Coarse graining phase space in collisionless gyrokinetic turbulence simulations

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Main References

"Particle continuum method: algorithmic unification of particle and continuum methods", S. Vadlamani, S. Parker, Y. Chen, C. Kim, Comput. Phys. Comm. 164 209 (2004)

"Coarse-graining phase space in delta-f particle-in cell simulations", Y. Chen and S. Parker, Phys. Plasmas 14, 082301 (2007)

"Coarse-graining the electron distribution in turbulence simulation of tokalamk plasmas", Y. Chen, S. Parker, G. Rewoldt, S. Ku, G. Park, C. Cheng Phys. Plasmas 15, 055905 (2008)

Outline

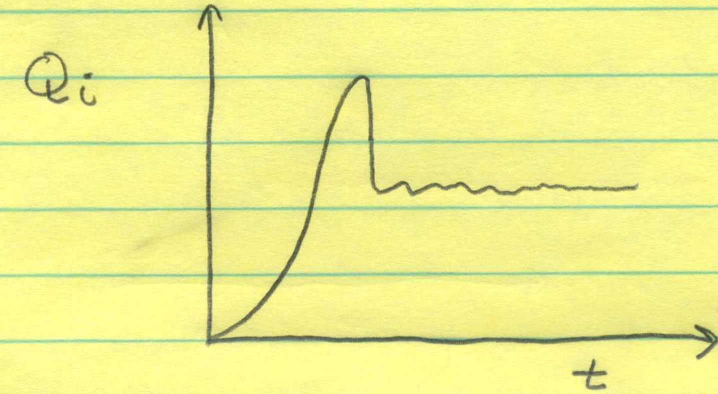
* Growing weight problem
    - DKE shear-less slab ITG model
    - "Entropy balance" equation
    - Growing weight problem

* Particle continuum method
    - Algorithm
    - Results

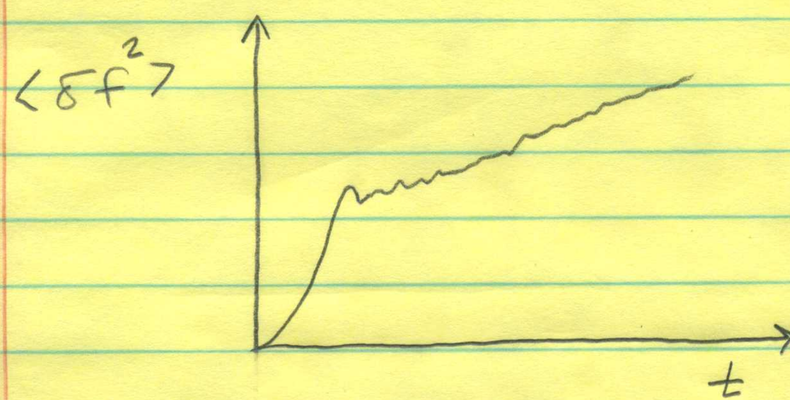
* 5D coarse graining procedure
    - Algorithm
    - Results show solution to the growing weight problem
    - Dissipation or effective collisionality

* 5D toroidal electromagnetic toroidal results
    - GEM code
    - Results using coarse-graining for electrons

"Growing Weight Problem"



Lee '88
Krommes '94



$\langle \delta f^2 \rangle$ grows algebraically

$$f(\underline{x}, \underline{v}, t) = f_0(\underline{x}, \underline{v}) + \delta f(\underline{x}, \underline{v}, t)$$

ITG - ion temperature gradient driven turbulence

5D $(\underline{x}, v_{\parallel}, \mu)$

toroidal, electrostatic

gryrokinetic ions, $\delta n_e = n_0 \dfrac{e\phi}{T_e}$

"Entropy Balance"

$$\int_{\text{all } \underline{x}} \int_{\text{all } \underline{v}} \frac{\delta f}{f_M} \times \text{GKE} \; d^3x \, d^3v$$

$$\Rightarrow \quad \frac{\partial F}{\partial t} = \kappa_n \Gamma + \frac{1}{2} \kappa_T Q_T - D$$

F: $\left\langle \frac{\delta f^2}{f_M} \right\rangle$

κ_n: $\frac{|\nabla n|}{n}$

Γ: space avged particle flux

κ_T: $\frac{|\nabla T|}{T}$

Q_T: space avged heat flux

D: Dissipation $\langle \delta f \, C(\delta f) \rangle$

For ITG, $\Gamma = 0$, $D = 0$

$$\Rightarrow \quad F = \frac{1}{2} \kappa_T Q \, t$$

$$\langle \delta f^2 \rangle \propto t$$

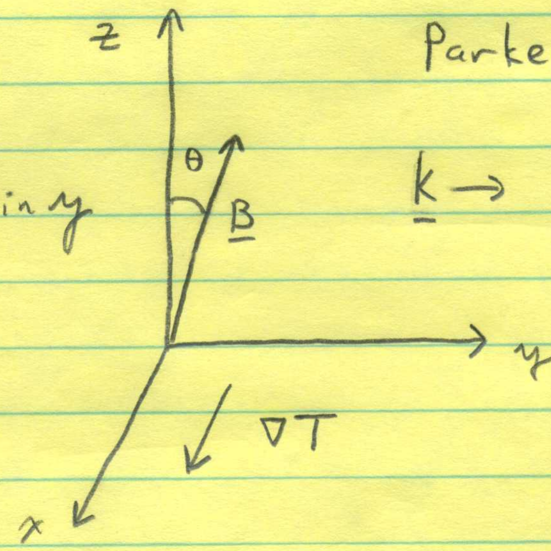
2D "Shear-less Slab" Problem

Parker '94

ITG Mode

x–y plane

bounded in x, periodic in y



$$\boxed{\delta n_e = n_0 e\phi / T_e}$$

$$k_\parallel = \theta k_y$$

$$\omega_{*T} \equiv \frac{|\nabla T_i|}{T} k_y \rho_i v_{ti}$$

$k_\parallel v_{ti}$ resonates with ω_{*T}

$\delta f = \delta f(x, y, v_\parallel, t)$ — Average over $v_\perp$

$$\boxed{\frac{\partial \delta f}{\partial t} + \underline{v}_E \cdot \nabla \delta f + v_\parallel \nabla_\parallel \delta f = \kappa v_{Ex} f_0 + \frac{q}{T} v_\parallel E_\parallel f_0}$$

$$\boxed{\delta n_e = \delta n_i}$$

$$\kappa = \kappa_n + \frac{1}{2}\left(\frac{v_\parallel^2}{v_t^2} - 1\right)\kappa_T$$

κ_n ↑ $\frac{|\nabla n|}{n}$ κ_T ↑ $\frac{|\nabla T_i|}{T}$

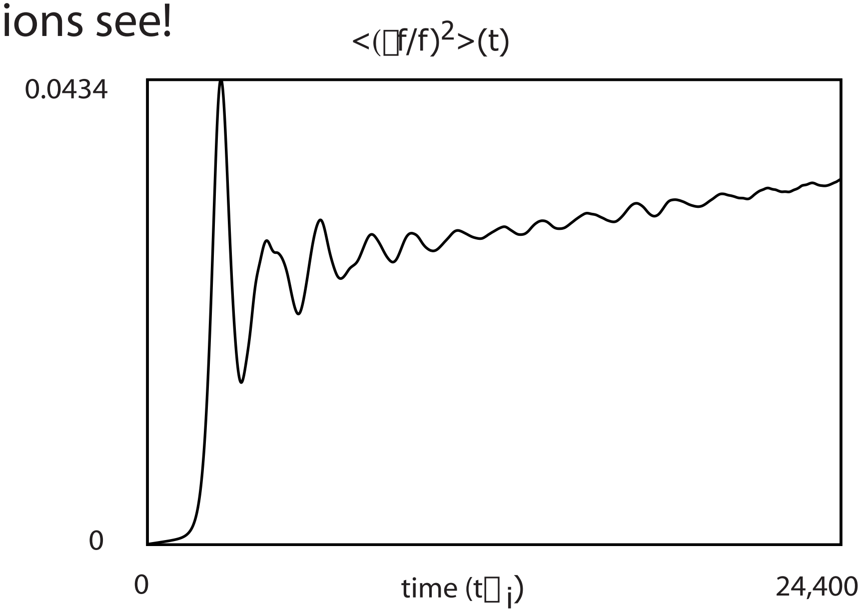
"The Growing Weight Problem"

Flux balances dissipation. If you have no dissipation, then df^2 has to grow.

See: Krommes and Hu (1994) and refs. therein

Simpy multiply the Vlasov eq. by f and integrate over (x,v).

This is real physics, and it is what df PIC simulations see!



"The Problem" is that if the particle weights get too be large there can be a noise problem.

BUT

1) easily tested for by particle # convergence

2) stationary state reached long before weights become large

δf Methods

Parker '93

Let $\underline{z} = (\underline{x}, \underline{v})$

$$f(\underline{z}, t) = f_0(\underline{z}) + \delta f(\underline{z}, t)$$

$$\dot{\underline{z}} = \dot{\underline{z}}^0 + \dot{\underline{z}}^1$$

$\dot{\underline{z}}^0$ ← equilibrium trajectory

$\dot{\underline{z}}^1$ ← perturbed trajectory

$$\frac{\partial \delta f}{\partial t} + \dot{\underline{z}} \cdot \frac{\partial}{\partial \underline{z}} \delta f = - \dot{\underline{z}}^1 \cdot \frac{\partial f_0}{\partial \underline{z}}$$

Follow characteristics: $\dot{\delta f} = - \dot{\underline{z}}^1 \cdot \dfrac{\partial f_0}{\partial \underline{z}}$

$$\delta f(\underline{z}, t) = \sum_i \delta f_i(t) \, \Delta V_i \, S^N[\underline{z} - \underline{z}_i(t)]$$

ΔV_i: phase space volume associated with particle i

S^N: "particle shape function"

Jargon: $w = \delta f \, \Delta V = \dfrac{\delta f}{g}$

w: "particle weight"

g: "Marker particle distribution function"

Particle-Continuum Methods

(really a class of a variety of methods)

Load particles on a uniform lattice (**x**, **v**)

Every M timesteps

deposit df on the phase space grid (grid points are the lattice points)

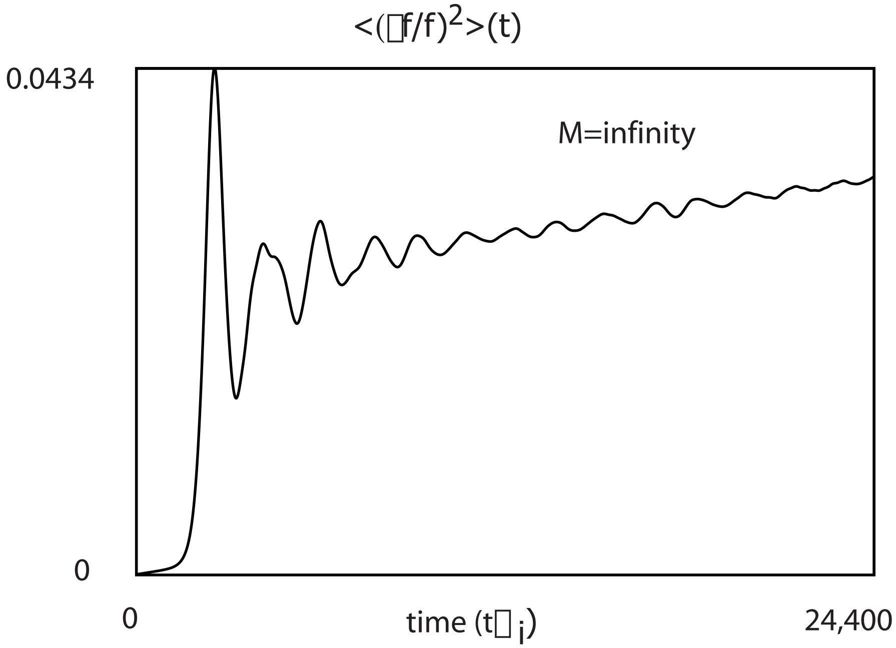
reset particle (**x**,**v**) to initial value

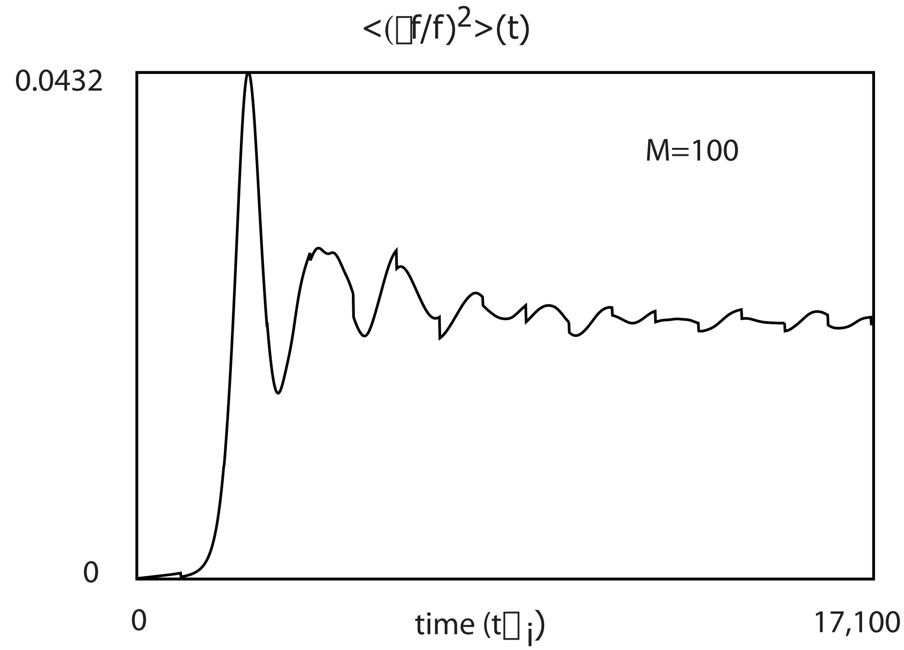
set particle df to grid point value

See: Vladlamani, et al. Comput. Phys. Comm. (2004) and Refs. therein.

Particle-Continuum method coarse-grains and df^2 saturates

Physically, this is what collisions would do on a very fine velocity dissipation scale



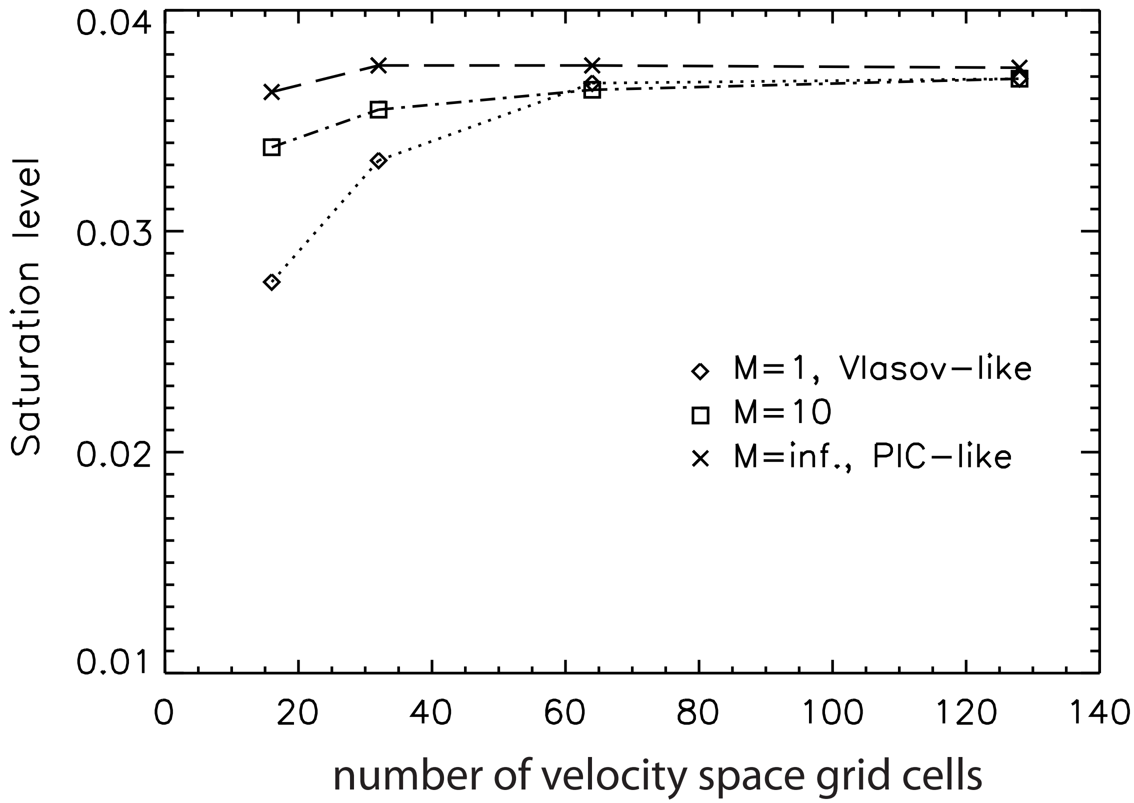


2D bounded slab ITG mode test problem

Results from: Vladlamani, et al. Comput. Phys. Comm. (2004)

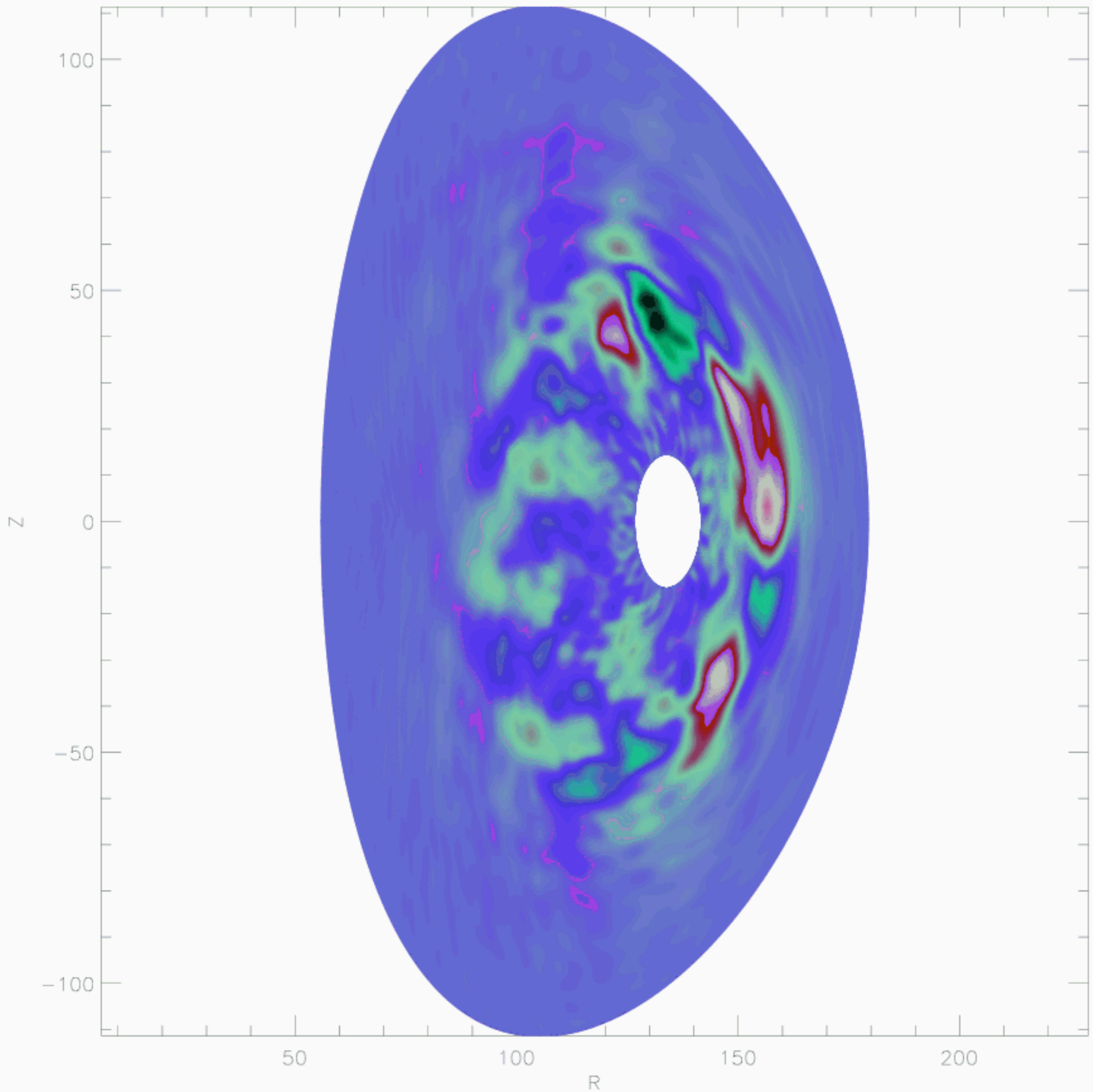
Particle limit converges quicker

(v-space grid cells = # of particles/cell)



The GEM Code

- $p_{\|}$ formulation, the split-weight scheme, high-β Ampere algorithm
- Use field-line-following coordinates
  - Cover $0 \leq \theta \leq 2\pi$
  - Radially global
  - Arbitrary size toroidal section
- Passing and trapped electrons
- Collisions
- Magnetic perturbations
- Nonlinear Landau damping effect
- Arbitrary shape tokamak equilibrium and equilibrium flow



Entropy Paradox

- The particle weight equation ($\kappa \propto \nabla f_0$, $\dot{\epsilon} = \frac{d}{dt}(mv^2/2)$)

$$\frac{dw}{dt} = \kappa\, v_{\rm Ex} + \frac{\dot{\epsilon}}{T_0}\,,$$

- Define $I = \left\langle w^2 \right\rangle /2$

$$\frac{dI}{dt} = \frac{1}{N}\sum_j \kappa\, v_{\rm Ex}\, w_j + \frac{1}{N}\sum_j \frac{\dot{\epsilon}_j}{T_0}\, w_j\,.$$

$$\frac{dI}{dt} \approx (\kappa_n - 1.5\kappa_T)\frac{\Gamma_p}{n_0} + \frac{\kappa_T}{n_0 T_0}\Gamma_e,$$

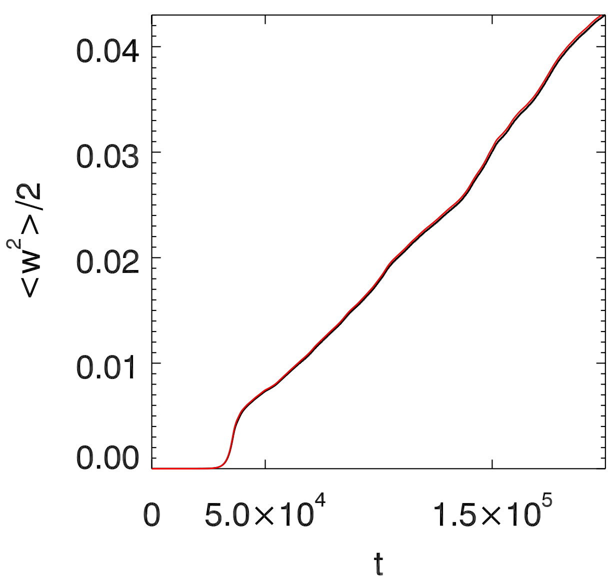
with

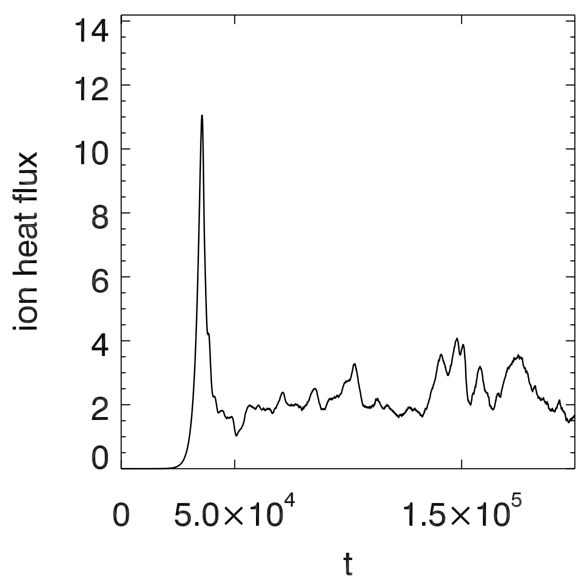
$$\Gamma_p = \frac{n_0}{N}\sum_j w_j\, v_{\rm Ex}\,,$$

$$\Gamma_e = \frac{n_0}{N}\sum_j w_j\, \epsilon_j\, v_{\rm Ex}\,.$$

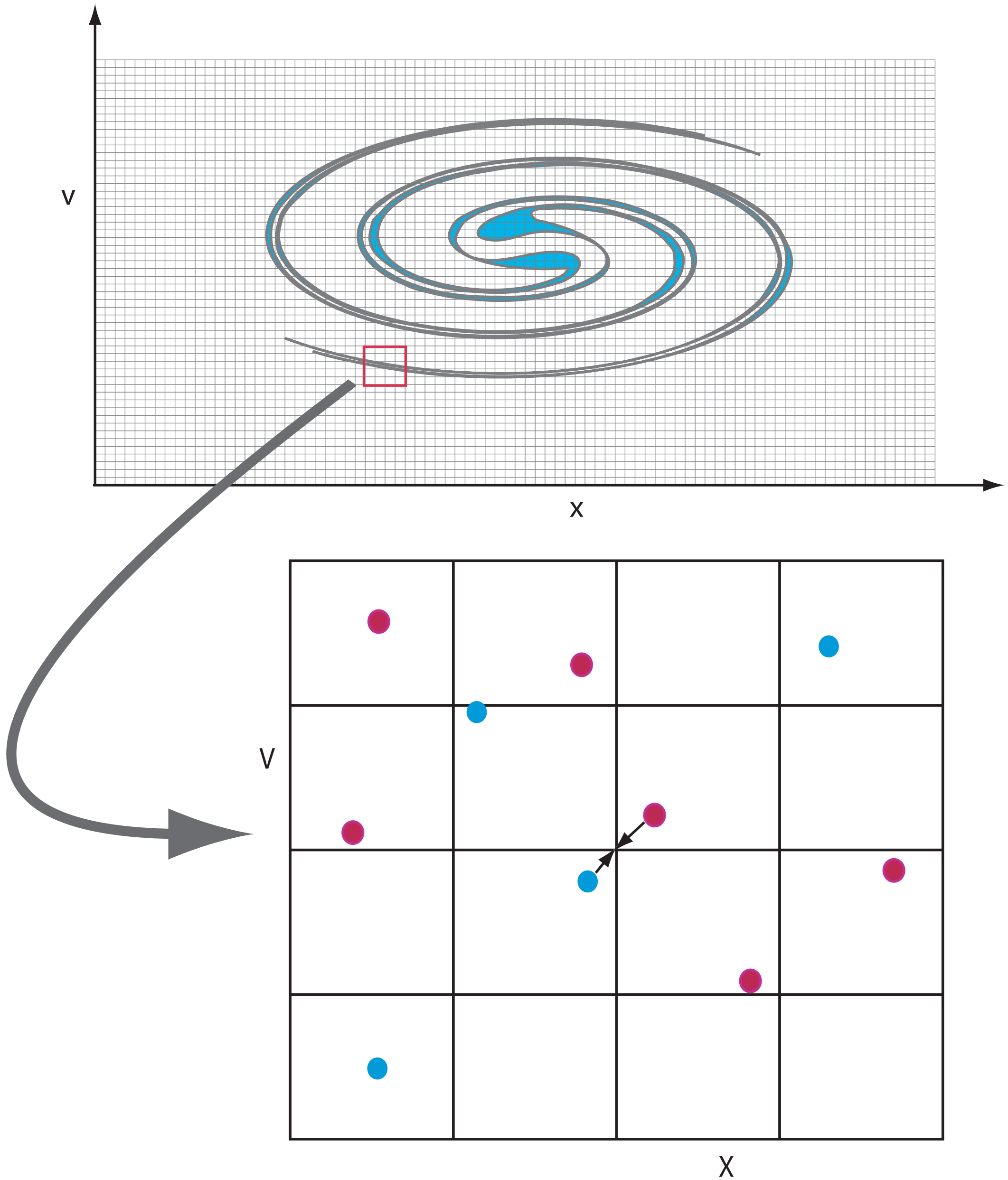
Entropy Paradox: In a stationary state with nonzero transport, the average particle weights will keep increasing.

Cyclone Base Case, with Adiabatic Electrons

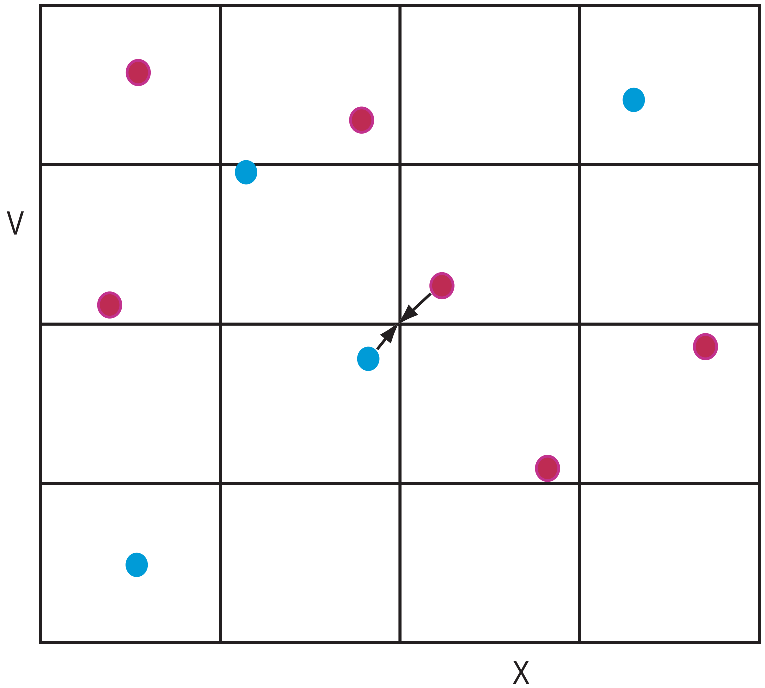




Discrete particle noise $\propto \frac{w}{\sqrt{N}}$—“The Growing Weight Problem”


v
x
V
X

Coarse-Graining Procedure



- Divide phase-space into 5D grids. Construct δf and marker distribution g on the grids
- Set the new particle weight to

$$w'(p) = \delta f(p)/g(p)$$

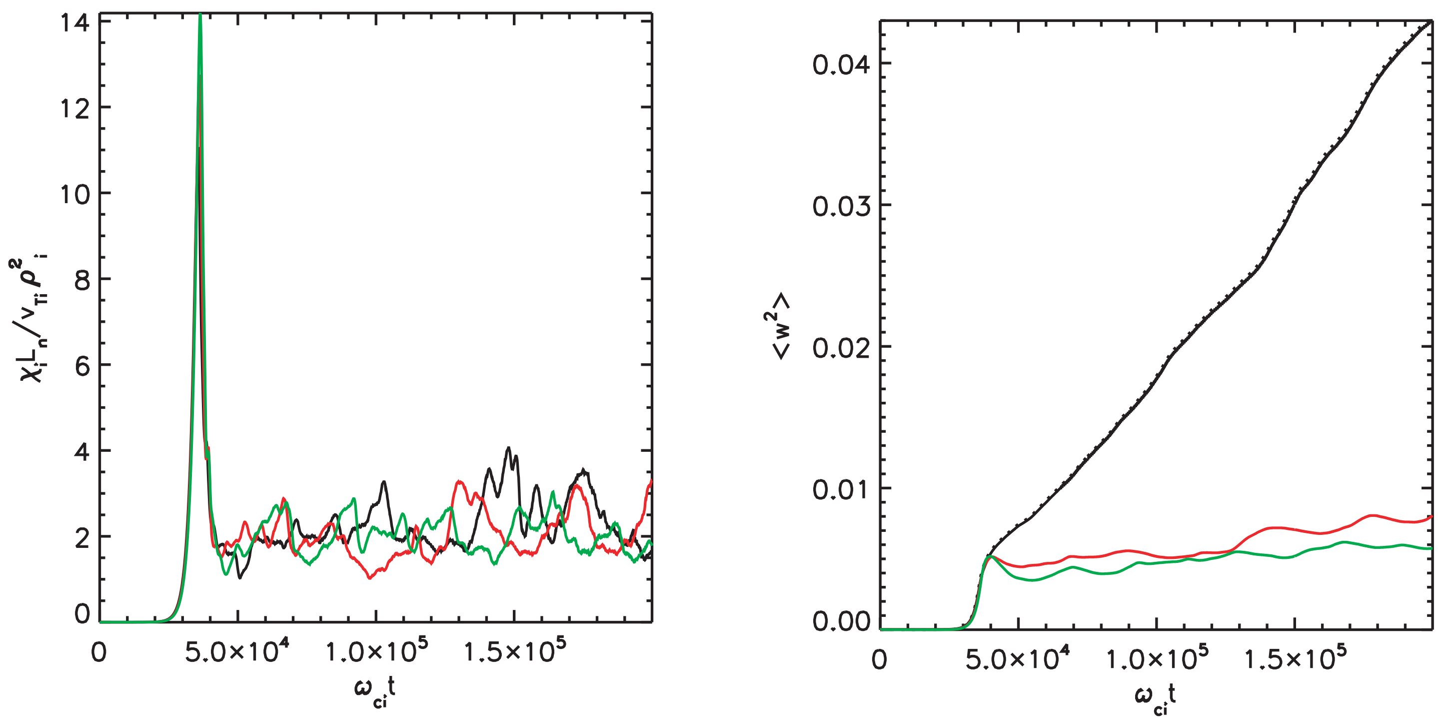
evaluated at the particle location using interpolation.

- To smooth in time, reset every N_s steps, and reset only a small fraction

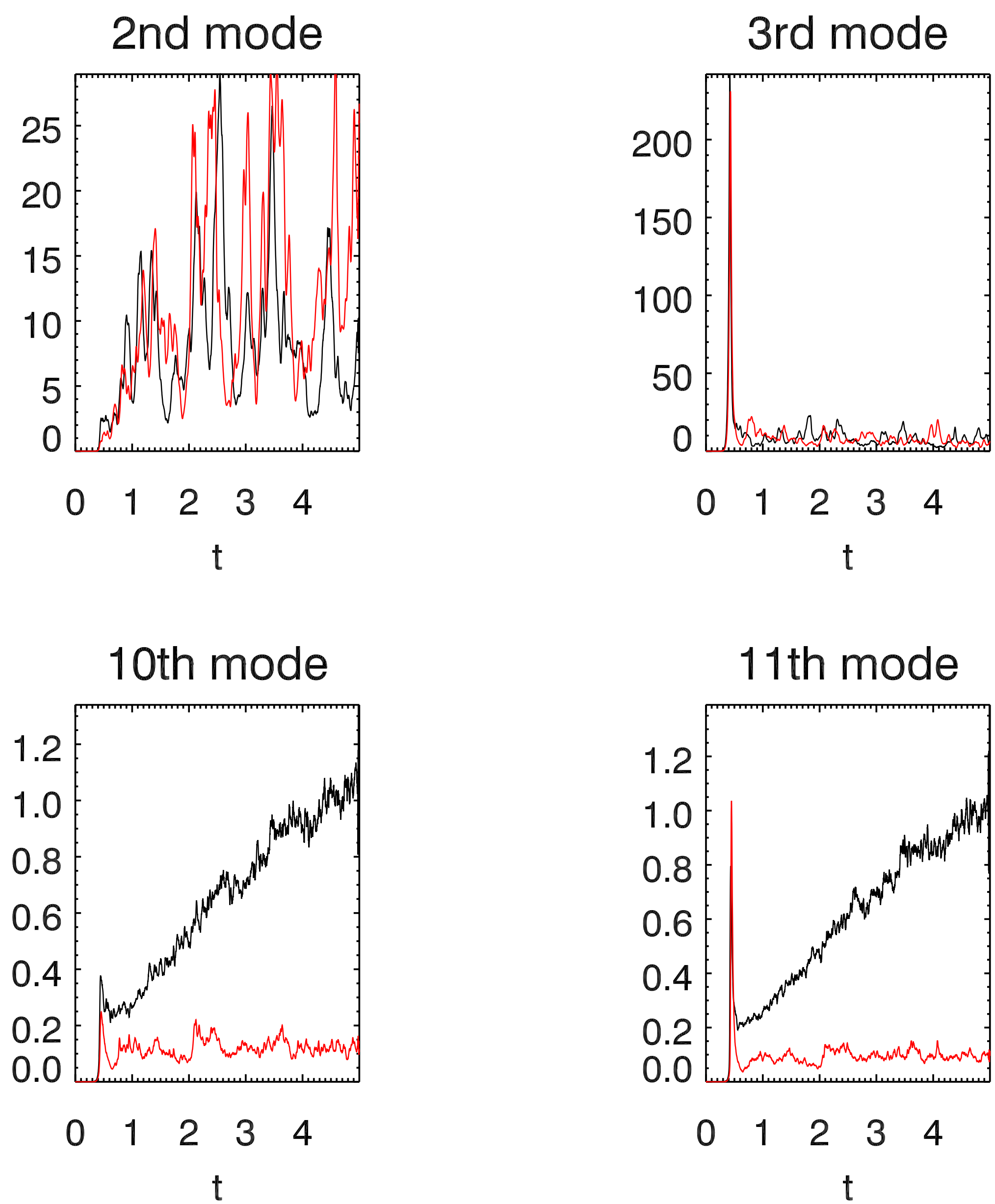
$$w^{\text{new}}(p) = (1-\delta)\, w^{\text{old}} + \delta w'(p)$$

- Can conserve number and energy by slightly adjusting weights

Coarse graining solves growing weight problem for Cyclone base case



□= 0.0 □= 0.05 □= 0.1



$$\rho^2(k_y, z_k) = \left\langle \mid \delta n(x, k_y, z_k) \mid^2 \right\rangle_x$$

Numerical dissipation

Denavit '72

Examine smoothing associate with interpolation to phase space grid

$$w \equiv \frac{\delta f}{g}$$ ← Marker particle distribution

$$w'(x_i) = \frac{1}{\Delta x} \int w(x) \, S(x - x_i) \, dx$$

(S ← particle shape function)

Assume $w(x) = w_0 e^{ikx}$

$$\Rightarrow \quad w'(x_i) = w(x_i) \left[1 - \frac{1}{24} (k \Delta x)^2 \right]$$

$$\left. \frac{\partial \delta f}{\partial t} \right|_{diss.} = \frac{\delta \, \Delta x^2}{24 \, M \Delta t} \frac{\partial^2 \delta f}{\partial x^2}$$

($M \Delta t$ ← time period between coarse graining)

$$w_{new} = (1 - \delta) \, w_{old} + (\delta) \, w'$$

$$C(\delta f) = -\frac{\partial}{\partial v}(\nu v + \nu v_T^2 \frac{\partial}{\partial v}\delta f)$$

$$\left.\frac{dI}{dt}\right|_c = -\nu v_T^2 \left\langle \left(\frac{\partial w}{\partial v}\right)^2 \right\rangle \approx -\nu v_{\mathrm{T}}^2 \frac{\langle w^2 \rangle}{(\triangle v)^2}$$

Krommes, Phys. Plasmas **6**, 1477 (1999)

$$\frac{dI}{dt} = \frac{1}{n_0 T_0}\kappa_T \Gamma_e - \left.\frac{dI}{dt}\right|_c = 0$$

$$\nu = \kappa_T \frac{\Gamma_e}{n_0 T_0}\left(\frac{\triangle v}{v_{\mathrm{T}}}\right)^2 \frac{1}{\langle w^2 \rangle}$$

$$\Delta v \sim 0.5 v_T \longrightarrow \nu/\Omega_c = 4 \times 10^{-6}$$

Coarse Graining Preserves True Collisional Effects

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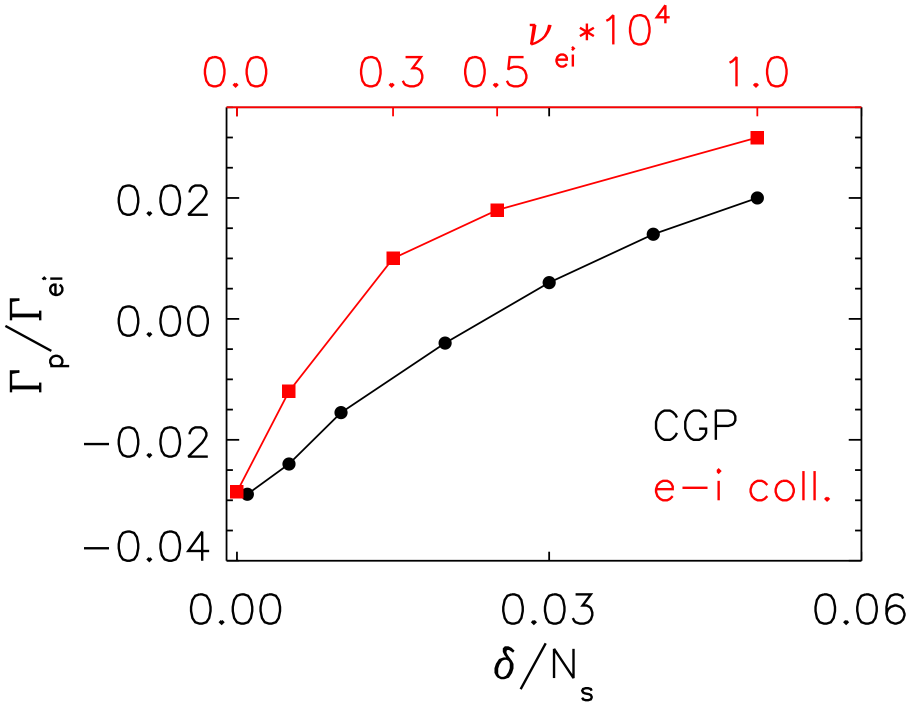
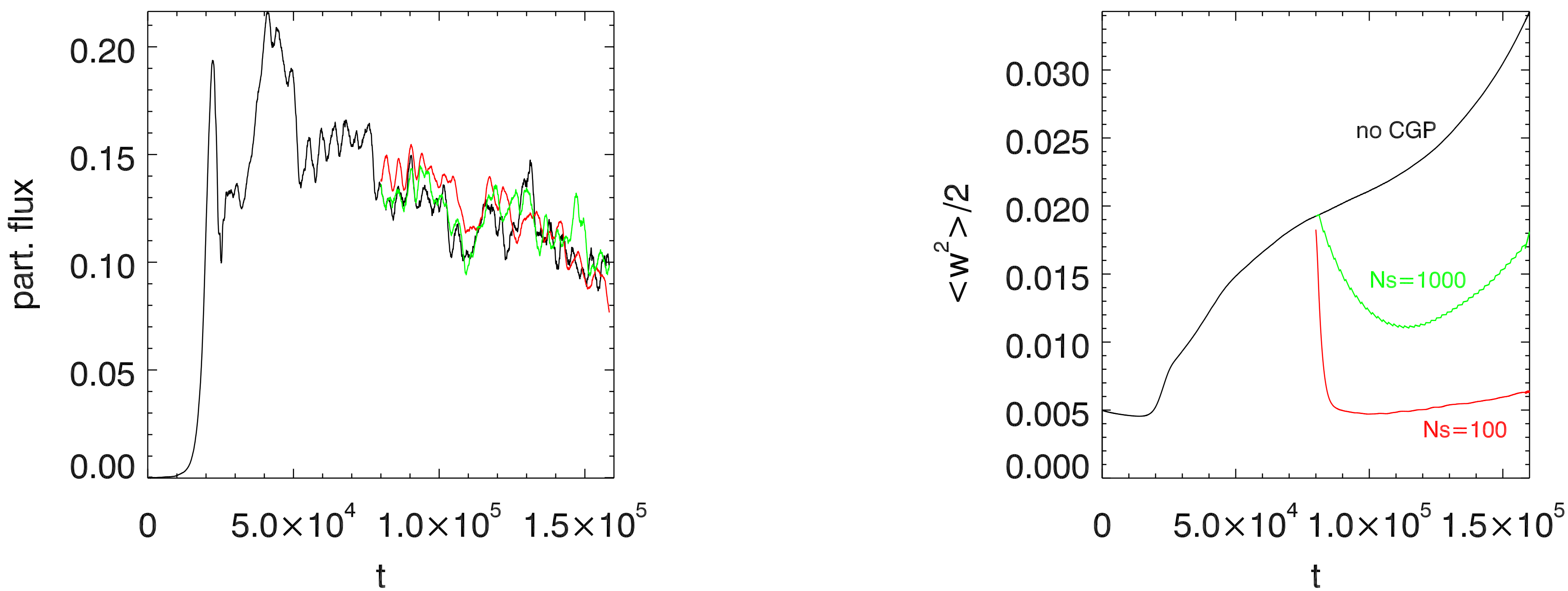


- $\Gamma_p < 0$ (particle pinch) observed in collisionless ITG simulations.
  - Due to passing electrons interacting with the long tail of the modes along **B** (Hallatschek and Dorland PRL **95**, 055002 (2005)).
- Pinch is sensitive to e-i collisions.
- Ratio of quasi-linear fluxes

$$\frac{\Gamma_p}{\Gamma_i} = \frac{\text{particle flux}}{\text{ion heat flux}}$$

Coarse-Graining Reduces Weights And Preserves Pinch



Parameters based on the Cyclone Base Case.

Core Simulation with Coarse-Graining Electrons

From TRANSP

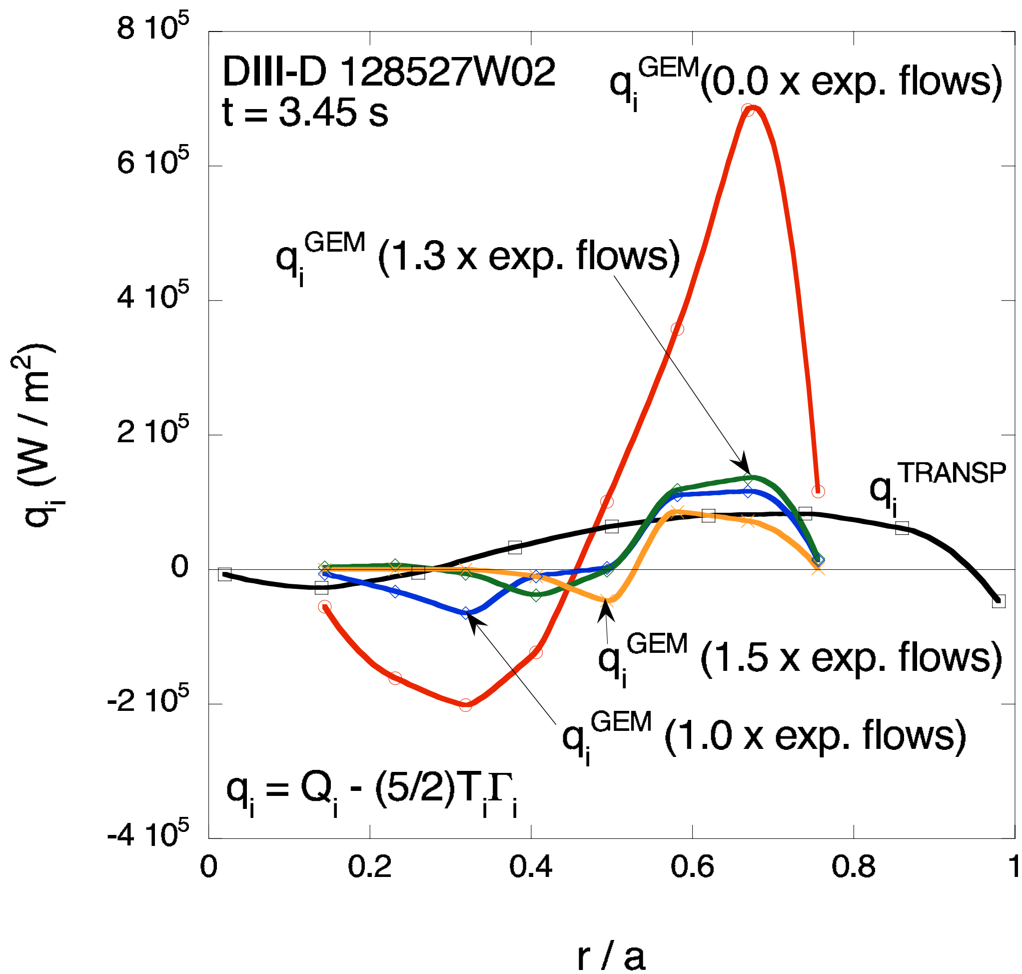
- The density and temperature profiles for each of the four plasma species, background deuterium, carbon impurity, hot beam deuterium, and electrons
- Radial profiles of the parallel flow velocities for each of the ion species

From NCLASS

- Radial profile of the equilibrium electrostatic potential is calculated from radial force balance

From JSOLVER

- Radial profiles of ellipticity, triangularity, major radius, and q



8 10^5
6 10^5
4 10^5
2 10^5
0
-2 10^5
-4 10^5
q_i (W / m^2)
DIII-D 128527W02
t = 3.45 s
q_i^GEM (0.0 x exp. flows)
q_i^GEM (1.3 x exp. flows)
q_i^TRANSP
q_i^GEM (1.5 x exp. flows)
q_i^GEM (1.0 x exp. flows)
q_i = Q_i - (5/2)T_iΓ_i
0
0.2
0.4
0.6
0.8
1
r / a

Coupled GEM-XGC Edge Simulation

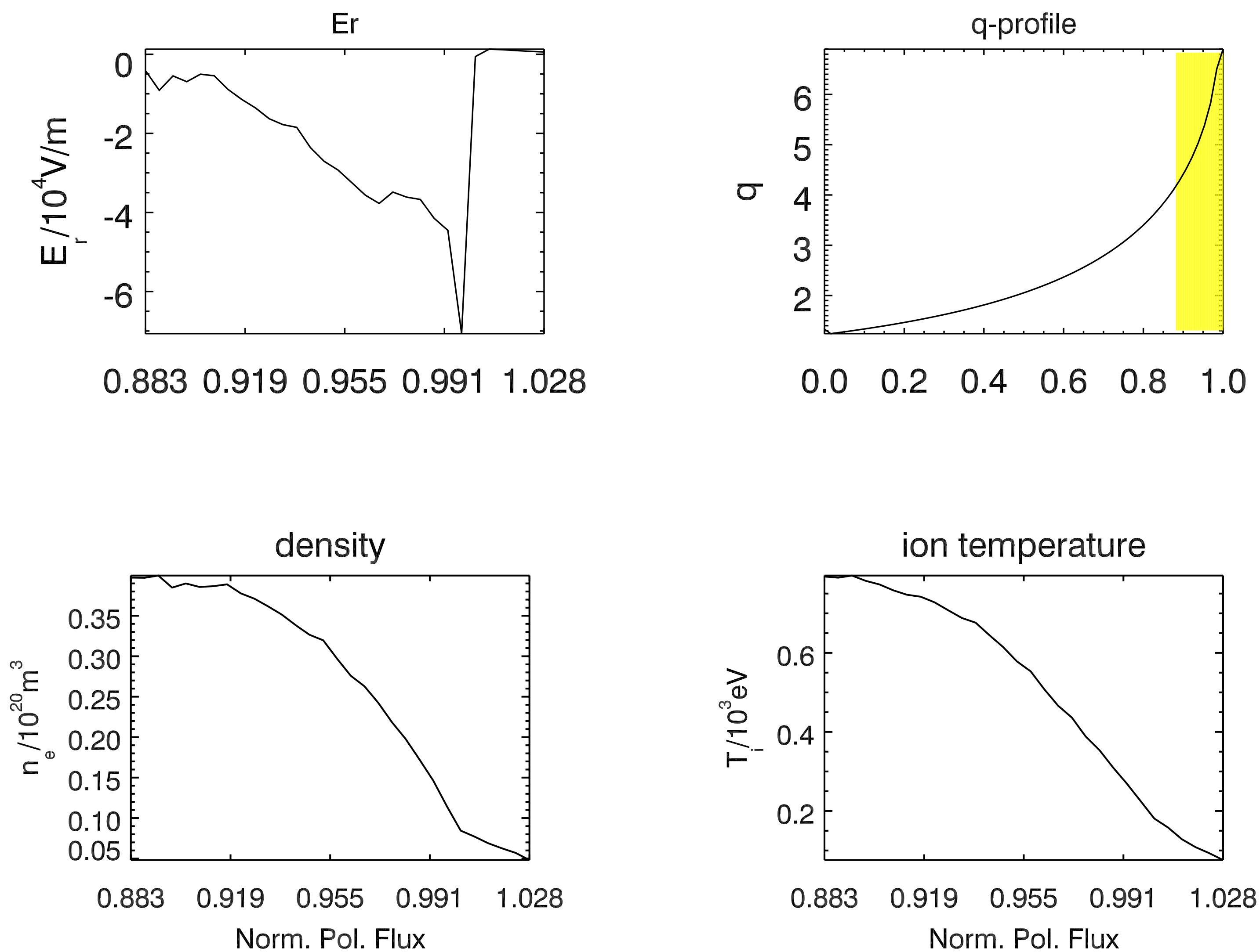
XGC

- Particle-in-Cell code for studying edge transport developed at **CPES** (PI: C-S Chang)
- Neoclassical and turbulent transport in one integrated code
- Realistic magnetic geometry containing X-point

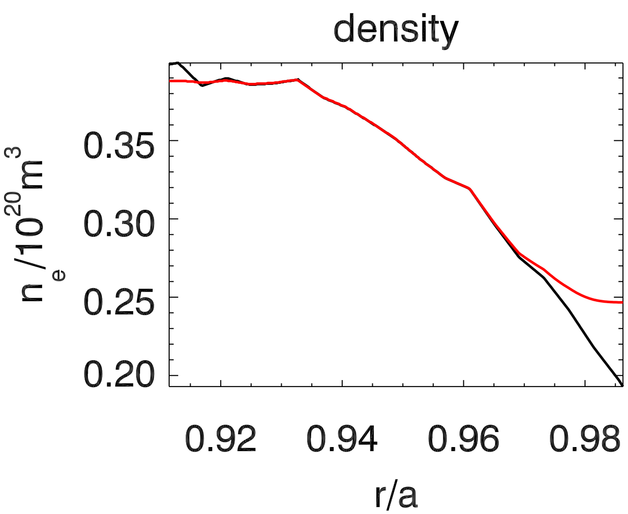
Coupling with GEM

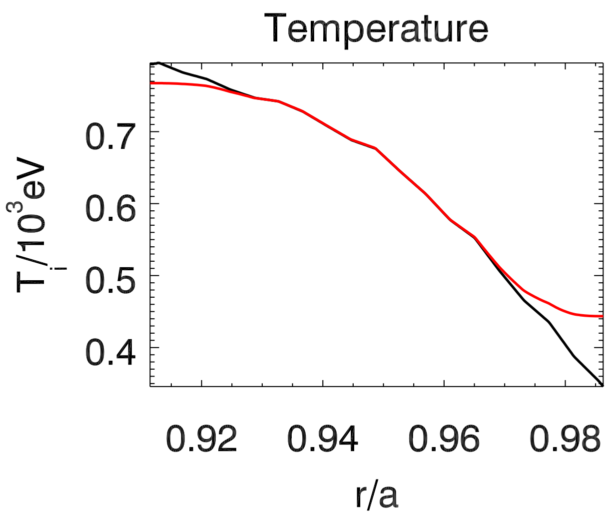
- Only profiles inside separatrix used
- $T_i(r)$, $T_e(r)$, $n(r)$, $E_r(r)$, $q(r)$, $\kappa(r)$, $\delta(r)$ and $R_0(r)$
- Fixed boundary condition in GEM, T and n profiles modified near simulation boundaries.

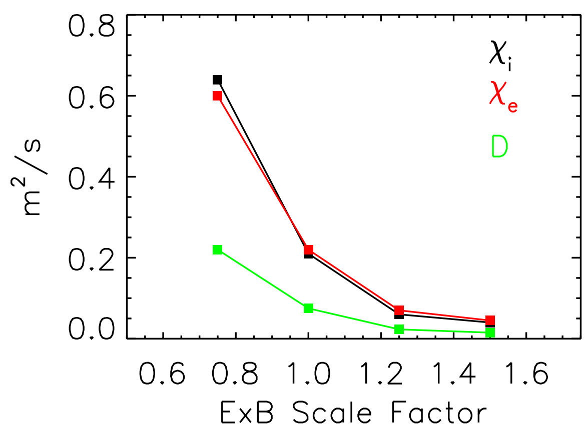
Profiles from XGC (DIII-D #096333 taken at 3337ms).

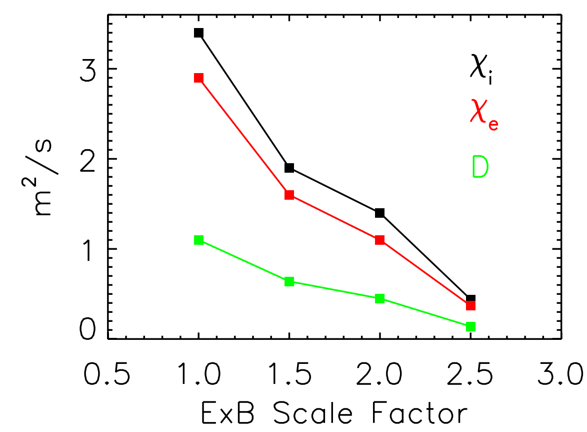


For GEM simulation $T(r)$, $n(r)$ flattened near boundaries

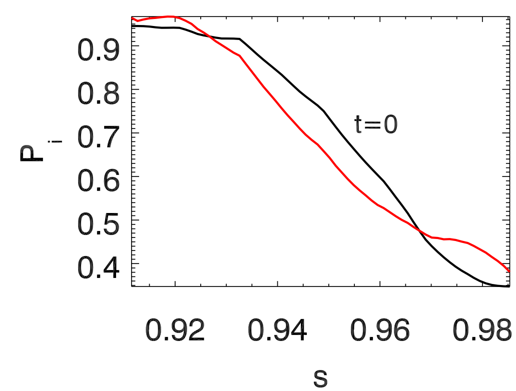


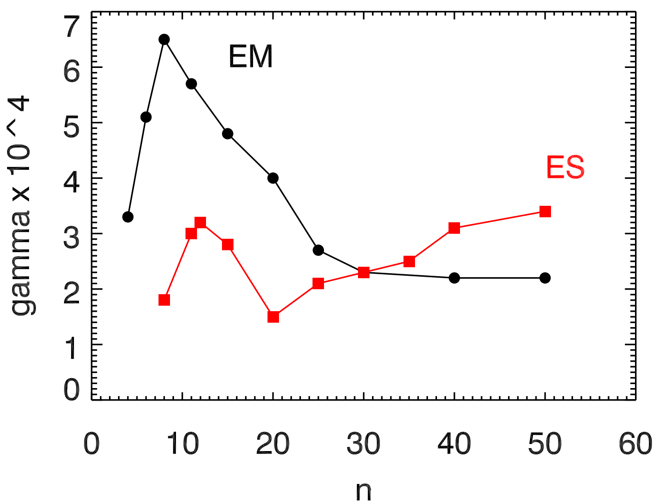


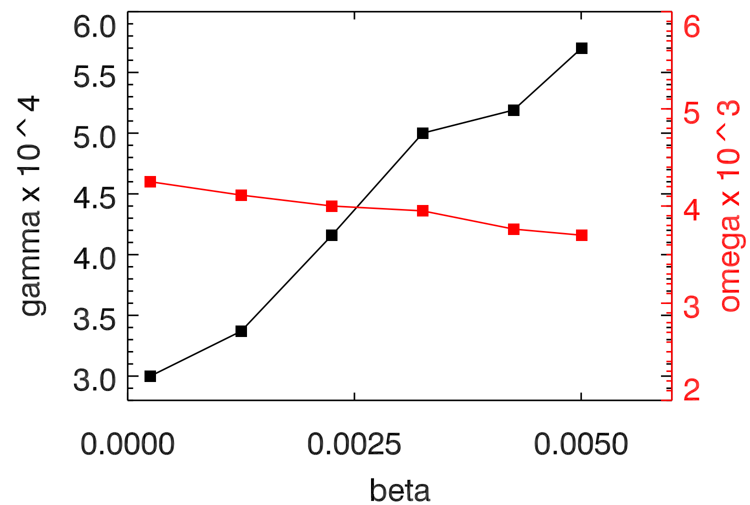




- Diffusivities obtained with averaged Γ and ∇T, ∇n at $r/a = 0.96$
- Significant profile relaxation in EM simulation
- Magnetic perturbation strongly enhances the instabilities, even with $\beta \sim 0.001$







- $\delta\mathbf{B}$ destabilizing for $n \sim 10$ ($k_\theta \rho_i \leq 0.2$), stabilizing for $n > 30$
  - high-n likely to be electron drift waves (Lang, Chen and Parker, Phys. Plasmas **14**, 082315 (2007))
- Test with flattened profiles shows ∇n drive most important, ∇T_i effect is small.
- low-n EM and ES modes appear to be the same branch

Summary

Growing weight problem is solved using new coarse graining procedure

Numerical dissipation can be quantified

Coarse graining is especially useful for electromagnetic turbulence with kinetic electrons