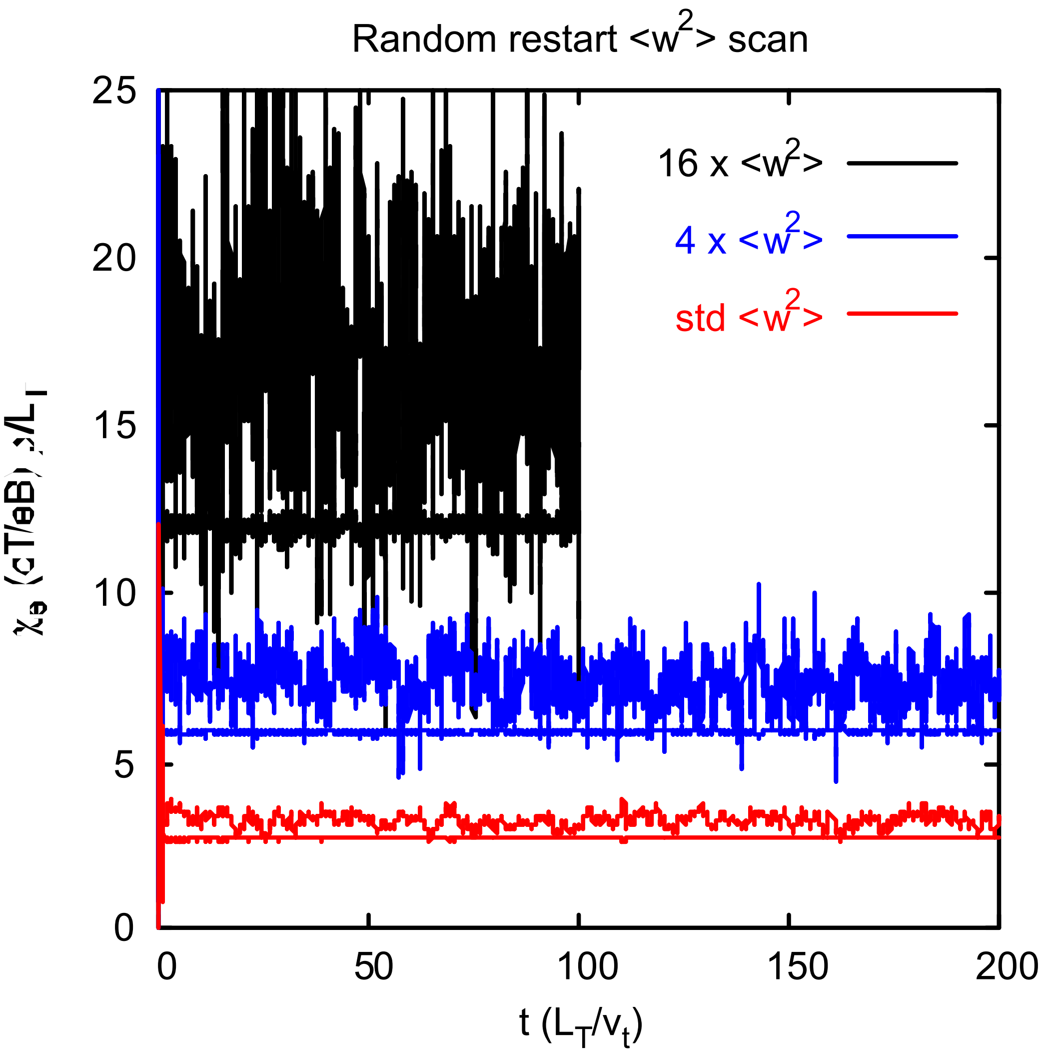
The Bolton/Lin "Noise Test":
Discrete particle noise suppresses ETG transport



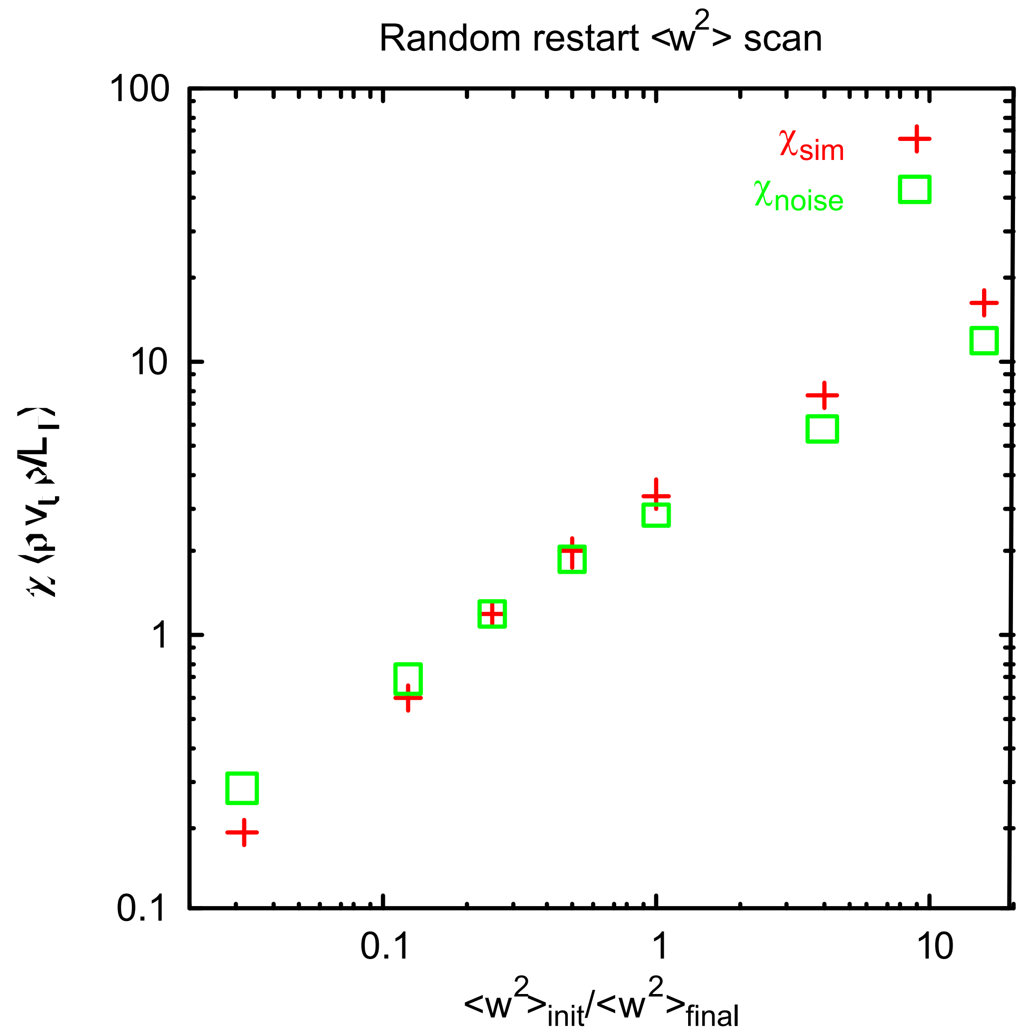
Predicted $\chi_{noise} \approx$ measured χ_e for every $\langle w^2 \rangle_{initial}$ in noise test



Predicted $\chi_{noise} \approx$ measured χ_e as $\langle w^2 \rangle_{initial}$ varies by factor of 512 in noise test



Scan to larger random weights



Discussion of results

- Large initial transients in $\chi_{etg}(t)$ seen by Dimits & by Z. Lin are larger than or comparable to Jenko & Dorland χ_{etg}. But this high χ_{etg} quickly drives weights so large that $k_\perp^2 D_{noise} \sim \gamma_{lin}$ and the turbulence is suppressed or significantly reduced.

- Scanning from 5-20 particles/cell appears to be converged (but isn't). Just wait longer and the weights build up to give the same noise level:

$$D_{noise} \propto \left[\frac{\langle w^2 \rangle}{n V_{smooth}} \right]^{1/2} \propto \left[\frac{\int_0^t dt' \, \chi(t')}{n V_{smooth}} \right]^{1/2}$$

- ETG eddies are radially very extended but still short scale in poloidal direction, so only takes a little bit of D_{noise} << Jenko-Dorland χ_{etg} to suppress or significantly reduce the turbulence. Radially extended ETG eddies more sensitive to noise than ITG is, requires many more particles to converge:

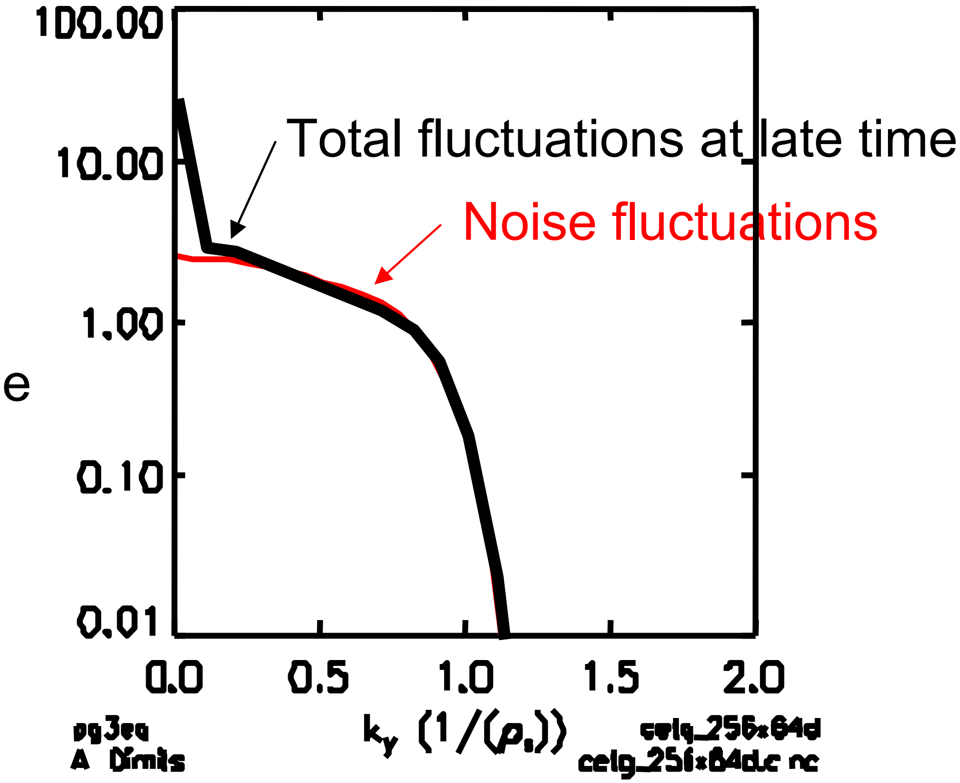
$$\boxed{D_{total} = \frac{\gamma - k_\perp^2 D_{noise}}{k_r^2} + D_{noise}}$$

Caveats

- Used guestimates of filtering/numerical parameters for Z. Lin's ETG simulations, based on Lin's previous ITG spectra.
- Neglected differences in zonal components of noise due to differences in ITG/ETG zonal flow dynamics.
- Fluctuation-dissipation theorem used uniform plasma dielectric in unsheared slab geometry. Probably good approximation at late times when noise dominates and turbulence is suppressed, but would be interesting to try a renormalized model of turbulent dielectric.
- Long-time scale variability often seen in $\chi(t)$ makes detection of trends harder
- At present have used just test-particle diffusion coefficients, assuming $\chi = (3/2)\, D_{test}$. Should calculate energy weighted thermal diffusion more consistently, including adiabatic constraints that allow heat transport but no net particle transport.
- Transition from turbulence-dominated state to noise-dominated state expected to be slower in Z. Lin's simulations then in Dimits' initial simulations (because of box size differences).

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.

- Resolves discrepancy, supports Jenko-Dorland result that ETG can give large transport.

- Renormalized calculation of χ_{noise} (also with no free parameters) 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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Summary

1. Continuum/Eulerian approach to gyrokinetic simulations
   - Introduction to one class of modern advection algorithms:
     high-order upwind with limiters
   - GYRO, GS2, &GENE continuum codes
     - demonstrated that 5-D continuum approach to gyrokinetics is feasible by using the latest most powerful advanced computers and a number of clever advanced algorithms.
     - These are the most comprehensive 5-D gyrokinetic turbulence codes in existence & the most widely used in the fusion program.
   - Interesting potential grad student projects!

2. Noise issues in PIC simulations of ETG turbulence
   - A very simple 2-page derivation of noise spectrum
   - Full noise theory agrees very well with Dimits PIC simulations, resolves previous PIC/continuum differences

Note: this talk focusses on the continuum approach to gyrokinetic simulations (except for part 2). The PIC approach to gyrokinetic simulations was covered in several previous graduate student seminar talks by W.W. Lee.