Equilibrium Statistical Mechanics of Gyrokinetic Fluctuations

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PPPL & U. of Maryland / Center for Multiscale Plasma Dynamics

APS-DPP Meeting, Chicago, November 8-12, 2010

Outline

- Short summary of 3 other projects with grad students:
  - Erik Granstedt: GYRO simulations of turbulence in density-gradient driven regimes that might be expected with lithium walls in LTX
  - Luc Peterson: GYRO simulations of ETG turbulence in NSTX, improved algorithms for TGYRO multiscale coupling of transport/turbulence codes
  - Jess Baumgaertel: GS2 calculations of gyrokinetic instabilities and turbulence in non-axisymmetric stellarator geometry

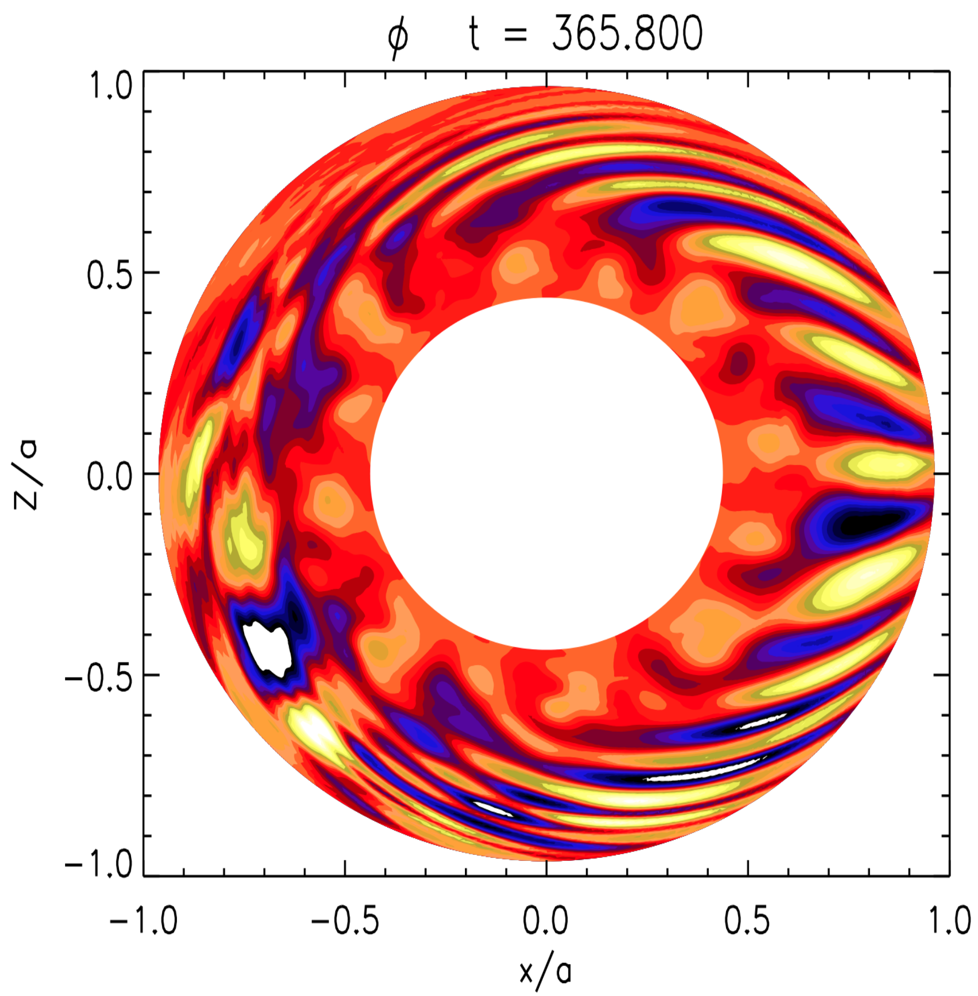
- Equilibrium statistical mechanics of gyrokinetic fluctuations
  - Review classic 2D/3D hydro/HM results by T.D. Lee, Kraichnan, Hasegawa-Mima (HM): inverse cascade in 2D because of 2 invariants. What happens in 2D gyrokinetics (GK) with many invariants?
  - Set up calculation: GK eqs., conserved quantities, Gibbs ensemble distribution function in extended phase space
  - Some interesting mathematical tricks
  - Plots of results: inverse cascade stronger in 2D GK than 2D HM
  - Recent interesting discovery of spontaneous spin up in bounded 2D hydro

Initial GYRO simulations of LTX

Lithium Tokamak eXperiment (LTX) exploring possible improved confinement with lithium walls: reduced recycling of cold neutrals will raise plasma temperature.

In ideal case $\nabla T=0$, but ∇n may drive TEM turbulence.

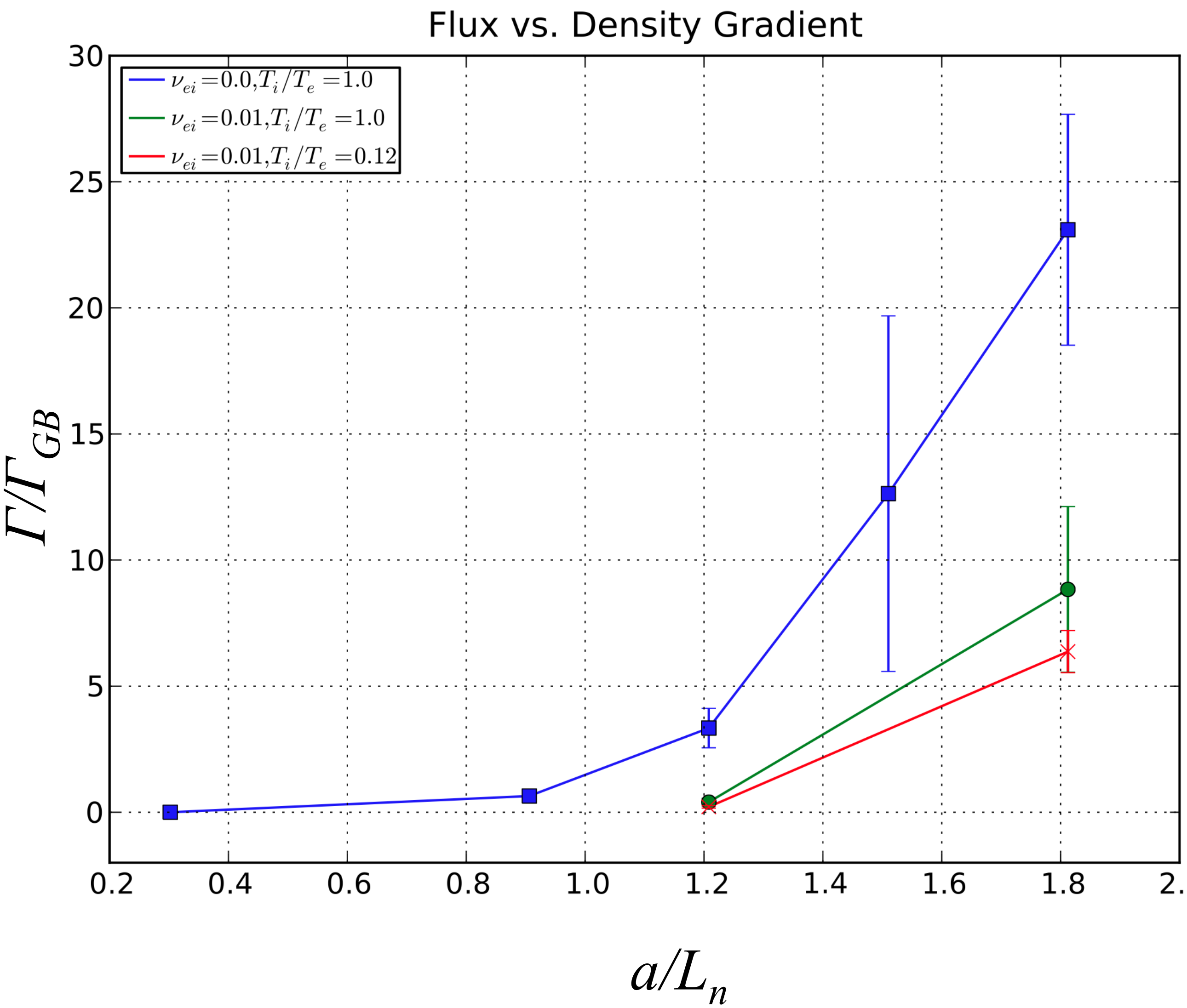
LTX $a/\rho_s \sim 25\text{-}35$ (at best ASTRA projections) making the whole plasma one large pedestal/edge region. Perhaps need improved outer boundary conditions to better model losses to wall? Spontaneous sheared flows may be important? 3D perturbations from VV eddy currents?



Granstedt (grad student) & Hammett

Beginning to use GYRO to study transport in ideal lithium-wall flat temperature regime

Exploring dependence of a critical R/L_n for TEM modes on collisionality and other parameters, in the small ρ/L flux-tube limit.

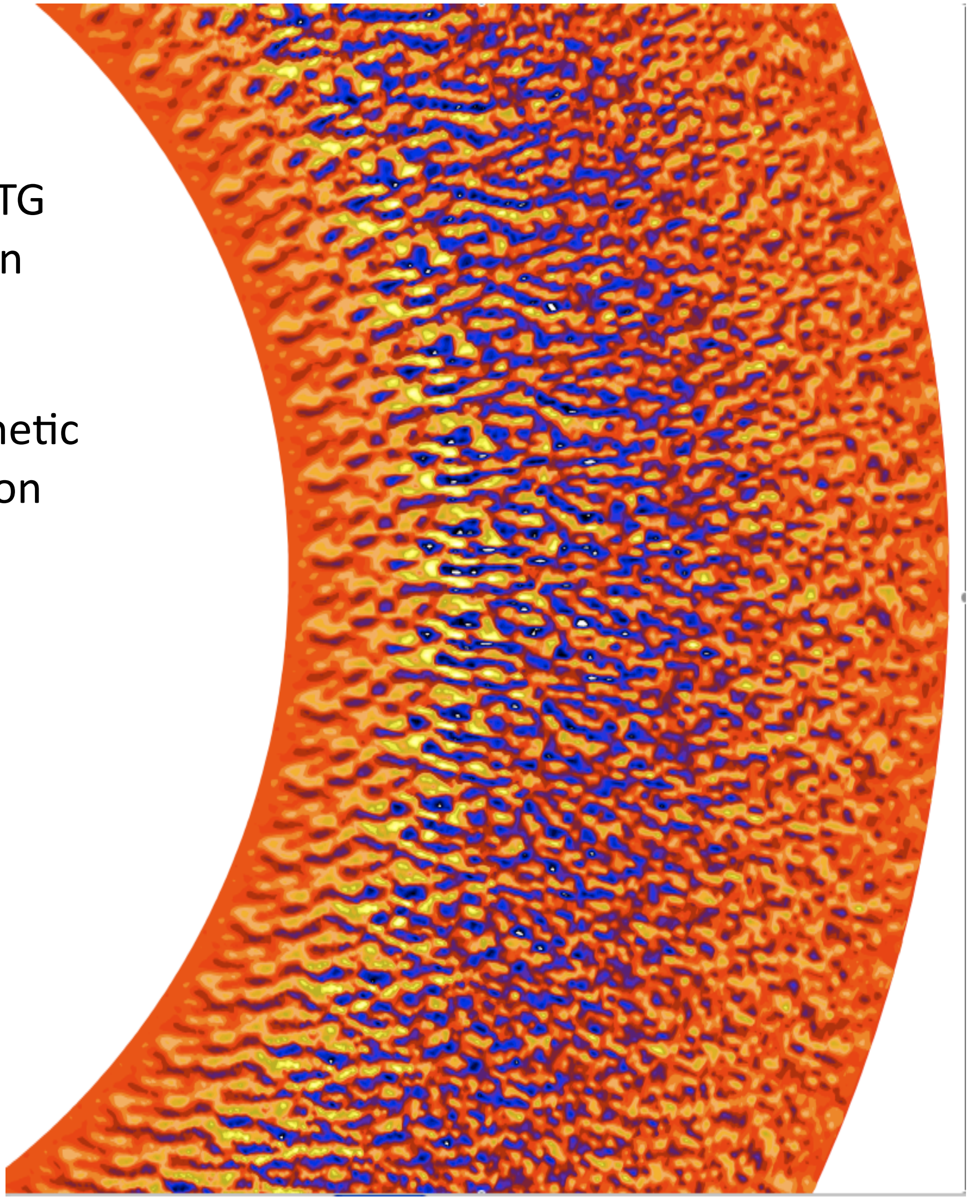


Granstedt (grad student) & Hammett

GYRO Simulations of ETG turbulence on NSTX

High resolution simulations of electron-scale ETG turbulence on NSTX using the GA GYRO code, in global/thick-annulus mode.

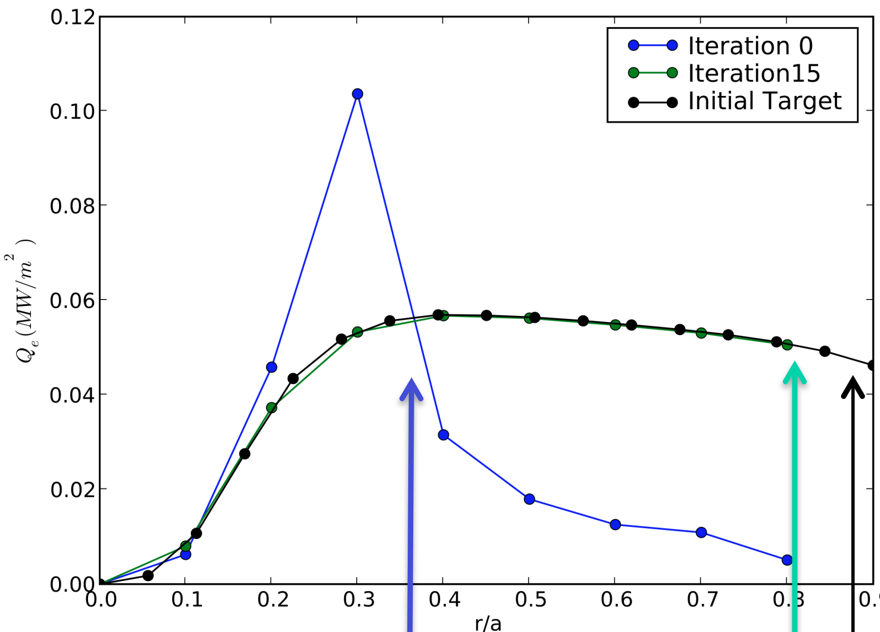
Will provide detailed validation tests of gyrokinetic codes, including synthetic diagnostic comparison with microwave scattering measurements.

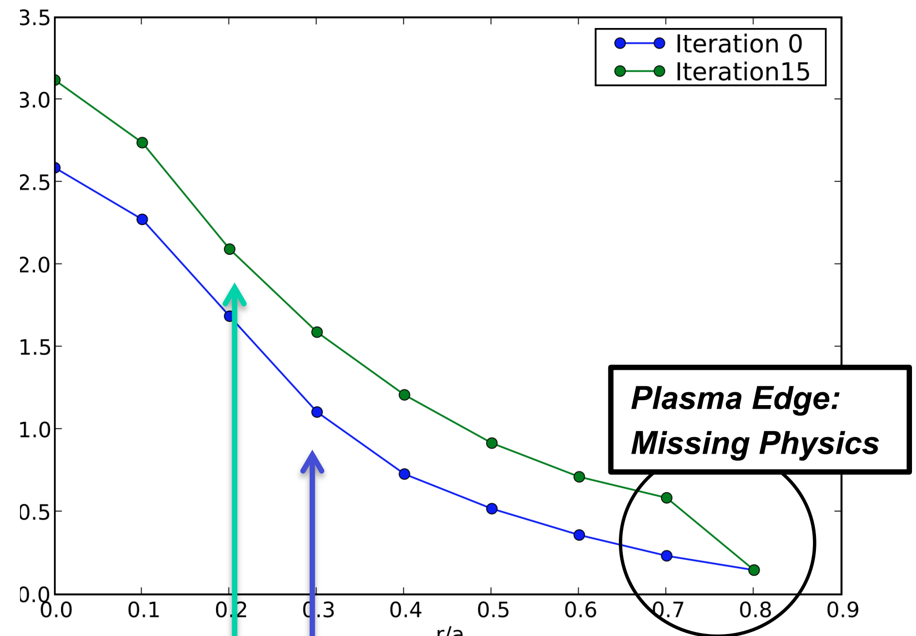


Peterson (grad student) & Hammett, CSPM collab.

TGYRO-TGLF Predicts Te for Low-Shear NSTX Discharge

$$Q_e \rightarrow T_e$$





Qe using Measured Te Profile

Qe using Predicted Te Profile

Measured Qe Profile

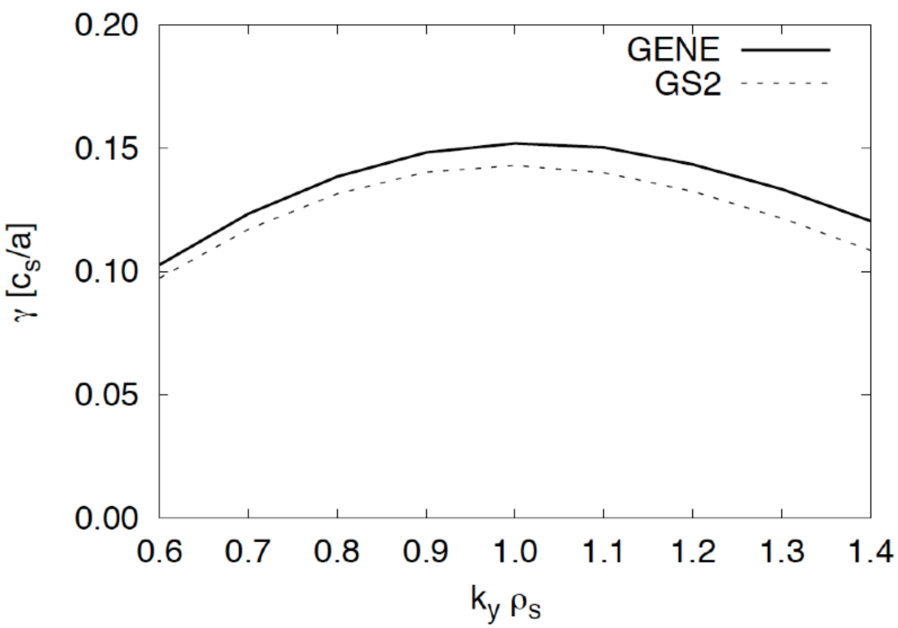
Measured Te Profile

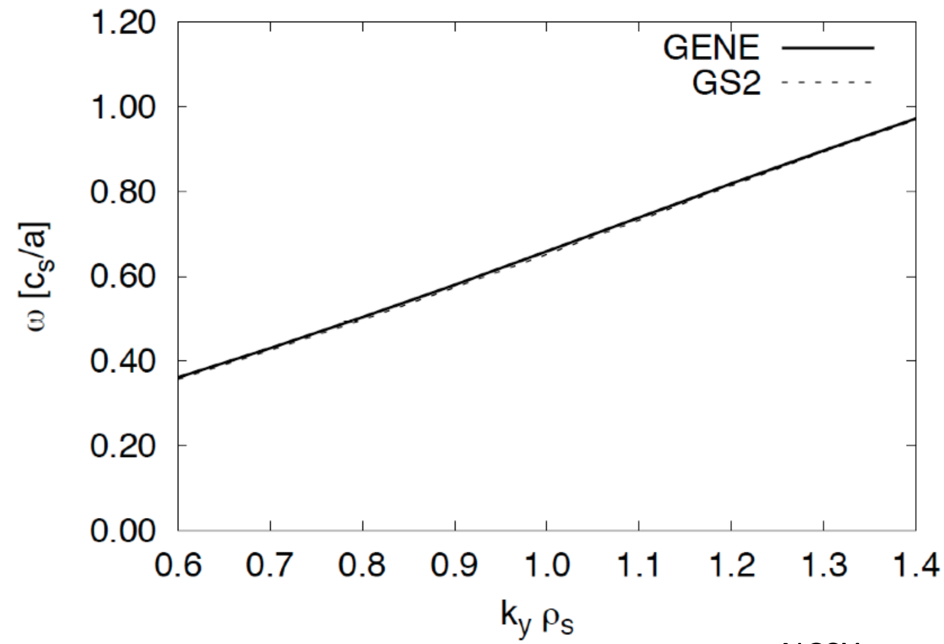
Predicted Te Profile

New Algorithm (Newton/Levenberg-Marquadt): < 15 iterations

Old Algorithm: No Convergence after 200 iterations

GS2 vs. GENE 3D benchmarks for stellarator geometry are close





NCSX case

Studying the nature of gyrokinetic turbulence in stellarators interesting, because stellarators:

- can have natural negative magnetic shear, & short connection length between regions of very high local magnetic shear: increase critical gradients & reduce turbulence?

- shaping flexibility → opportunities to optimize GK transport (Mynick et al. PRL 10)

Baumgaertel (grad student), Xanthopolous, Hammett, Mikkelsen
From D. Gates et al., 2010

Motivation for Studying Statistical Mechanics of Truncated Conservative Equations

- Very useful early studies of 2-D & 3-D hydrodynamics and fluid drift-wave turbulence
- Here we extend to higher dimensionality of gyrokinetics (2 x + 1 v, or 3 x+ 2 v)
- Kraichnan: prediction of inverse cascade in 2-D fluid turbulence because of simultaneous conservation of energy and enstrophy invariants
- Equilibrium spectrum predicted by statistical mechanics provides a rare analytic nonlinear result for testing codes.
- Equilibrium spectrum can also be used to test turbulence theories (DIA & relatives)
- Provide general insight into properties of the equations and resulting nonlinear dynamics, can help guide formulation of turbulence theories
- Interesting questions about relative cascade rates in various directions in phase space, mechanisms of irreversible particle heating at small scales, ion vs. electron heating.
- Improved turbulence theories could lead to improved subgrid models for nonlinear gyrokinetic codes.

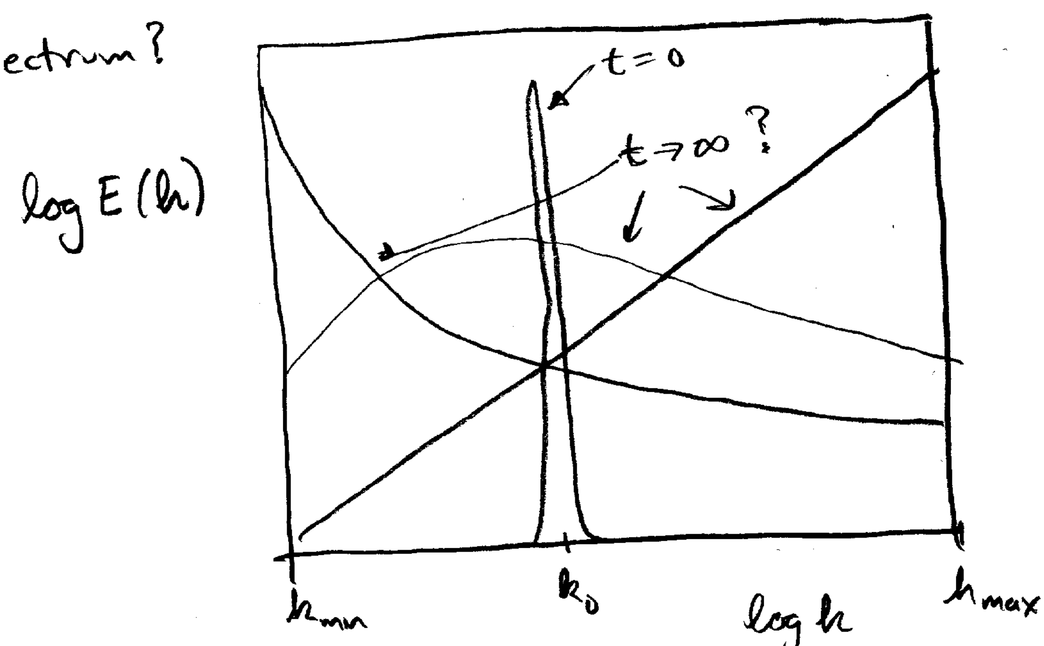
Equilibrium Statistical Mechanics of Gyrokinetic Fluctuations

Greg Hammett & Jian-Zhou Zhu
(U. Maryland / CMPD Postdoc)

(preprint available on request)

Numerical Gedanken Experiment:

Initialize fluctuations in a conservative gyrokinetic code with dissipation & driving instabilities turned off (uniform plasma background $\nabla n = \nabla T = 0$). (Can be done in GS2 & other GK codes.) Initial fluctuations localized in k. Modes will nonlinearly interact & couple energy to other modes. What is the long time, steady-state or ensemble-averaged spectrum?



Amazingly, an analytic solution can be found, using techniques from T. D. Lee (1952) et al.

General technique: statistical mechanics of truncated set of Fourier modes for Euler's nonlinear hydrodynamic equations, first worked out by T.D. Lee (1952) (related to Onsager earlier work on point vortices)

- Other contributions: Kraichnan, Montgomery, J.B. Taylor, …
- 3D PIC: Landon, 3D GK PIC: Krommes et al., Hammett & Nevins

2 Main Motivations for this study:

1. Insights into complex nonlinear system
   - Could help in developing statistical turbulence theories (like DIA/EDQNM/RMC) for gyrokinetic plasma turbulence
   - Could help in designing effective sub-grid models for gyrokinetic simulations

2. Rare analytic nonlinear benchmark test for gyrokinetic continuum codes (like previous GK PIC tests).

Classic Hydro Results

3D

$$E(k) \propto k^2$$

Only 1 invariant.

⇒ Forward cascade of energy to small scales.

Equipartition of energy $|V_k|^2$ among Fourier modes

$$E_{TOT} = \int dk\, E(k) = \int d^3k\, |V_k|^2 = 4\pi \int dk\, k^2 |V_{|k|}|^2$$

2D

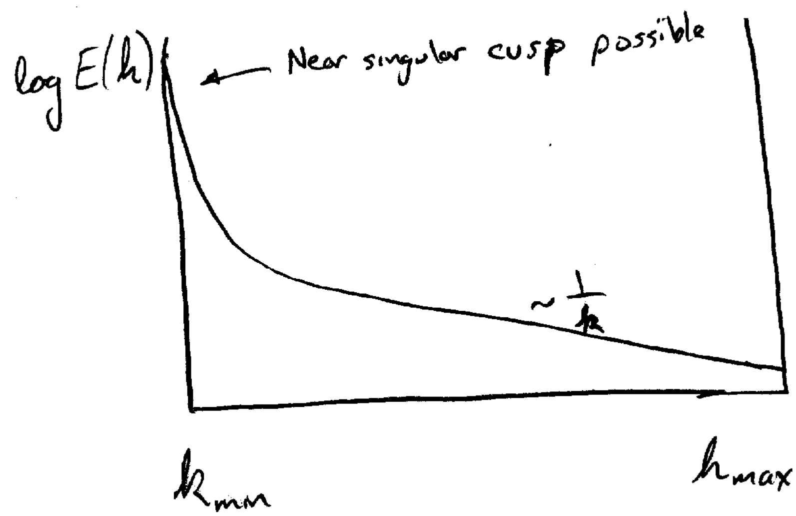
$$E(k) \propto \frac{k}{\beta + \alpha k^2}$$

2 invariants:
Energy + Enstrophy

⇒ Inverse cascade of Energy to large scales

(+ Forward cascade of enstrophy to small scales)

$\beta < 0$ "Negative temperature" state possible with energy condensing to largest wavelengths



Big difference between 3D & 2D Hydro because

3D has 1 invariant

2D has 2 (quadratic) invariants
(that are "rugged" + survive
Fourier-truncation.)

What happens in 2D Gyrokinetics
where there are many (N+1) invariants?
N = # of velocity grid points

GK Eqs. in 2D Limit

(Following notation of Plunk, Cowley, et al.)

Gyro-averaged Particle Distribution Function → g

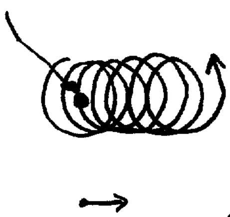
Gyro-averaged potential → $\overline{\Phi}$

$$\frac{\partial g(\underset{\sim}{x}, v_\perp, t)}{\partial t} + \underbrace{\{\overline{\Phi}, g\}}_{\underbrace{\hat{z}\times}\nabla\overline{\Phi}\cdot\nabla g} = 0$$

$v_\perp$: fast gyration velocity

$\hat{z}\times\nabla\overline{\Phi}\cdot\nabla g$: slow E×B drift

$\underset{\sim}{x}$ = guiding-center position



slow E×B drift

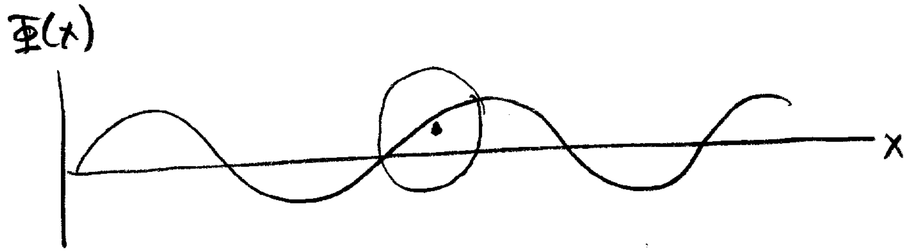
$$\overline{\Phi}(\underset{\sim}{x}, v_\perp, t) = \sum_{\underset{\sim}{k}} J_0(k_\perp v_\perp)\,\Phi_k\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}$$

$$J_0(k_\perp v_\perp) = \frac{1}{2\pi}\int d\theta\, e^{i k_\perp v_\perp \cos\theta}$$

Normalized units:

$v_t = 1$

$\rho_i = 1$



$$\Phi_k = \frac{2\pi}{\tau(\underset{\sim}{k}) + 1 - \Gamma_0(k_\perp^2)}\int dv_\perp\, v_\perp\, J_0(k_\perp v_\perp)\, g_k(v_\perp, t)$$

$$\boxed{\Phi_k \approx \beta(\underset{\sim}{k}) \sum_{i=1}^{N} \underbrace{\Delta v_i\, v_i\, J_0(k_\perp v_i)}_{w_i(k_\perp)}\, g_{k,i}(t)}$$

(Gauss-Legendre choice of points + weights can give super-exponential convergence $\sim (\Delta v)^N \sim \frac{1}{N^N}$; introduced by Kotschenreuther for GS2)

GK Eq. in Fourier space:

$$\frac{\partial g_{\underset{\sim}{k},i}}{\partial t} = \sum_{\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}} \hat{z}\cdot \underset{\sim}{p}\times\underset{\sim}{q}\; J_0(p_\perp v_i)\, \Phi_{\underset{\sim}{p}}(t)\, g_{\underset{\sim}{q},i}(t)$$

Conservation Properties of GK Eqs.:

Multiply GK. Eq. by g:

$$\frac{\partial}{\partial t}\frac{1}{2}g^2(\underset{\sim}{x}, v_\perp, t) + \underbrace{\hat{z}\times\nabla\Phi\cdot\nabla\frac{1}{2}g^2}_{} = 0$$

$$= \nabla\cdot\left[\left(\hat{z}\times\nabla\Phi\right)\frac{1}{2}g^2\right]$$

vanishes after integrating over all space

So $G(v_\perp) = \frac{1}{V}\int d^2x\, \frac{1}{2}g^2(\underset{\sim}{x}, v_\perp, t) = \text{const.}$

related to perturbed entropy.

(Higher order "Casimir invariants" $\propto \int d^2x\, g^p$ for $p>2$ not preserved by simple Fourier truncation of quadratic nonlinearity)

Two classes of quadratic invariants:

$$G_i = G(v_i) = \frac{1}{2}\sum_{\underset{\sim}{k}} |g(\underset{\sim}{k}, v_i)|^2$$

$$E = \pi\sum_{\underset{\sim}{k}}\frac{1}{\beta(k)}|\Phi_{\underset{\sim}{k}}|^2 = \pi\sum_{\underset{\sim}{k}}\beta(\underset{\sim}{k})\sum_i w_i\, g^*_{\underset{\sim}{k},i}\sum_j w_j\, g_{\underset{\sim}{k},j}$$

(Proved in Gabriel Plunk's thesis & other places.)

Statistical Mechanics for GK

Define $\underset{\sim}{g} \equiv \{ g_{\underset{\sim}{k},i} \}$ uniquely specifies the state of a system at a given time.

Can think of an ensemble of systems prepared in similar ways (with some constraints on I.C.'s):

$\mathbb{P}(\underset{\sim}{g}, t)$ = Probability a system is in state $\underset{\sim}{g}$ at time t.

Hyper phase space: $N_{TOT} = N_{\underset{\sim}{k}} N$ dimensional

$$\int dg_{\underset{\sim}{k}_1,1} \int dg_{\underset{\sim}{k}_2,1} \cdots \int dg_{\underset{\sim}{k}_1,2} \cdots \int dg_{N_{TOT}} \; \mathbb{P} = \int d\underset{\sim}{g} \, \mathbb{P} = 1$$

$\mathbb{P}(\underset{\sim}{g}, t)$ obeys a conservation law:

($\underset{\sim}{g}$ is indep. variable here & dep. var. in GK. Eq.)

$$\frac{\partial \mathbb{P}}{\partial t} + \frac{\partial}{\partial \underset{\sim}{g}} \cdot \left(\dot{\underset{\sim}{g}} \, \mathbb{P} \right) = 0$$

($\dot{\underset{\sim}{g}}$ given by G.K. Eq. in $\underset{\sim}{k}$ space.)

& $\mathbb{P}(\underset{\sim}{g}, t)$ obeys a Liouville theorem:

$$\boxed{\frac{\partial \mathbb{P}}{\partial t} + \dot{\underset{\sim}{g}} \cdot \frac{\partial \mathbb{P}}{\partial \underset{\sim}{g}} = 0}$$

or $\frac{D\mathbb{P}}{Dt} = 0$

$\mathbb{P}(\underset{\sim}{g}(t), t) = \text{const}$ along trajectories in hyper phase-space.

Liouville theorem holds because:

$$\frac{\partial}{\partial \underset{\sim}{g}} \cdot \dot{\underset{\sim}{g}} \Rightarrow \frac{\partial}{\partial g_{\underset{\sim}{k},i}} \dot{g}_{\underset{\sim}{k},i} = 0$$

↖ does not depend on $g_{\underset{\sim}{k}}$.

$$\dot{g}_{\underset{\sim}{k},i} = \sum_{\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}} \hat{z}\cdot \underset{\sim}{p}\times\underset{\sim}{q}\, J_0(p_\perp v_i)\, \Phi_{\underset{\sim}{p}}\, g_{\underset{\sim}{q},i}$$

If $\underset{\sim}{q}=\underset{\sim}{k}$ then $\underset{\sim}{p}=\underset{\sim}{k}-\underset{\sim}{q}=0$ & nonlinearity vanishes.

Because a Liouville theorem holds, all the results (& assumptions) of classical statistical mechanics can be used.

If dynamics is sufficiently mixing, so an Ergodic Hypothesis holds, then can use a microcanonical ensemble:

$$\mathbb{P}(\underset{\sim}{g}) \propto \delta(E(\underset{\sim}{g})-E_0)\prod_i \delta(G_i(\underset{\sim}{g})-G_{i0})$$

A Gibbs canonical ensemble is a good approx. to this for a large # of D.O.F.

Gibbs canonical ensemble:

Find $\mathbb{P}$ that is as uniform as possible

(maximizes entropy $\propto -\int d\underline{g}\, \mathbb{P} \log \mathbb{P}$)

subject to constraints on the average values

of the conserved quantities. $\Rightarrow$

$\log \mathbb{P}$ is a linear combination of conserved quantities:

$$\boxed{\mathbb{P}(\underline{g}) \propto \exp\left[-\left(\alpha_0 E + \sum_i \alpha_i G_i\right)\right]}$$

$$\propto \exp\left[-\frac{1}{2}\left(\sum_{i=1}^{N} \alpha_i \sum_{\underline{k}} |g_{\underline{k},i}|^2 + \alpha_0 2\pi \sum_{\underline{k}} \beta(\underline{k}) \sum_i w_i(\underline{k})\, g^*_{\underline{k},i} \sum_j w_j(\underline{k}) g_{\underline{k},j}\right)\right]$$

$$\propto \exp\left[-\frac{1}{2}\sum_{\underline{k}} \sum_i \sum_j g^*_{\underline{k},i}\left[\delta_{ij}\alpha_i + \alpha_0 2\pi\beta(\underline{k}) w_i(\underline{k}) w_j(\underline{k})\right] g_{\underline{k},j}\right]$$

$$\propto \exp\left[-\frac{1}{2}\sum_{\underline{k}} \underline{g}^*_{\underline{k}} \cdot \underline{\underline{M}}_{\underline{k}} \cdot \underline{g}_{\underline{k}}\right]$$

↑ vector of different velocity values at a given $\underline{k}$.

$\mathbb{P}$ has form of a Multivariate Gaussian distribution

Can find covariance matrix $\frac{1}{2}\langle \underline{g}^*_{\underline{k}}\, \underline{g}_{\underline{k}} \rangle = \underline{\underline{C}}_{\underline{k}} = \underline{\underline{M}}_{\underline{k}}^{-1}$

$$\frac{1}{2}\langle g^*_{\underline{k},i}\, g_{\underline{k},j}\rangle = C_{\underline{k},i,j}$$

All very nice; but $\underset{\approx}{M}_{\underset{\sim}{k}}$ is a dense $N \times N$ matrix

& finding its inverse would seem to be difficult.

$\alpha_0 = 0$ limit: $\underset{\approx}{M} \Rightarrow$ diagonal & easily inverted.

Small $\alpha_0 \Rightarrow$ Matrix Taylor series expansion

& discover it can be summed to all orders.

$\Rightarrow$ Special case of Sherman – Morrison formula.

2D GK Equilibrium Spectrum Results

$$D_{\underset{\sim}{k}} = \frac{\pi}{\beta(\underset{\sim}{k})} \langle |\Phi_{\underset{\sim}{k}}|^2 \rangle = \frac{\pi \beta(\underset{\sim}{k}) \sum_i w_i^2(\underset{\sim}{k})/\alpha_i}{1 + \alpha_0 \, 2\pi \beta(\underset{\sim}{k}) \sum_i w_i^2(\underset{\sim}{k})/\alpha_i}$$

$$G_{\underset{\sim}{k},i} = \frac{1}{2} \langle |g_{\underset{\sim}{k},i}|^2 \rangle = \frac{1}{2\alpha_i} \left[1 - \frac{\alpha_0 \, 2\pi \beta(\underset{\sim}{k}) w_i^2(\underset{\sim}{k})/\alpha_i}{1 + \alpha_0 \, 2\pi \beta(\underset{\sim}{k}) \sum_i w_i^2(\underset{\sim}{k})/\alpha_i} \right]$$

where α_i's & α_0 are determined by initial conditions:

$$E_0 = \sum_{\underset{\sim}{k}} D_{\underset{\sim}{k}} = E_0(\underset{\sim}{\alpha})$$

$$G_{i0} = \sum_{\underset{\sim}{k}} G_{\underset{\sim}{k},i} = G_{i0}(\underset{\sim}{\alpha})$$

Wrote a nonlinear root solver to determine $\underset{\sim}{\alpha}$ for specified I.C.'s.

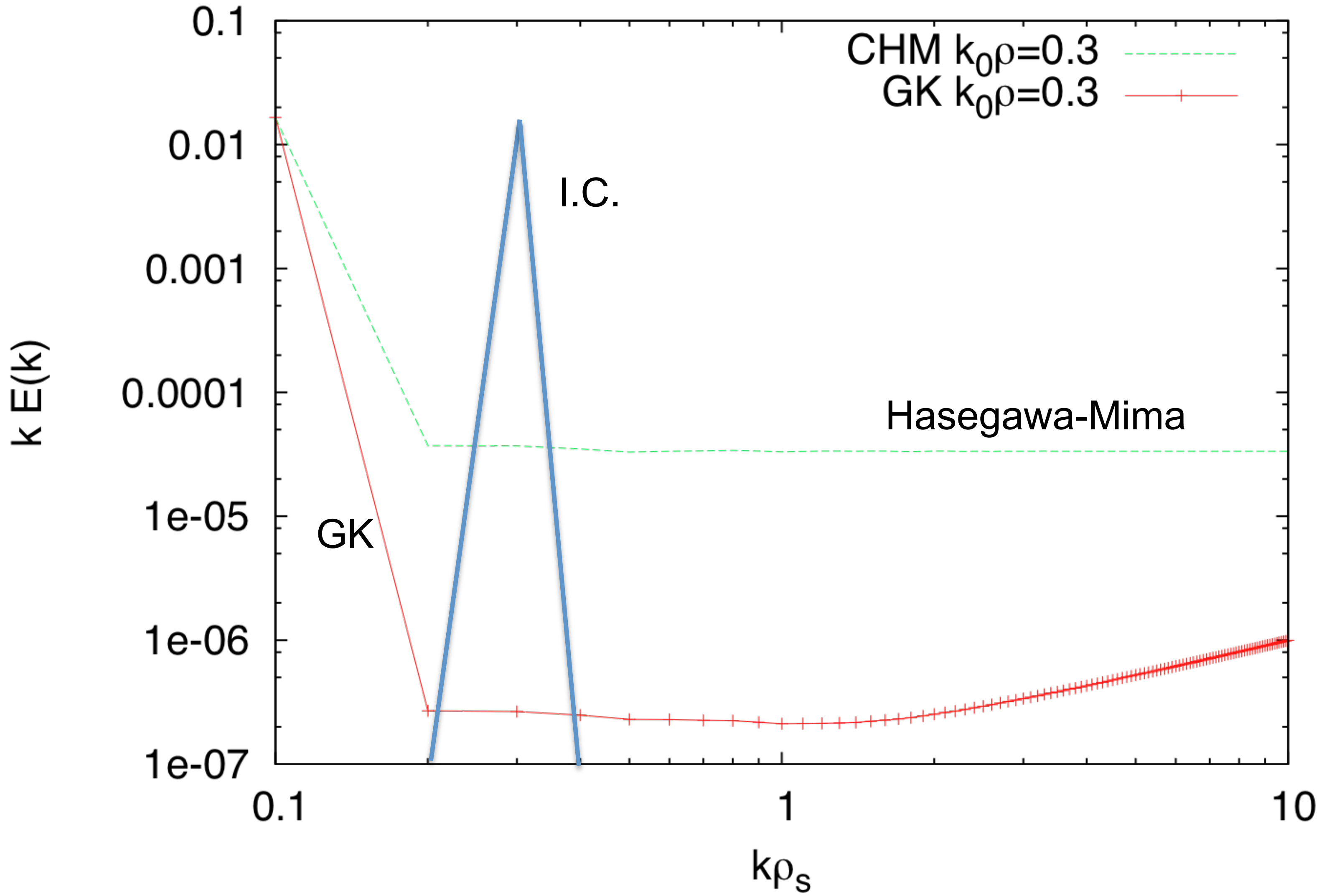
Consider E_0 & G_{i0} given by I.C:

$$g(\underset{\sim}{x}, v_\perp) = \cos(k_0 x) \frac{e^{-v_\perp^2/2}}{2\pi} J_0(k_0 v_\perp)$$

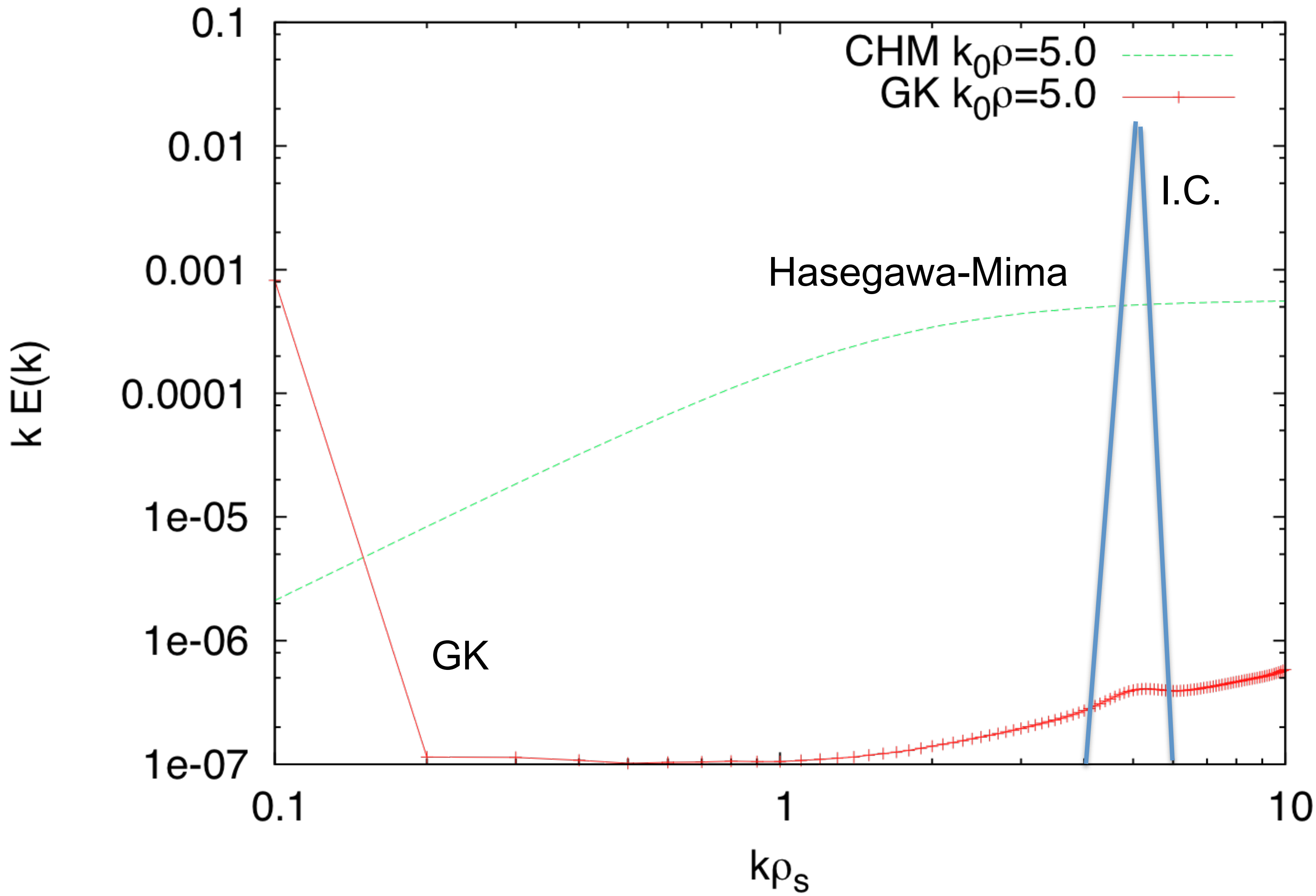
Plots of resulting spectra find stronger inverse cascade than for Hasegawa-Mima.

Entropy related invariant G_i not the same as the HM enstrophy invariant, which exists only if $T_i = 0$.

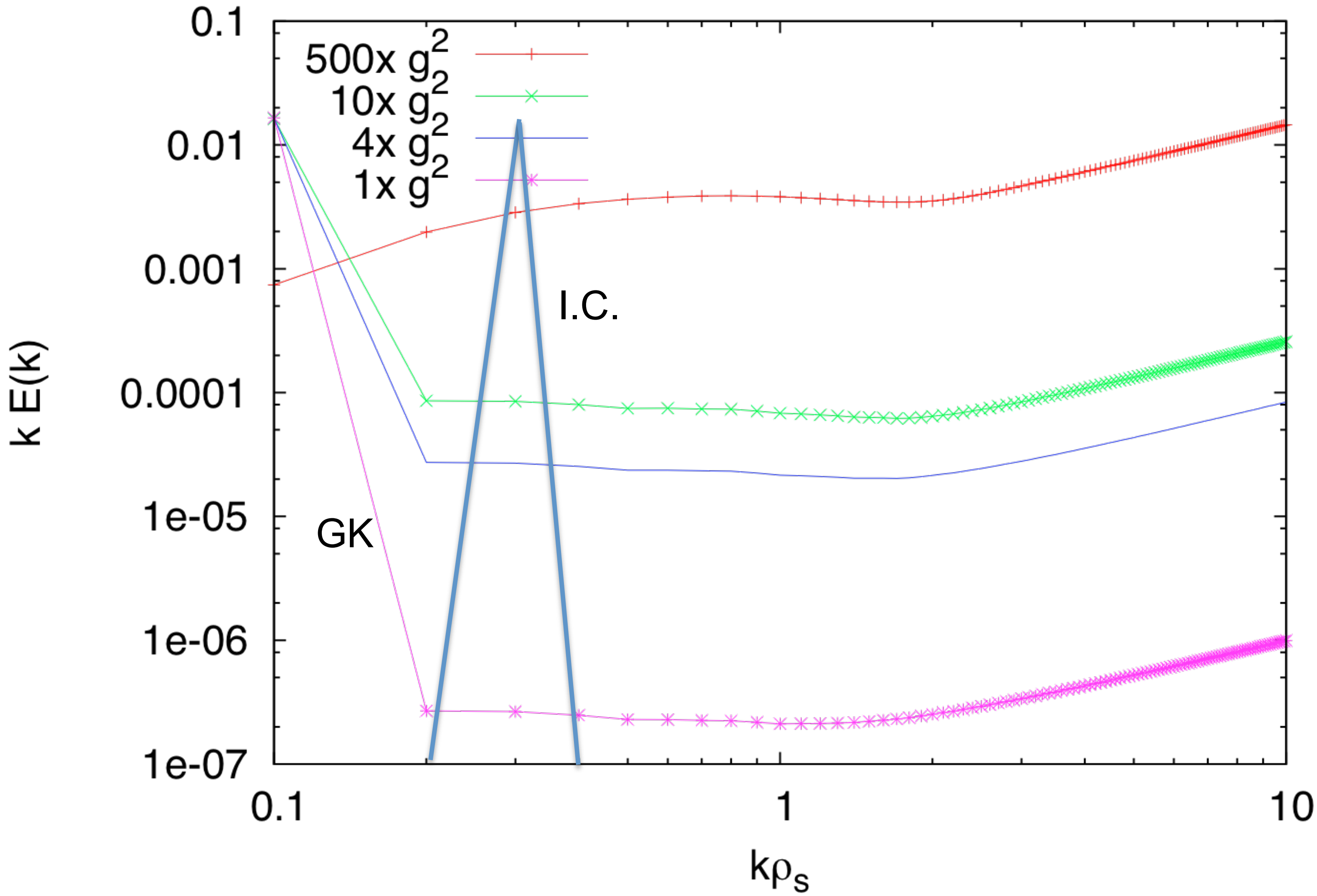
Both gyrokinetic and HM spectra show inverse cascade of energy relative to initial condition



If I.C. is at high k, near k_{max}, then inverse energy cascade in HM is limited because the forward enstrophy cascade is limited. But GK shows a stronger inverse cascade.



Adding an incoherent part to g that has zero velocity integral (so does not contribute to the electrostatic energy) but increases the $G(v) \sim \langle g^2 \rangle$ quantities, causes an increase in the high-k tail.



3D GK Equil. Spectra

Only 1 invariant, generalized free energy.

$$\langle |\Phi_k|^2 \rangle = \frac{\overline{g^2}}{N N_k} \frac{\Gamma_0(k_\perp^2)}{(\tau + 1 - \Gamma_0(k_\perp^2))(\tau+1)}$$

Equiv. to PIC result of Krommes et al. + Nevins + Hammett

Equipartition in $k_\parallel$ (except $\tau(k)=0$ for $k_\parallel=0$ ZF's).

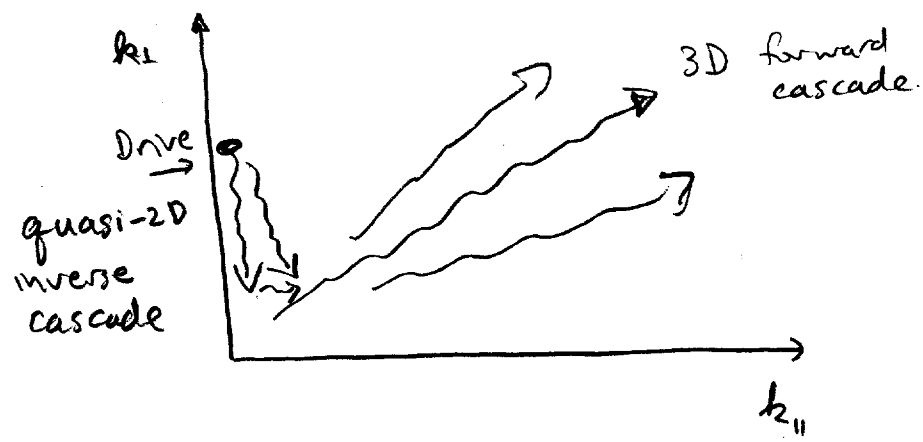
for $N_{particles} \Longleftrightarrow N N_k$

$$\langle w^2 \rangle \Longleftrightarrow \overline{g^2} = \frac{1}{V} \int d^3x \int d^3v \; \frac{g^2}{F_0}$$

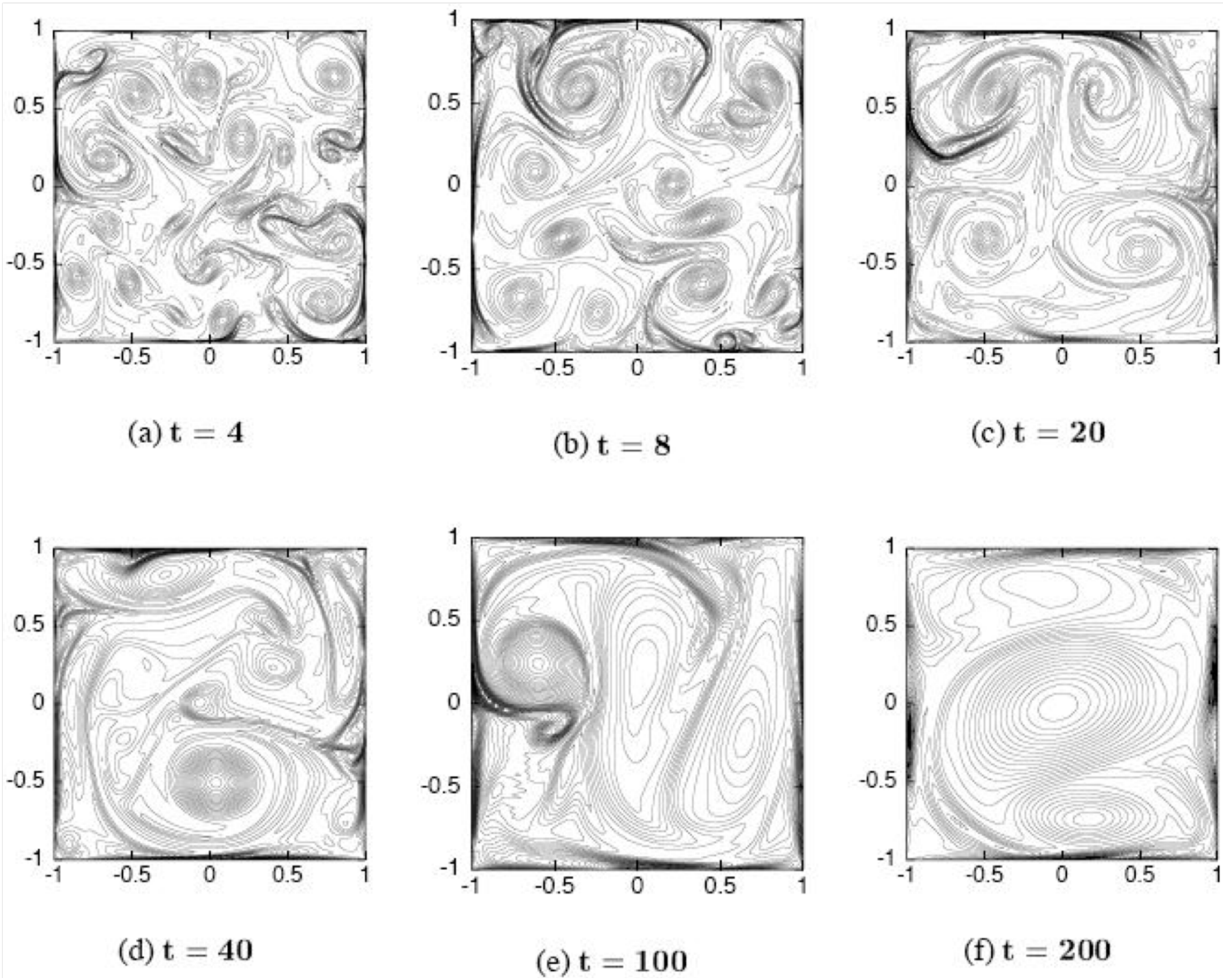
"Test particle superposition principle"

$\Rightarrow$ "Test mode superposition principle"

2D/3D GK implications!

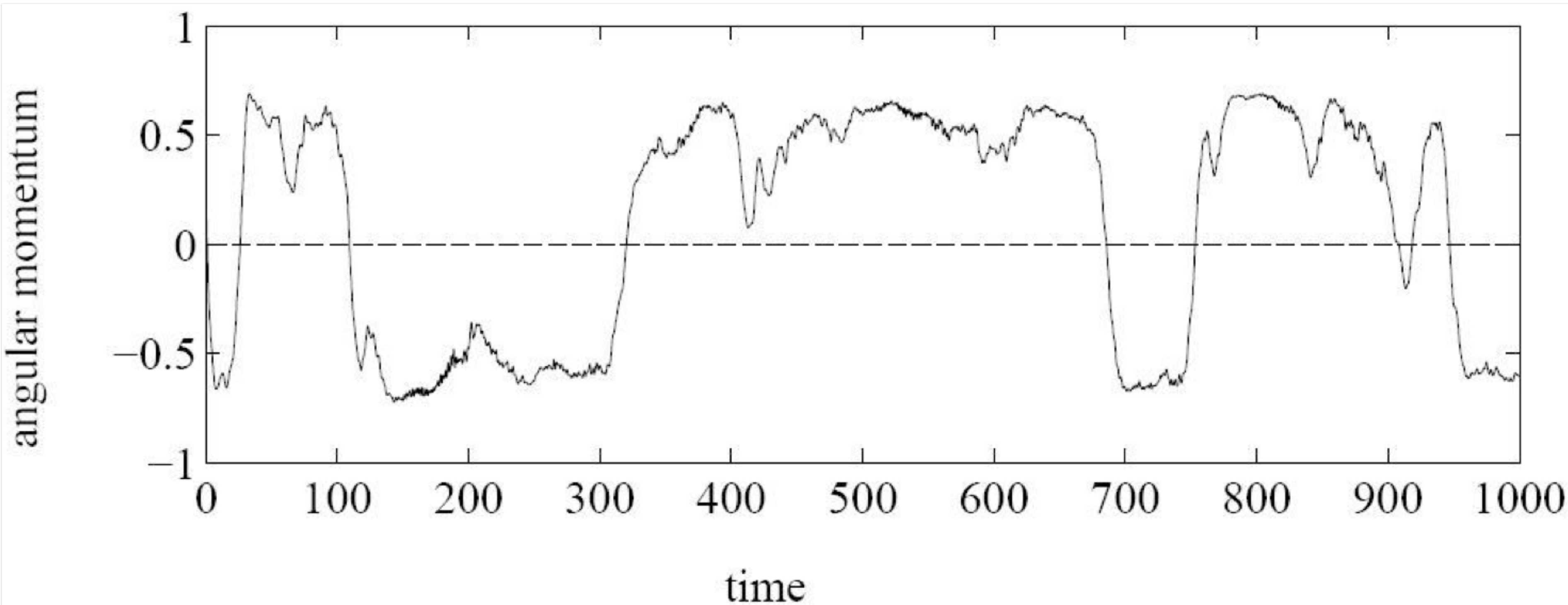


Spontaneous spin-up in 2-D bounded hydro discovered



Decaying 2D turbulence sim., Clercx 1997 (from van Heijst and Clercx 2009)

Spontaneous spin-up in 2-D bounded hydro is large: ~50% of kinetic energy in net solid body rotation



J.B. Taylor, Borchardt, & Helander PRL09: statistical equilibrium theory explains spontaneous spin-up, influence of boundary shape

Driven 2D turbulence sim., Molenaar et al. 2004(from van Heijst and Clercx 2009)

Possible Future Work

- Multiple kinetic species, including kinetic electrons & ions
- Add $\delta B_{\perp}$, study characteristics of stochastic magnetic field, impact on zonal flows
- Include ∇B and curvature drift terms.
- Study spontaneous spinup possibilities?
- Extend δf to full F formulation w/ $E_{//}$ nonlinearities
- Test in GS2 or other GK codes.
- EDQNM or other statistical theories for GK, should be able to reproduce these spectra in the unforced, dissipationless limit
- EDQNM or other statistical theories for more realistic case of driven, dissipative, GK turbulence

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  - Set up calculation: GK eqs., conserved quantities, Gibbs ensemble distribution function in extended phase space
  - Some interesting mathematical tricks
  - Plots: inverse cascade stronger in 2D GK than 2D HM
  - Recent interesting discovery of spontaneous spin up in bounded 2D hydro