Numerical Aspects of Drift Kinetic Turbulence: Illposedness, Regularization and Apriori Estimates of SGS Terms

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# Outline

- Introduction and motivation
- A new 4D drift kinetic code
  - Higher -- order numerical method
- Numerical results
  - Comparison with different methods
  - Ill-posedness and regularization
- LES for plasma turbulence
  - Primer on hydrodynamic turbulence
  - Quantification of SGS terms
- Summary and future work



## Introduction

- GOAL: Develop "sub-grid-scale" models for kinetic and gyrokinetic plasma turbulence simulations
  - To compute plasma turbulence at a coarse-grain resolution without sacrificing physics accuracy
  - Fully resolved simulations are prohibitively expensive
- Motivation for current investigation
  - CPES (US DOE Scidac Center) is addressing the issue of coupling "coarse-grained" XGC0 simulations with "fine-grained" XGC1 simulations
  - Hydrodynamic turbulence simulations frequently employ "large eddy simulation (LES)" methodology to capture "sub-gridescale (SGS)" physics

## Introduction – Present Work

- Investigate numerical aspects of plasma turbulence simulations in the context of drift-kinetic turbulence in 4D
  - 5D and 6D fully-resolved simulations are still computationally expensive
- Developed an Eulerian drift-kinetic code
  - Investigate a variety of numerical algorithms
- Perform "Direct Numerical Simulations", i.e., fullyresolved simulations
  - What does fully-resolved mean?
  - Role of collisions (models) and regularization of the equations
- Quantify the SGS terms
  - a priori estimates: perform DNS, filter and examine SGS terms
  - a posteriori: perform LES and compare with filtered DNS to examine the efficacy of the SGS model

# Background

- Science question: In gyrokinetic plasma turbulence, what are the mechanisms of energy cascade from large to small scales?
  - A good exposition of the nonlinear route to dissipation in phase space given by Schekochihin et al. (Plasma Phys. Control. Fusion 2008, Astrophysiical J. Supp. 2009)
  - If the collision frequency is small, the distribution function develops small features in velocity space
  - Collisionless (Landau) damping redistributes generalized energy: electromagnetic fluctuations are converted to entropy fluctuations
  - In order for any heating to occur, the entropy fluctuations must cascade in phase space to collisional scales. Collisions, even if infrequent, are necessary to complete the cascade and satisfy Boltzman H-theorem. Collisions are necessary for the system to converge to a statistical steady-state
- Other relevant papers
  - Howes (PRL 2008), Tatsuno et al. (PRL 2009), Howes (PRL 2011): AstroGK code
  - A. Bañón Navarro et al. (PRL 2011): GENE code. Also discuss SGS modeling for plasma turbulence
  - Watanabe and Sugama (PoP 2004) and many others by this group.
  - Grandgirard et al. (Plasma Phys. & Controlled Fusion, 2008): GYSELA code
- GYSELA code (Grandgirard et al., J. Comput. Phys. 2006)
  - Solves the 4D drift kinetic and 5D gyrokinetic systems
  - Semi-Lagrangian approach (splitting second order)
  - Second-order Poisson solver



# **4D Drift-kinetic Vlasov Equation**

$$\frac{\partial f}{\partial t} + \vec{v}_{GC} \cdot \vec{\nabla}_{\perp} f + v_{\parallel} \frac{\partial f}{\partial z} + \dot{v}_{\parallel} \frac{\partial f}{\partial v_{\parallel}} = 0$$

where 
$$\vec{\nabla}_{\perp} = \left(\frac{\partial}{\partial r}, \frac{1}{r}\frac{\partial}{\partial \theta}\right)$$

- distribution function  $f(x,y,z,v_{\parallel},t)$  in 4D

- drift velocity 
$$\vec{v}_{GC} = \frac{\left(\vec{E} \times \vec{B}\right)}{B^2}$$
,  $\vec{B} = B\vec{e}_z$  in the "toroidal" direction

-  $v_{\parallel}$  : velocity along the magnetic field lines

$$\dot{v}_{\parallel} = \frac{q}{m_i} E_z$$
, q: ion charge, m: ion mass

Adiabatic electrons



#### Poisson equation in cylindrical geometry

$$\left[ -\nabla_{\perp} \left[ \frac{n_0(r)}{B\Omega_0} \nabla_{\perp} \phi \right] + \left[ \frac{en_0(r)}{T_e(r)} \left( \phi - \left\langle \phi \right\rangle \right) \right] = n_i - n_0$$

#### linearized polarization term

- φ: electric potential;
- $\vec{E} = -\vec{\nabla}\phi$  electric field;
- ion cyclotron frequency  $\Omega_0 = q_i B_0 / m_i$ ;
- Te: electron temperature profile;
- no: electron density profile;
- ion density profile  $n_i(r,\theta,z,t) = \int dv_{\parallel} f(r,\theta,z,v_{\parallel},t)$

- 
$$\langle \cdot \rangle = \frac{1}{L_z} \int dz$$
, average on the magnetic field lines

adiabatic response of the electrons

# **Initial and Boundary Conditions**

Local Maxwellian as the equilibrium part:  $f = f_{ea} + \delta f$ -

$$f_{eq}(r, v_{\parallel}) = \frac{n_0(r)}{(2\pi T_i(r)/m_i)^{1/2}} \exp\left(-\frac{m_i v_{\parallel}^2}{2T_i(r)}\right)$$

- Perturbation:  $\delta f = f_{eq}g(r)h(v_{\parallel})\delta p(\theta,z)$ 

where 
$$g(r)$$
 and  $h(v_{\parallel})$  are exponential functions

$$\delta p(\theta, z) = \sum_{m,n} \varepsilon_{mn} \cos\left(\frac{2\pi n}{L_z}z + m\theta + \phi_{mn}\right)$$

where  $\epsilon_{mn}$  and  $\phi_{mn}$  are the random amplitude and random phase for the mode (m,n)

Periodic boundary condition on  $\theta$  and z Boundary condition on r: zero flux of f Homogeneous Neumann (Dirichlet) boundary condition for potential in r at 0 (r<sub>max</sub>)



## Normalization

- Temperature  $\hat{T} = \frac{T}{T_{e0}}$ , where  $\frac{T_e(r_0)}{T_{e0}} = 1$ ; Time  $\hat{t} = \Omega_0 t$ , where  $\Omega_0 = q_i B_0 / m_i$  length  $\hat{l} = (\Omega_0 / c_s)!$
- Velocity  $\hat{v} = \frac{v}{c_s}$ , normalized to the sound speed  $c_s = \sqrt{\frac{T_{e0}}{m}}$
- Potential & electric field  $\hat{\Phi} = (q_z / T_{z0}) \Phi, \quad \hat{E} = (1/c_s B_0) E$

#### Normalized equations:

- Vlasov equation:  $\frac{\partial f}{\partial t} + \vec{v}_{GC} \cdot \vec{\nabla}_{\perp} f + v_{\parallel} \frac{\partial f}{\partial z} + E_z \frac{\partial f}{\partial v_{\parallel}} = 0$ Poisson equation:

$$-\nabla_{\perp} \left[ \frac{n_0(r)}{B} \nabla_{\perp} \phi \right] + \frac{n_0(r)}{T_e(r)} \left( \phi - \left\langle \phi \right\rangle \right) = n_i - n_0$$
  
Initial condition: 
$$f_{eq}(r, v_{\parallel}) = \frac{n_0(r)}{\left(2\pi T_i(r)\right)^{1/2}} \exp\left(-\frac{v_{\parallel}^2}{2T_i(r)}\right) \tag{KAUST}$$

# **Numerical Method**

In the uniform field case, the Liouville theorem is applicable

$$\vec{\nabla}_{\perp} \cdot \vec{v}_{GC} + \frac{\partial v_{\parallel}}{\partial z} + \frac{\partial v_{\parallel}}{\partial v_{\parallel}} = 0$$

Hence the Vlasov equation can be written in <u>conservative</u> form:

$$\frac{\partial f}{\partial t} + \vec{\nabla}_{\perp} \cdot \left(\vec{v}_{GC} f\right) + \frac{\partial}{\partial z} \left(v_{\parallel} f\right) + \frac{\partial}{\partial v_{\parallel}} \left(\dot{v}_{\parallel} f\right) = 0$$

Time evolution for

$$\frac{\partial f}{\partial t} = -divy$$

2<sup>nd</sup> and 3<sup>rd</sup> order TVD Runge-Kutta. 2<sup>nd</sup> order scheme written below:

$$f^{n+1} = \frac{\left(f_1 + f_2\right)}{2}$$
$$f_1 = f^n + \Delta t \cdot f^{'n}$$
$$f_2 = f^n + \Delta t \cdot f_1^{'}$$



# **Numerical Method**

For numerical stability, it was empirically found that the following form of the equations leads to a much more robust and stable numerical simulations and requires no filtering (δf numerics on full-f equation)

$$f' = f - f_{eq}$$
$$\frac{\partial f'}{\partial t} + \nabla_{\perp} \cdot \boldsymbol{v}_{\perp} f' + \frac{\partial v_{\parallel} f'}{\partial z} + \frac{\partial v_{\parallel} f'}{\partial v_{\parallel}} + S = 0$$
$$S = E_{\theta} f_{eq} \frac{T'_i(r)}{T_i(r)} \left[ \frac{v_{\parallel}^2}{2T_i(r)^2} + \frac{n'_0(r)}{n_0(r)} - \frac{1}{2} \right] - E_z f_{eq} \frac{v_{\parallel}}{T_i(r)}$$



# Numerical Method Cont.

- Finite volume discretization:

$$c\frac{\partial f}{\partial x} = \frac{\partial F_x}{\partial x} = \frac{F_x\left(i + \frac{1}{2}, j\right) - F_x\left(i - \frac{1}{2}, j\right)}{\Delta x}$$

-High order upwind discretization

1st, 3rd, 5th and 7th order options in the code

-Central finite difference discretization

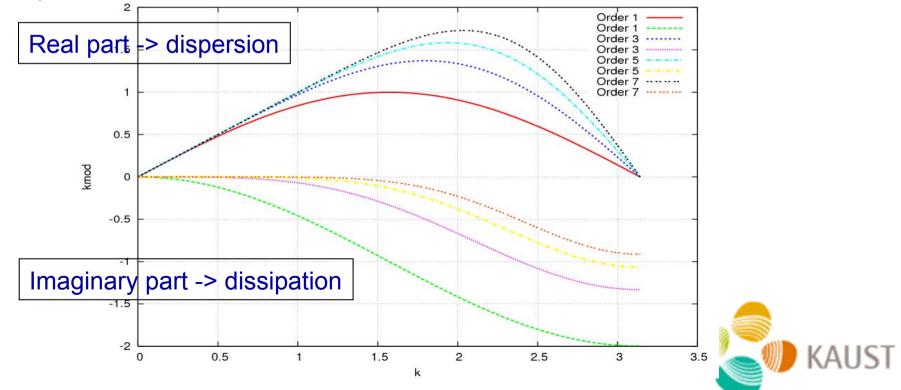
2<sup>nd</sup>, 4<sup>th</sup> order, 2<sup>nd</sup> and 4<sup>th</sup> order tuned finite difference options in the code - Example: 5<sup>th</sup> order upwinding flux calculation:

$$F\left(i+\frac{1}{2}\right) = \frac{1}{30}F(i-2) - \frac{13}{60}F(i-1) + \frac{47}{60}F(i) + \frac{9}{20}F(i+1) - \frac{1}{20}F(i+2) \quad \text{if } c > 0$$
$$\frac{1}{30}F(i+3) - \frac{13}{60}F(i+2) + \frac{47}{60}F(i+1) + \frac{9}{20}F(i) - \frac{1}{20}F(i-1) \quad \text{if } c < 0$$

References: 1) Hill and Pullin, J. Comput. Phys. 2004, for tuned finite differences 2) Pirozzoli, J. Comput. Phys. 2002. for upwind-biased fluxes

#### **Numerical Method - Dispersion & Dissipation**

- Drift-kinetic PDEs have no natural dissipation
  - Unless collision operator is included
- In the absence of physical dissipation (except Landau damping), we may resort to "numerical" dissipation to provide high-frequency cut-off (Note that the centered finite differences have no numerical dissipation)
- For 1st, 3rd, 5th and 7th order upwind methods, the dissipation and dispersion characteristics are shown in the figure below



#### **Poisson Solver**

Average on z and subtracted from original Poisson equation

Poisson: 
$$-\nabla_{\perp} [a \nabla_{\perp} \phi] + b (\phi - \langle \phi \rangle) = n_i - n_0$$
, where  $a = \frac{n_0}{R}$ 

 $b = \frac{n_0(r)}{T_a(r)}$ 

Fourier expansion:

$$\phi(r,\theta,z) = \sum_{m} \sum_{n} \phi^{m,n}(r) \exp(im\theta) \exp(inz)$$

Results in a penta-diagonal solve:

$$A\hat{\phi}(i-2) + B\hat{\phi}(i-1) + C\hat{\phi}(i) + D\hat{\phi}(i+1) + E\hat{\phi}(i+2) = \hat{R}$$
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## Poisson Solver Cont.

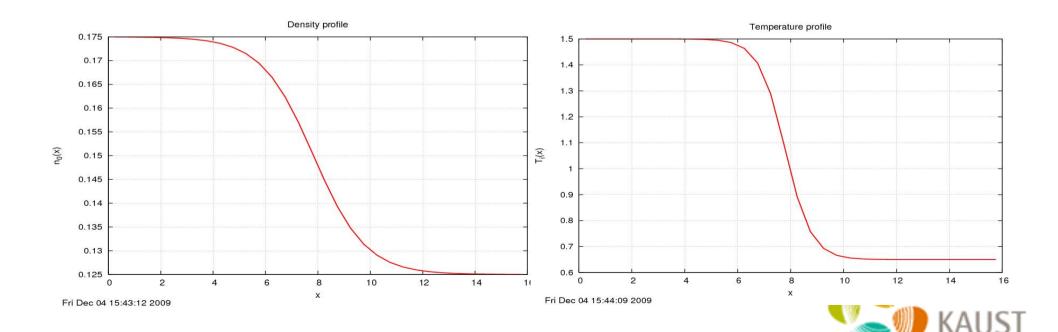
$$A = \frac{a(r)}{12\Delta r^{2}} - \frac{1}{12\Delta r} \left( \frac{da(r)}{dr} + \frac{a(r)}{r} \right) \qquad B = -\frac{4a(r)}{3\Delta r^{2}} + \frac{2}{3\Delta r} \left( \frac{da(r)}{dr} + \frac{a(r)}{r} \right),$$

$$C = \frac{5a(r)}{2\Delta r^{2}} + \frac{n^{2}a(r)}{r} + b(r) \qquad D = -\frac{4a(r)}{3\Delta r^{2}} - \frac{2}{3\Delta r} \left( \frac{da(r)}{dr} + \frac{a(r)}{r} \right),$$

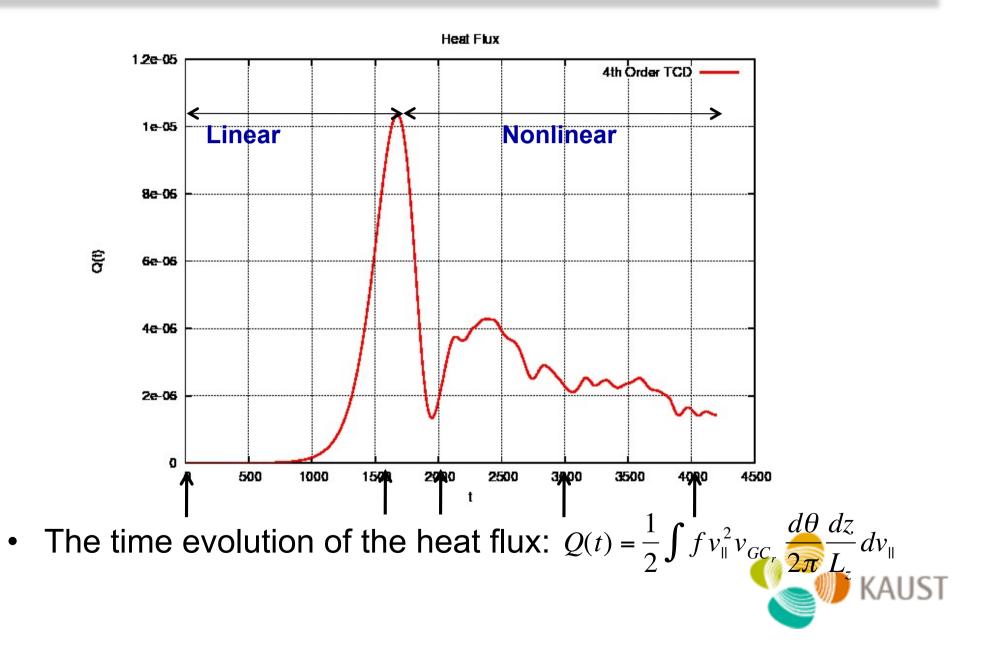
$$E = \frac{a(r)}{12\Delta r^{2}} + \frac{1}{12\Delta r} \left( \frac{da(r)}{dr} + \frac{a(r)}{r} \right)$$
Together with Neumann and Dirichlet boundary condition:
$$\begin{pmatrix} C + B & D + A & E \\ B - A & C & D & E \\ A & B & C & D & E \\ \dots & \dots & \dots & \dots & \dots \\ A & B & C & D & E \\ \dots & \dots & \dots & \dots & \dots \\ A & B & C & D & E \\ A & B & C & D & E \\ \dots & \dots & \dots & \dots & \dots \\ A & B & C & D & E \\ A & B & C & D & E \\ \dots & \dots & \dots & \dots & \dots \\ A & B & C & D & E \\ A & B & C$$

# **Numerical Results**

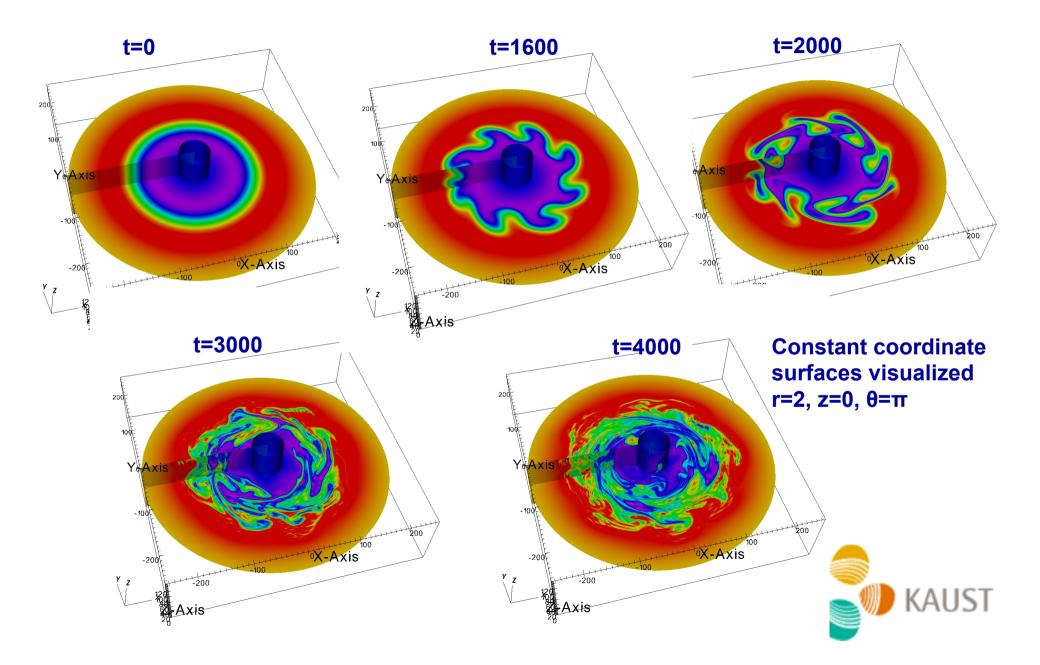
- Domain: [0:15] x [0:2π] x [0:1500] x [-8:8]
- Mesh resolution: 256x256x32x256 (512 procs Shaheen)
- Time step dt=0.1
- 4<sup>th</sup> Order tuned centered finite difference
- Density and temperature profiles



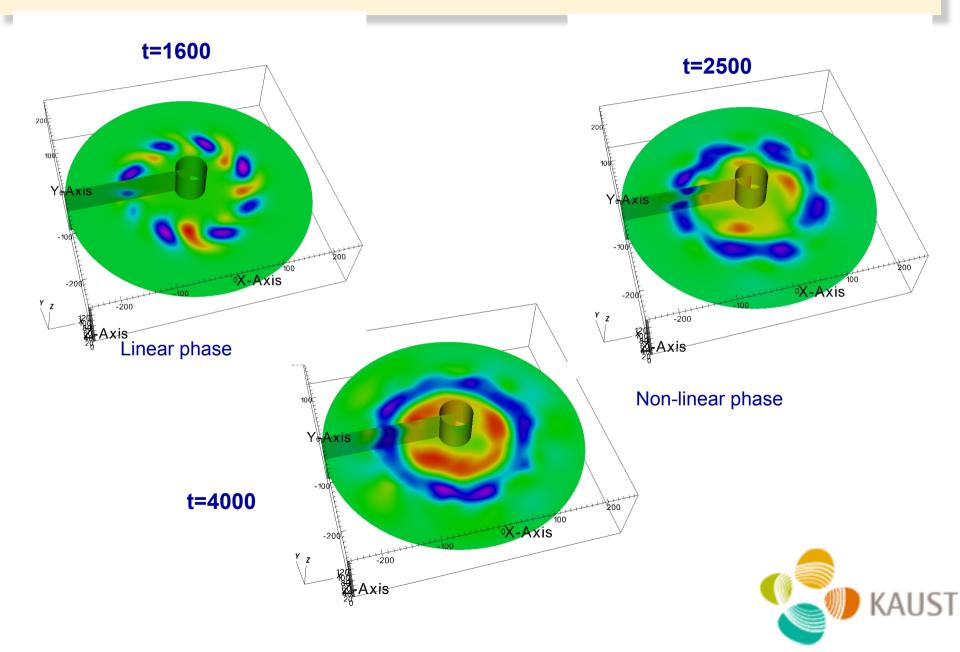
### Numerical Results – Higher Order Moments



#### **Numerical Results - Distribution Function**



# **Numerical Results - Potential**



# **Energy conservation**

• Variation of the kinetic energy:

$$\delta \varepsilon_{kin} = \int m_i \frac{v_{\parallel}}{2} (f - f_{eq}) dV dv_{\parallel}$$

• Variation of the potential energy:

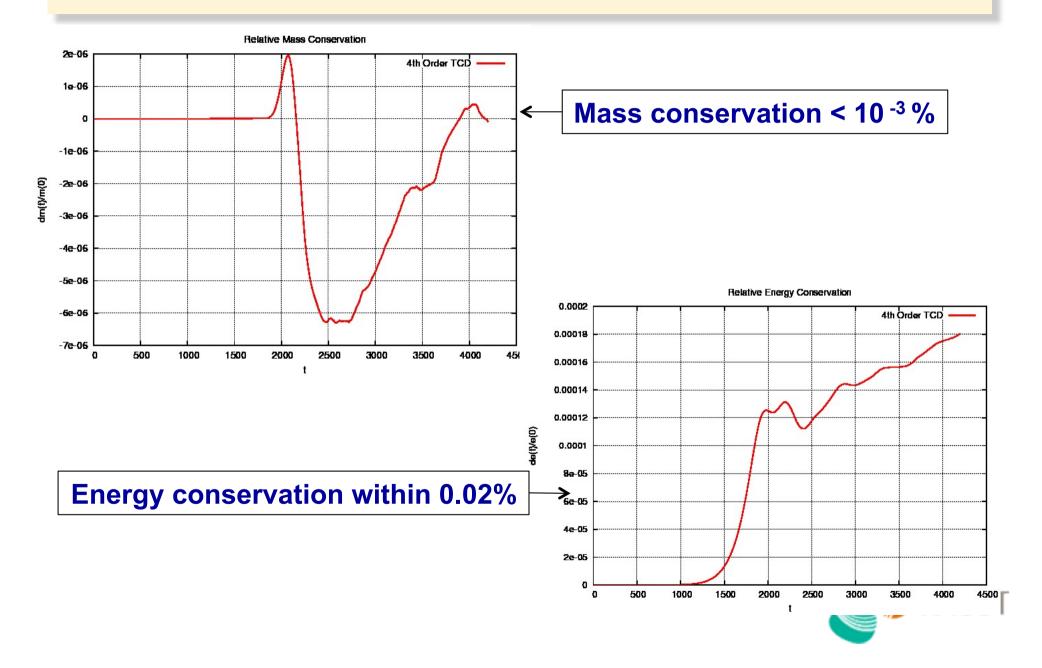
$$\delta \varepsilon_{pot} = \frac{q_i}{2} \int (n_i - n_0) \phi dV$$

Conservation of the total energy

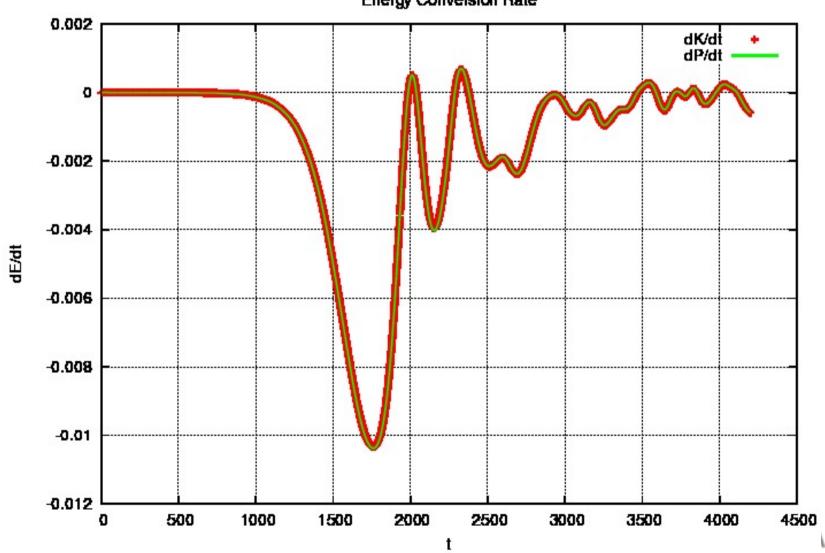
$$\delta \varepsilon_{tot} = \delta \varepsilon_{kin} + \delta \varepsilon_{pot} = \text{constant}$$



# **Numerical Results - Conservation**

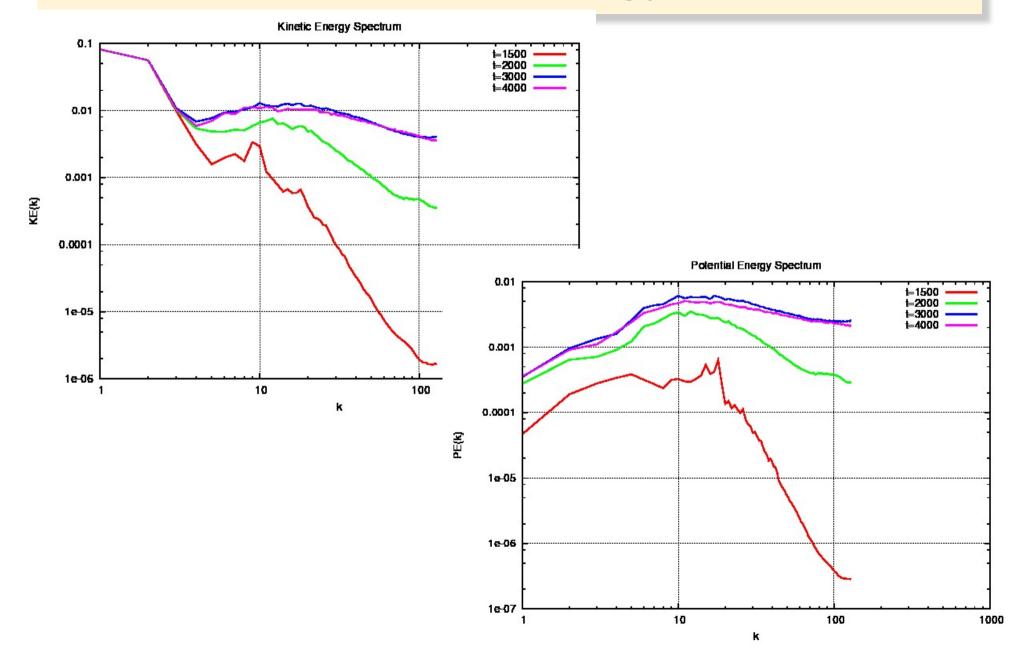


# Numerical Results – Energy Conversion



**Energy Conversion Rate** 

# **Numerical Results - Energy Spectrum**



### Vlasov-Poisson System – III-posedness

- From the numerical results, and in particular the energy spectrum, we observe generation of small scales
  - What is the physical cut-off?
- <u>Claim</u>: The drift-kinetic Vlasov-Poisson system of equations is scale-free
  - $-x \rightarrow \alpha x', t \rightarrow \alpha t', B \rightarrow B'/\alpha, \Phi = \Phi'/\alpha^2, E \rightarrow E'/\alpha, f = f', n = n', v_{\parallel} = v'_{\parallel}$
  - With this transformation the equations are unchanged
- In the nonlinear regime, there is no physical cut-off for the small scales. The system of equations is ill-posed and requires either a physical cut-off mechanism or a numerical regularization
  - Without regularization the generation of small scales proceeds ad-infinitum
  - Convergence with mesh refinement will not be achieved
  - In fact, after a certain critical time the code ought to blow up as energy keeps piling at the small-scales
  - Frequently the phrase "velocity space filamentation" is used (see, for example, Klimas, JCP 1987 and references therein for a discussion of this)
  - Tatsuno et al. (PRL 2008) introduce a non-dimensional number D (a la Reynolds number) to characterize the scale separation in gyrokinetic turbulence

$$\frac{\delta v_{\perp c}}{v_{\rm th}} \sim \frac{1}{k_{\perp c}\rho} \sim D^{-3/5}, \qquad D = \frac{1}{\nu \tau_{\rho}},$$



## Vlasov-Poisson System – Regularization

- A Laplacian "viscosity" term in the Vlasov equation
  - Motivated by shock-hydrodynamics
  - Viscosity coefficient depends on the local gradients so that in relatively smooth regions this term is inactive
  - Results presented so far used this regularization
- A hyperviscosity term in the Vlasov equation
  - Motivated by hydrodynamic turbulence simulation literature
  - 4<sup>th</sup> order hyperviscosity term which provides a numerical cut-off at high wave numbers.
    - Employed, for example, A. Bañón Navarro et al., Free Energy Cascade in Gyrokinetic Turbulence, PRL, 2011. Also by Howes et al. PRL 2008
- Implicit numerical dissipation provided by upwinding methods
- Collision physics model
  - Example: Howes et al. (PRL 2011) work on gyrokinetic simulations of solar wind used collision models developed by Abel (PoP 2008) and Barnes (PoP 2009)
  - Most of the recent papers acknowledge that we need collisions to provide the physical cut-off



# **Model Collision Operator**

 Generalization of the operator defined in Rathman and Denavit

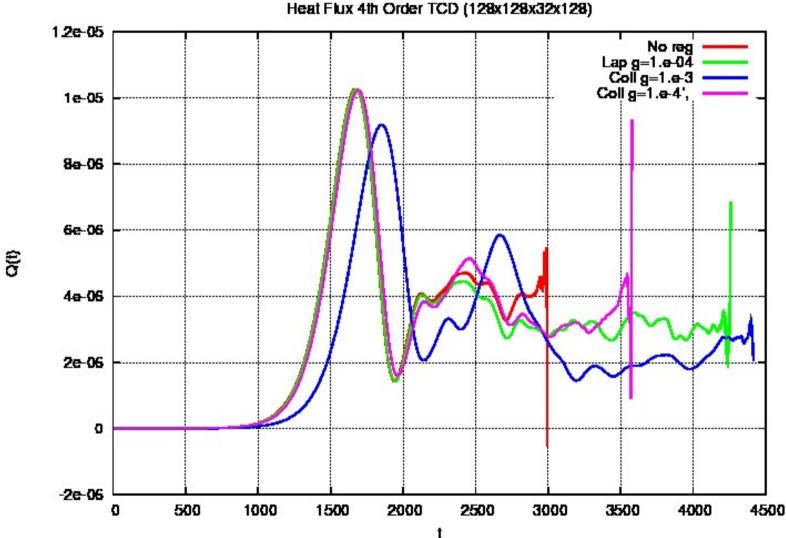
$$\frac{\partial f}{\partial t} + \vec{v}_{GC} \cdot \vec{\nabla}_{\perp} f + v_{\parallel} \frac{\partial f}{\partial z} + \dot{v}_{\parallel} \frac{\partial f}{\partial v_{\parallel}} = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

• 4<sup>th</sup> order central difference for discretization

$$f' = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$
$$f'' = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2}$$

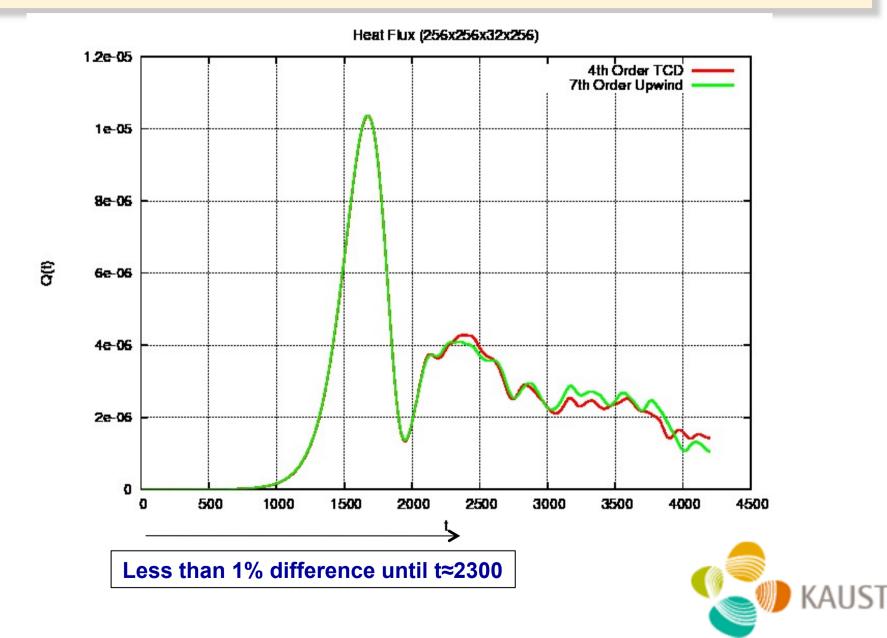


# **Regularization of Central FD Scheme**

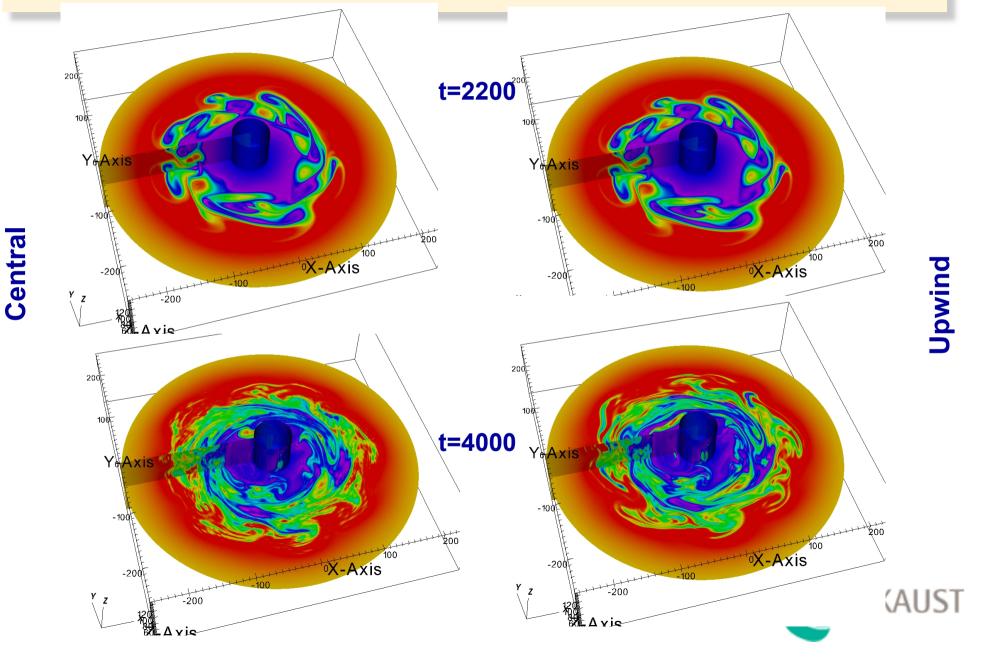




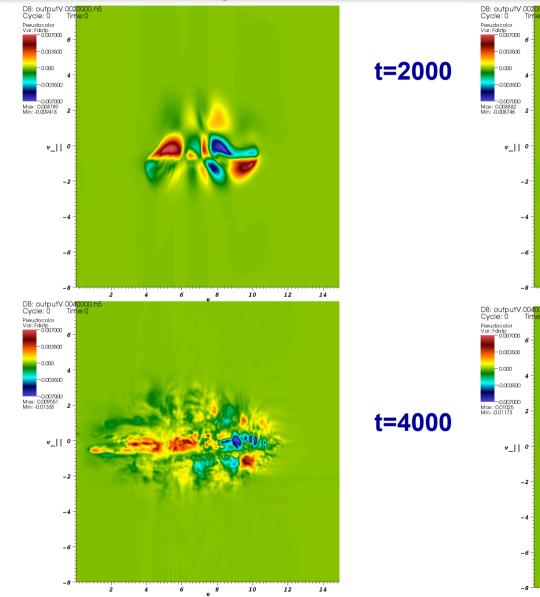
# **Comparing Central vs. Upwind**



# Comparing Central vs. Upwind



# Distribution function $f(r, 3\pi/2, 0, v_{\parallel})$ Central vs. Upwind

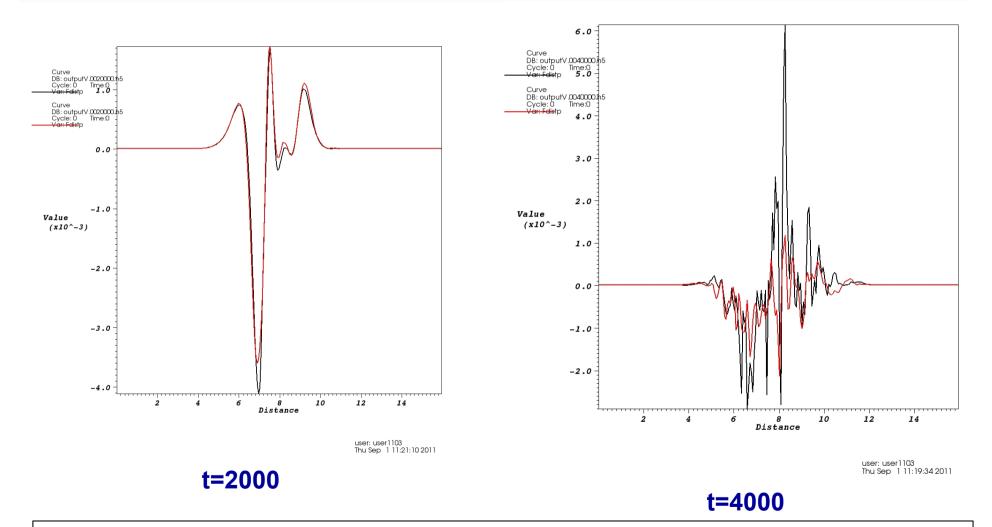


Central



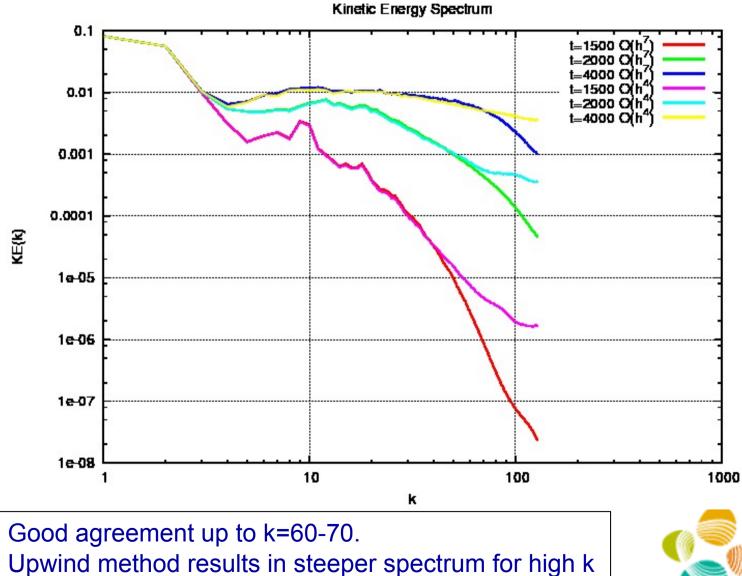
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# Distribution function $f(7.5,3\pi/2,0,v_{\parallel})$ Central vs. Upwind



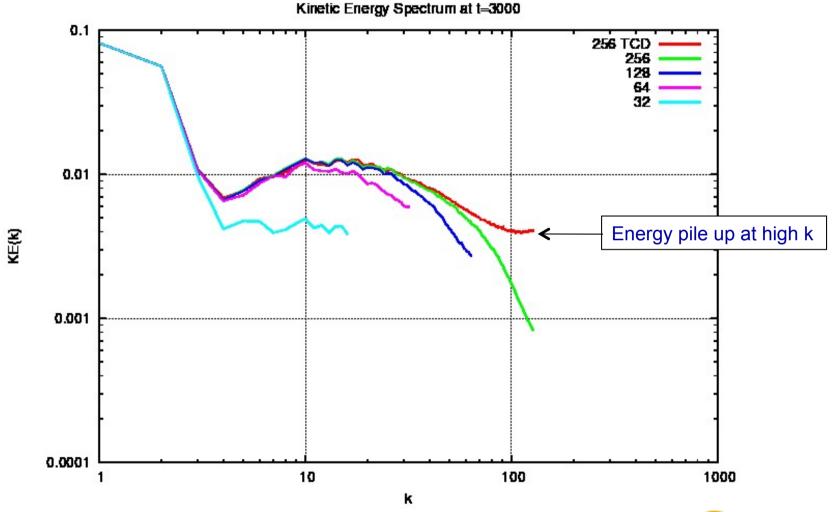
Good agreement until early non-linear stage. Upwind method gives smoother distribution function at late times compared with central FD.

## Kinetic Energy Spectrum: Central vs. Upwind



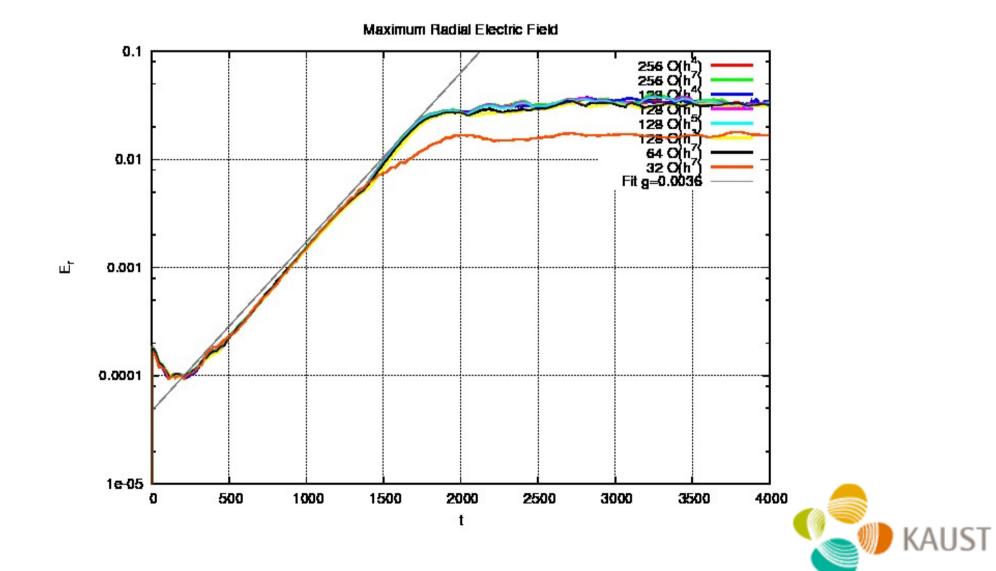


### Kinetic Energy Spectrum: Mesh Resolution

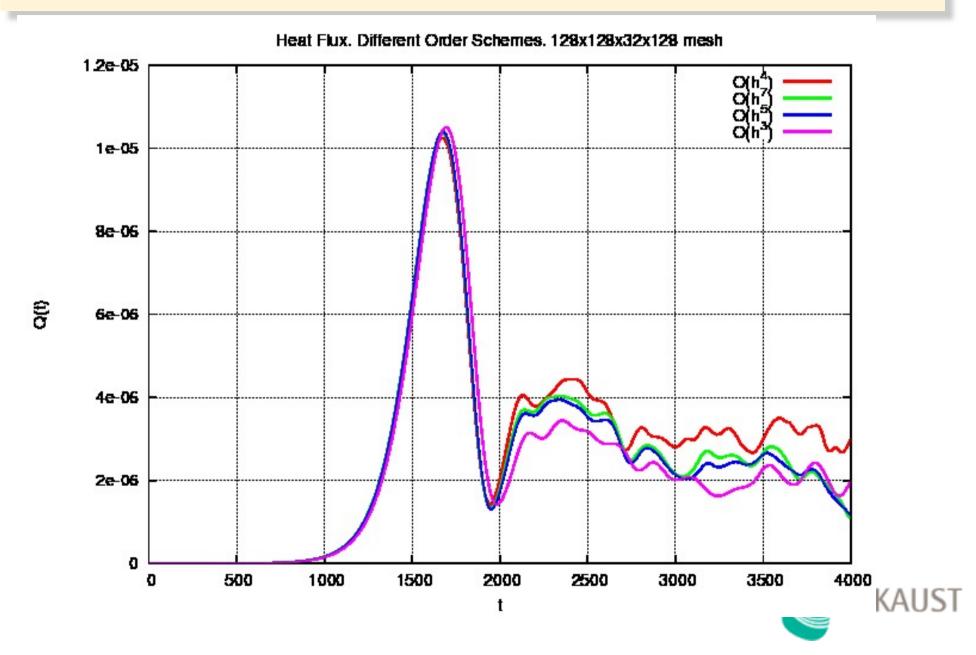




#### Radial Electric Field: Different Methods and Mesh Resolutions



#### Heat Flux: Comparison of Order



## Hydrodynamics Turbulence - Primer

#### Central idea

 For high Reynolds numbers, there exists a range of scales (aka the inertial range) in which effects of viscosity, boundaries, and large scale structures. Dimensional analysis leads to the wellknown universal power-law spectrum (Kolmogorov 1941)

 $E(k) = c_K \varepsilon^{2/3} k^{-5/3}$ 

#### DNS: Direct Numerical Simulation

- All scales, i.e. turbulent fluctuations resolved up to the Kolmogorov scale where dissipation takes place
- Computationally expensive for large Reynolds numbers
  - No of grid points scales as Re<sup>9/4</sup>
- LES: Large Eddy Simulation
  - Only those turbulent fluctuations resolved as determined by the mesh resolution. Scales smaller than the mesh, i.e. s<u>ub-grid-</u> <u>scales</u> must be modeled



## Filtering the Navier Stokes Equations

- Consider a filter  $G_{\Delta}(\mathbf{x})$ 
  - For example a Gaussian filter  $G_{\Delta}^{\text{gaus}}(\mathbf{x}) = [6/(\pi\Delta^2)]^{3/2} \exp(-6x^2/\Delta^2)$
- Convolve the velocity field with the filter (~ below indicates the convolved velocity field)
  - $-\Delta$  is the filter width below which the scales are eliminated
- The resulting equations, which are amenable to numerical discretization at spatial resolution  $\Delta$ , are

$$\partial_t \tilde{\mathbf{u}} + \tilde{\mathbf{u}} \cdot \nabla \tilde{\mathbf{u}} = -\frac{1}{\rho} \nabla \tilde{\rho} + \nu \nabla^2 \tilde{\mathbf{u}} - \nabla \cdot \boldsymbol{\tau}^{\Delta}, \ \nabla \cdot \tilde{\mathbf{u}} = 0$$

 The additional term above dubbed the "SGS (sub-grid-scale)" stress tensor is

$$\tau_{ij}^{\Delta} = \widetilde{u_i u_j} - \widetilde{u_i} \widetilde{u_j}.$$

- SGS stress tensor must be modeled in terms of the resolved (filtered) velocity field Leonard, Adv. Geophysics, 1974

Leonard, Adv. Geophysics, 1974 Pope, "Turbulent Flows", Cambridge, 2000 Rogallo & Moin, Ann. Rev. Fluid Mech, 1984 Lesieur & Metais, Ann. Rev. Fluid Mech, 1996



# "LES" for Kinetic Equations

- Present work explores applying similar ideas to kinetic equations (Vlasov, Fokker-Planck)
  - Question: Can we filter the 6D kinetic equation and derive analogous SGS terms which must be modeled if all scales are not resolved?
  - Benefit: It is likely that even a modest reduction in size may result in vast savings in computations

• Filter the kinetic 
$$\frac{\partial f_{\alpha}}{\partial t} + v \cdot \nabla f_{\alpha} + \frac{q_{\alpha}}{m_{\alpha}} (E + v \times B) \frac{\partial f_{\alpha}}{\partial v} = C_{\alpha,\beta}(f_{\alpha})$$
  
 $f = \overline{f} + f' \qquad \overline{f} = \int G_{\Delta}(x - x', v - v') f dx' dv'$   
 $\frac{\partial \overline{f}}{\partial t} + v \cdot \nabla \overline{f} + \overline{a} \frac{\partial \overline{f}}{\partial v} + \boxed{a' \frac{\partial f'}{\partial v}} = 0$   
Extra term resulting from  
correlations between sub-grid  
quantities; a' contains sub-grid  
magnetic and electric fields

# Examining the SGS terms

Define  $f = \overline{f} + f'$ the filtered field has  $\overline{f} = \overline{f}$  and  $\overline{f'} = 0$ 

Filtered Vlasov equation:  $(v_{\parallel} = \overline{v}_{\parallel})$ 

$$\frac{\partial f}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} \left( r \overline{v}_{GC_r} \overline{f} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \overline{v}_{GC_{\theta}} \overline{f} \right) + \frac{\partial}{\partial z} \left( v_{\parallel} \overline{f} \right) + \frac{\partial}{\partial v_{\parallel}} \left( \overline{\dot{v}}_{\parallel} \overline{f} \right) + SGS = 0$$

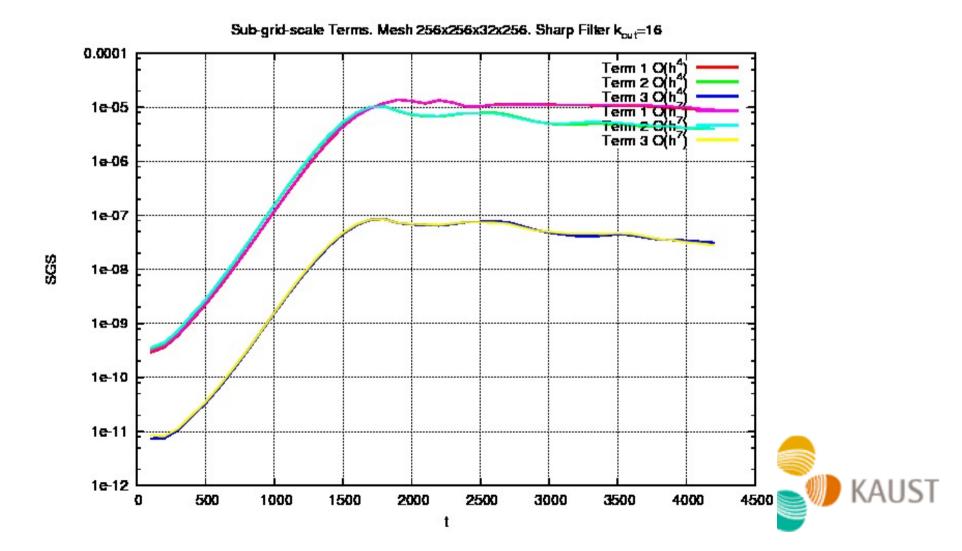
Calculate the last three SGS terms

$$SGS = \frac{1}{r} \frac{\partial}{\partial r} \left[ r \left( v_{GC_r} f - v_{GC_r} f \right) \right] + \frac{1}{r} \frac{\partial}{\partial \theta} \left[ v_{GC_{\theta}} f - v_{GC_{\theta}} f \right] + \frac{\partial}{\partial v_{\parallel}} \left[ \dot{v_{\parallel}} f - \dot{v_{\parallel}} f \right]$$

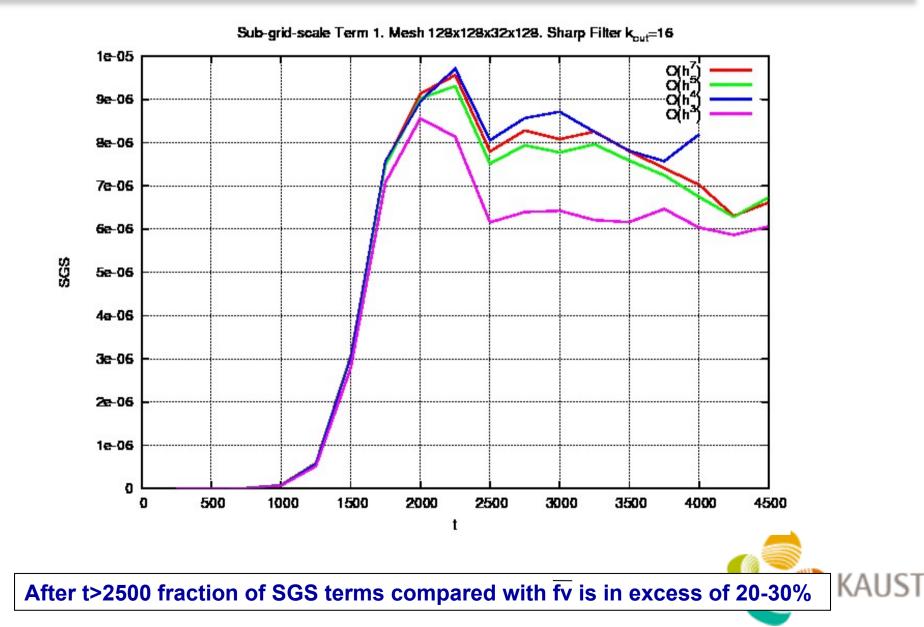


#### **Numerical Results: SGS Terms**

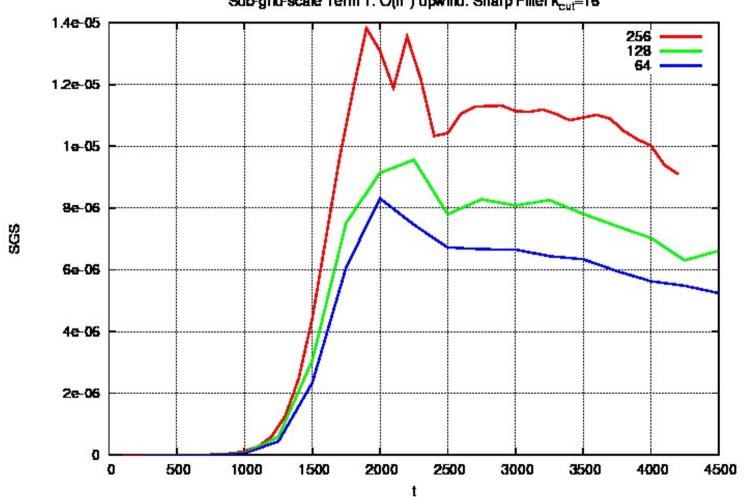
- SGS terms evaluated by filtering the simulation results
  - Filter is a "sharp cut-off" in Fourier space  $k_c=16$



### SGS Terms: Comparison of Order



## SGS Terms: Mesh Resolution



Sub-grid-scale Term 1.  $O(h^7)$  upwind. Sharp Filter  $k_{cut}$ =16



# Summary & Future Work

- Numerical results presented from a recently developed Eulerian Vlasov code
  - High-order fluxes with 4th order Poisson solver
  - Regularization (either diffusion/hyperdiffusion/upwinding/model collisions) required for code stability
  - A true DNS will require cut-off provided by physical collisions which must be resolved
  - Presented preliminary estimates of SGS terms which are in excess of 20-25%.
    - Under-resolved simulations will miss this contribution unless modeled
    - Back-scatter effects from fine to coarser scales will render these missed SGS terms even more important
- <u>Main challenge:</u> Developing physically accurate models for SGS terms in terms of resolved quantities especially because cascade to fine scales is not as straightforward as in hydro turbulence
- Future Work
  - Extend to 5D gyrokinetic
  - More diagnostics and quantification of SGS terms
  - Develop SGS models



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