Turbulence, shocks, and stochastic heating: updates from the Gkeyll Project

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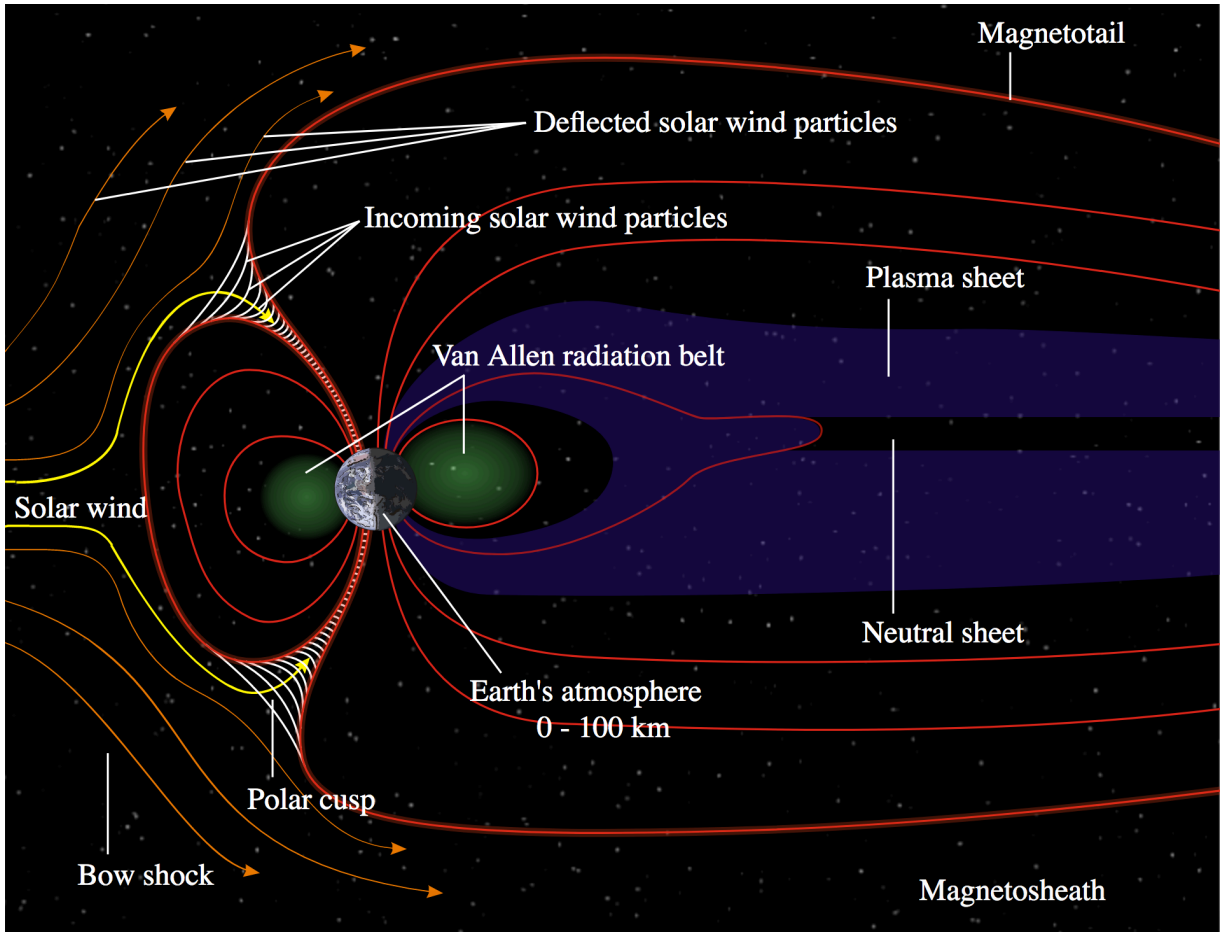
The Gkeyll Project has three major parts,

"It is one thing to mortify curiosity, another to conquer it"

- Multifluid models: treat each species as fluid, include some kinetic effects. Beyond single-fluid MHD or Hall-MHD (J. Ng, L. Wang, C. Dong, A. Bhattacharjee)
- Gyrokinetic models(N. Mandell, T. Bernard, M. Francisquez, **E. Shi**, G. Hammett)
- Vlasov-Maxwell model (J. Juno, P. Cagas, J TenBarge, B. Srinivasan)

Study of Earth's magnetosphere is of fundamental importance

- Impact on operations of satellites; solar storms can cause damage to power-lines and other electronic equipment
- **We would like to simulate the complete (global) magnetosphere with *advanced* plasma fluid models**



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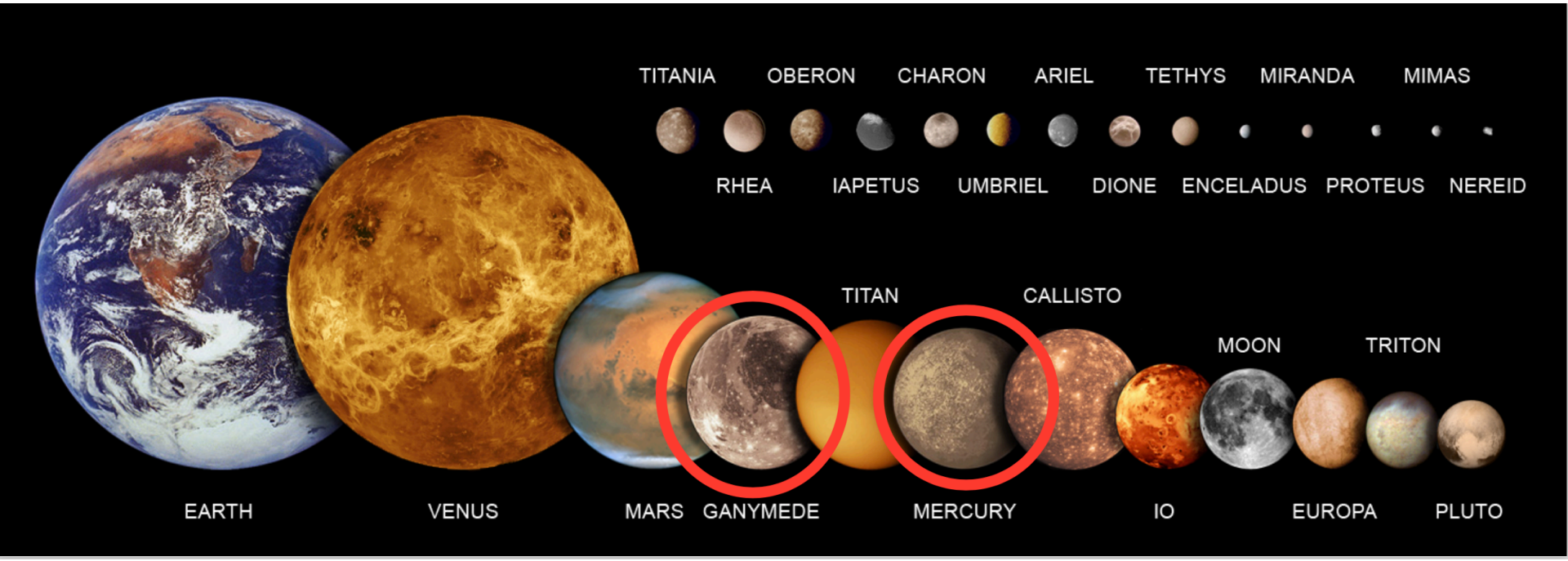
Resolving all scales is practical only for smaller solar system bodies



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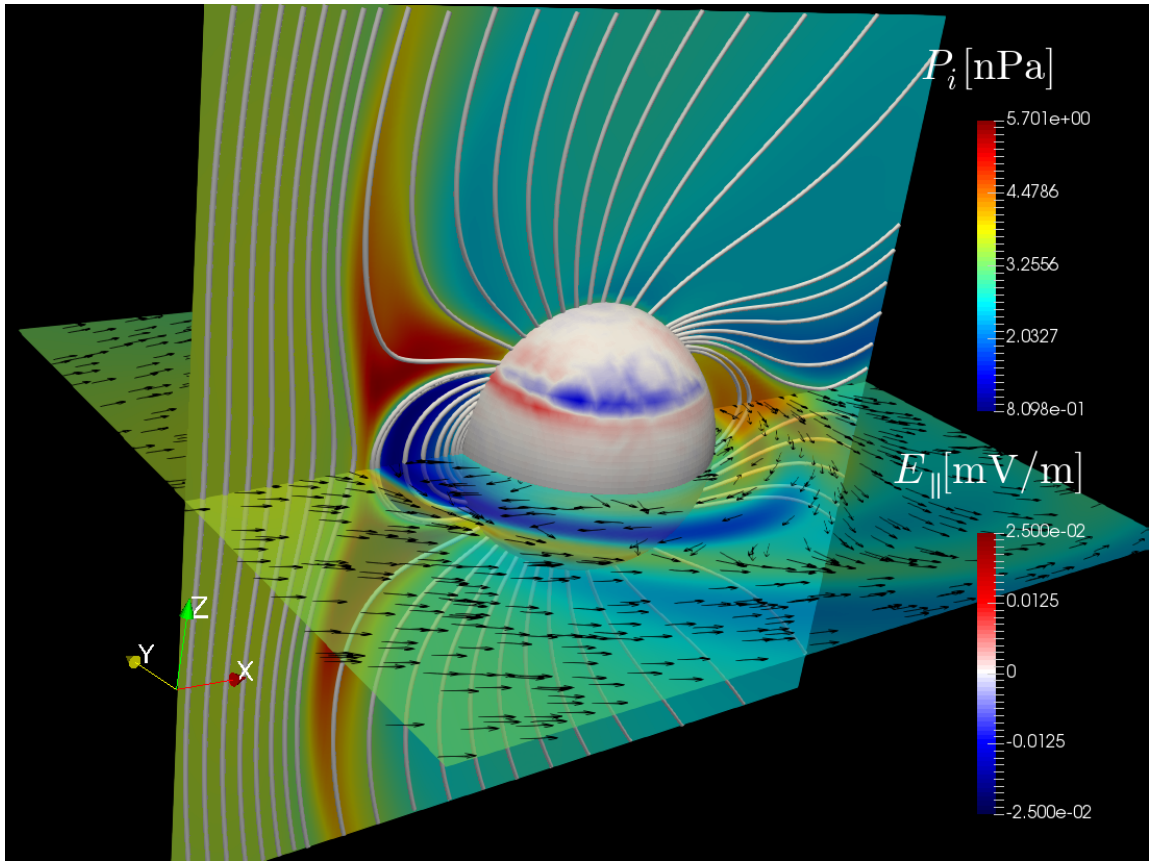
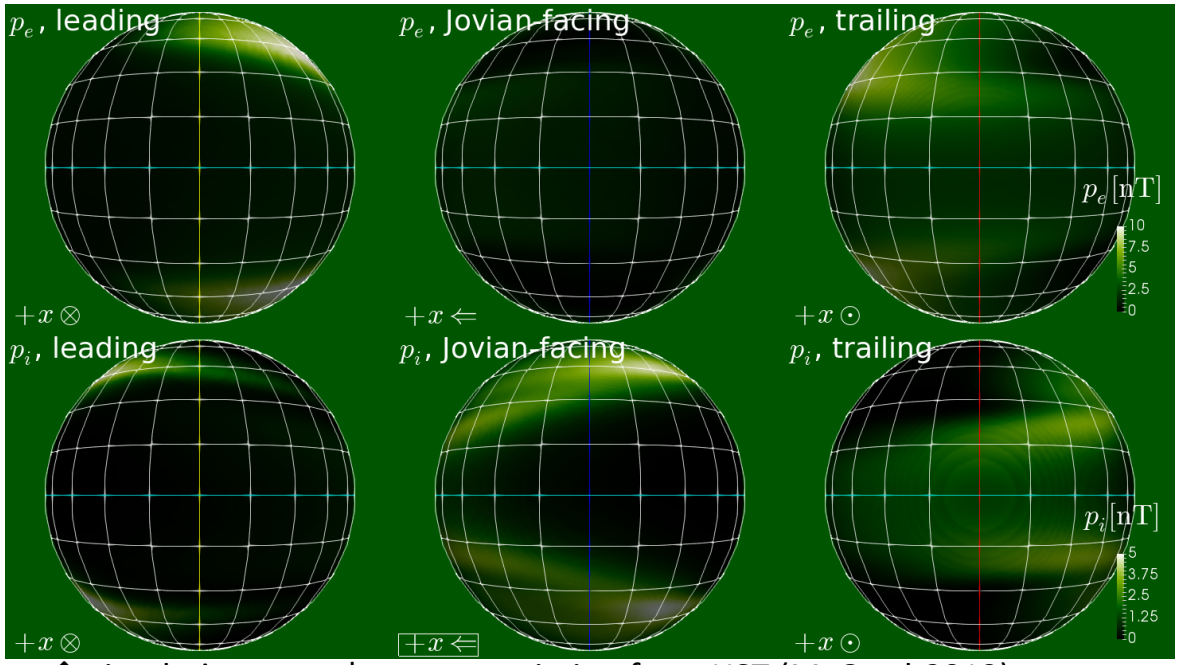
Earth is very large, has a very strong magnetic field. As test, choose Jupiter's moon Ganymede and the inner planet Mercury. Plenty of data from **Galileo** mission to Jupiter, **Hubble Space Telescope** and **Messenger** mission to Mercury.

Multifluid simulations of Ganymede give insight into reconnection and asymmetric flows

- Domain is 60^3 Rg and uses highly non-uniform 800^3 mesh
- Multifluid model retains all six components of pressure tensor; Hall currents; electron inertia
- New insight into reconnection electric fields; instabilities; surface brightness

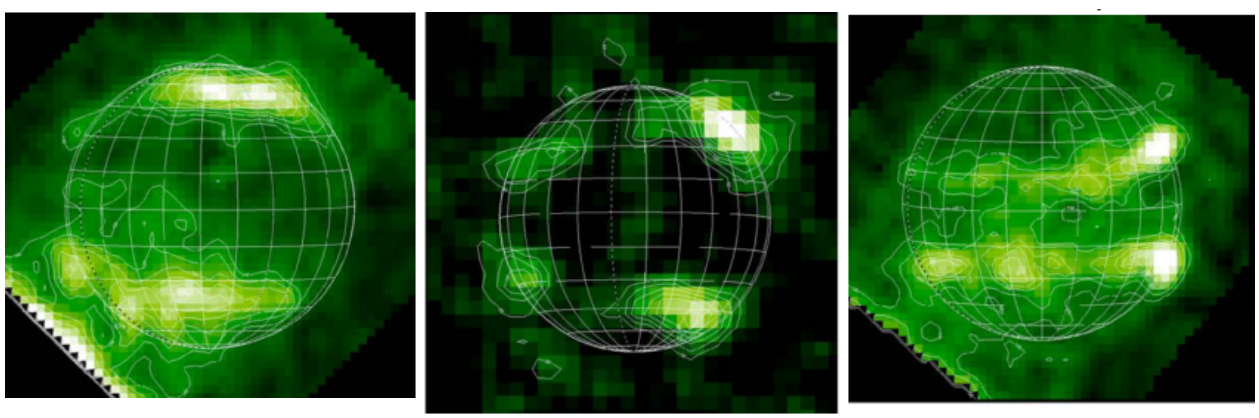


Hubble Space Telescope measurements capture Ganymede's "Northern lights"



Parallel electric field at moon surface from simulations

↑ simulation ↓oxygen emission from HST (McGrath2013)



Oxygen emission measured by **Hubble Space Telescope**

Gkeyll solves a general class of Hamiltonian evolution equations

Evolution of distribution function can be described as Hamiltonian system

$$\frac{\partial f}{\partial t} + \{f, H\} = 0$$

$f(t, \mathbf{z})$ is distribution function, $H(\mathbf{z})$ is Hamiltonian and $\{g, f\}$ is the Poisson bracket operator. The coordinates $\mathbf{z} = (z^1, \ldots, z^N)$ label the N-dimensional phase-space.
Defining $\boldsymbol{\alpha} = (\dot{z}^1, \ldots, \dot{z}^N)$, where $\dot{z}^i = \{z^i, H\}$, gives

$$\frac{\partial}{\partial t}(\mathcal{J} f) + \nabla_{\mathbf{z}} \cdot (\mathcal{J} \boldsymbol{\alpha} f) = 0$$

where $\mathcal{J}$ is Jacobian of the (potentially) non-canonical coordinates. Note that flow in phase-space is incompressible, i.e. $\nabla_{\mathbf{z}} \cdot (\mathcal{J} \alpha) = 0$.
We need three ingredients: Hamiltonian, Poisson Bracket, and field equation.

Long wavelength limit of gyrokinetics with straight $\mathbf{B}$ field

From the Hamiltonian

$$H = \frac{1}{2} m v_{\|}^2 + \mu B + q\phi$$

and Poisson bracket

$$\{F, G\} = \frac{1}{m}\left(\frac{\partial F}{\partial z}\frac{\partial G}{\partial v_{\|}} - \frac{\partial G}{\partial v_{\|}}\frac{\partial G}{\partial z}\right) - \frac{c}{qB}\mathbf{b}\cdot\nabla F \times \nabla G.$$

we obtain a *long wavelength limit of gyrokinetics in straight field lines*

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial z}\left(v_{||} f\right) + \nabla\cdot\left(\vec{v}_E f\right) + \frac{\partial}{\partial v_{||}}\left(\frac{q}{m} E_{||} f\right) = C[f] + S$$

The electrostatic field is determined by

$$-\nabla_\perp \cdot \left(\epsilon_\perp \nabla_\perp \phi\right) = 4\pi \sum_s q \int d^3 v f \equiv 4\pi \varrho_{gc}$$

where $\epsilon_\perp(\vec{x}) = c^2/v_{A0}^2 = c^2 4\pi n_0(\vec{x}) m_i / B^2$ is the plasma perpendicular dielectric coefficient.

It is important to preserve quadratic invariants of Hamiltonian systems

For any Hamiltonian system we can show that

$$\int_K H\{f,H\}\,d\mathbf{z} = \int_K f\{f,H\}\,d\mathbf{z} = 0$$

The first of this leads to conservation of total energy (on use of field equations), while the second leads to conservation of $\int_K f^2 d\mathbf{z}$ (called *enstrophy* for incompressible fluids, and related to entropy).

- Energy conservation in Hamiltonian systems is *indirect*: we evolve the distribution function and field equation. In fluid models, in contrast, the energy conservation is *direct*, as we evolve the total energy equation (in addition to density and momentum density equations). Hence, ensuring energy conservation for Hamiltonian system is non-trivial, and difficult in finite-volume schemes.
- Energy conservation can be ensured using the famous finite-difference *Arakawa* scheme (widely used in climate modeling and one of the top-twenty algorithms ever published in JCP). However, Arakawa scheme is *dispersive* and can lead to huge oscillations for grid-scale modes.

Discontinuous Galerkin algorithms represent state-of-art for solution of hyperbolic partial differential equations

- DG algorithms hot topic in CFD and applied mathematics. First introduced by Reed and Hill in 1973 for neutron transport in 2D.
- General formulation in paper by Cockburn and Shu, JCP 1998. More than 700 citations.
- DG combines key advantages of finite-elements (low phase error, high accuracy, flexible geometries) with finite-volume schemes (limiters to produce positivity/monotonicity, locality)
- Certain types of DG have excellent conservation properties for, low noise and low dissipation.
- DG is inherently super-convergent: in FV methods interpolate p points to get pth order accuracy. In DG interpolate p points to get $2p-1$ order accuracy.

DG combined with FV schemes can lead to best-in-class explicit algorithms for hyperbolic PDEs.

Essential idea of Galerkin methods: L_2 minimization of errors on a finite-dimensional subspace

Consider a general time-dependent problem

$$f'(x,t) = G[f]$$

where $G[f]$ is some operator. To approximate it expand $f(x)$ with a finite set of basis functions $w_k(x)$,

$$f(x,t) \approx f_h(x,t) = \sum_{k=1}^{N} f_k(t) w_k(x)$$

This gives discrete system

$$\sum_{k=1}^{N} f'_k w_k(x) = G[f_h]$$

How to determine f'_k in an optimum manner?

Essential idea of Galerkin methods: L_2 minimization of errors on a finite-dimensional subspace

Answer: Do an L_2 minimization of the error, i.e. find f'_k such that

$$E_N = \int \left[\sum_{k=1}^{N} f'_k w_k(x) - G[f_h] \right]^2 dx$$

is minimum. For minimum error $\partial E_N / \partial f'_m = 0$ for all $k = 1, \ldots, N$. This leads to the linear system that determines the coefficients f'_k

$$\int w_m(x) \left(\sum_{k=1}^{N} f'_k w_k(x) - G[f_h] \right) dx = 0$$

for all $m = 1, \ldots, N$.
Projection of residual on the basis set chosen for expansion leads to minimum errors in the L_2 sense. For this reason DG/CG schemes are constructed by projecting residuals of PDEs on basis sets.

What does a typical L_2 fit look like for discontinuous Galerkin scheme?

Discontinuous Galerkin schemes use function spaces that allow *discontinuities* across cell boundaries.

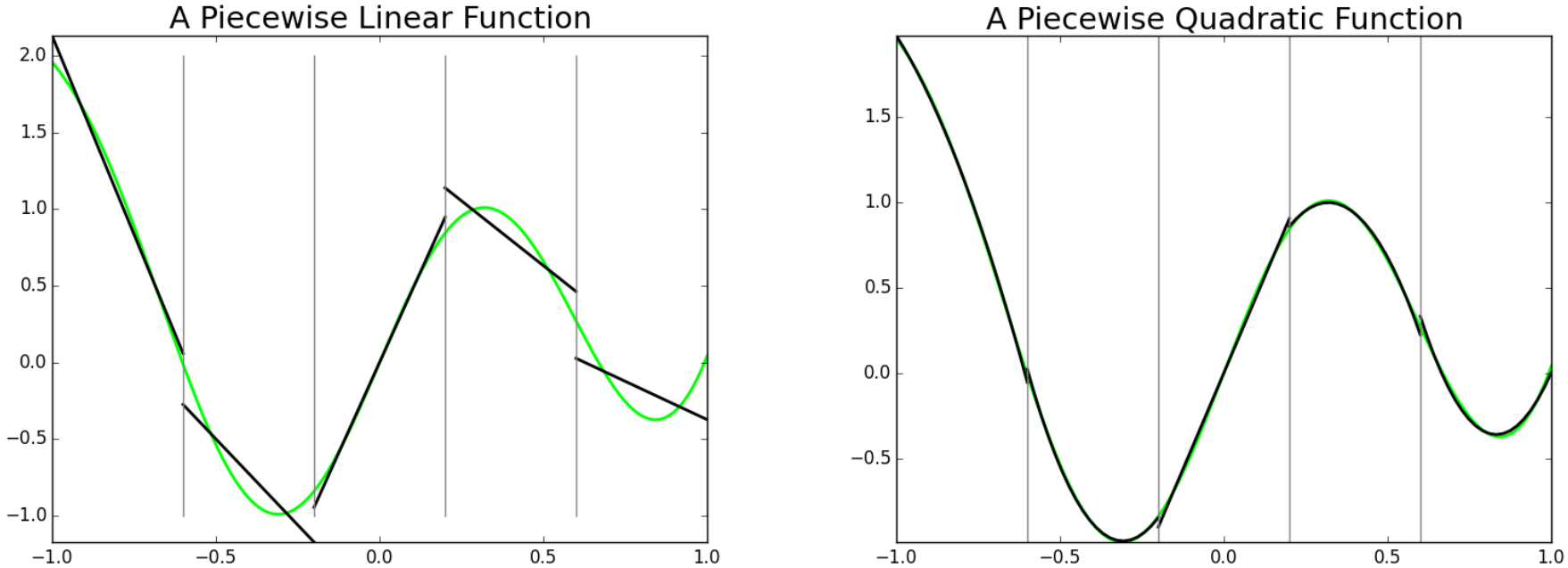


Figure: The best L_2 fit of $x^4 + \sin(5x)$ with piecewise linear (left) and quadratic (right) basis functions.

How to discretize Hamiltonian systems? Use discontinuous space to discretize distribution function, and continuous space for fields

Defining $\boldsymbol{\alpha} = (\dot{z}^1, \ldots, \dot{z}^N)$ as the phase-space velocity vector (assume $\mathcal{J}$ is constant)

$$\frac{\partial f}{\partial t} + \nabla \cdot (\boldsymbol{\alpha} f) = 0$$

Discrete problem is stated as: find f_h in our selected approximation space, such that for all test functions w the discrete weak-form

$$\int_{K_j} w \frac{\partial f_h}{\partial t}\, d\mathbf{z} + \oint_{\partial K_j} w^- \mathbf{n} \cdot \boldsymbol{\alpha}_h \hat{F}\, dS - \int_{K_j} \nabla w \cdot \boldsymbol{\alpha}_h f_h\, d\mathbf{z} = 0$$

is satisfied. Here $\hat{F} = \hat{F}(f_h^-, f_h^+)$ is a numerical flux function.
The discrete Poisson equation is obtained in a similar way (integration by parts), except, the basis set now is global The discrete Poisson equation is obtained in a similar way (integration by parts), except, the basis set now is global

$$\oint_{\partial\Omega} \psi \epsilon_\perp \nabla_\perp \phi_h \cdot \mathbf{n} dS - \int_\Omega \epsilon_\perp \nabla_\perp \psi \cdot \nabla_\perp \phi_h\, d\mathbf{x} = -4\pi \int_\Omega \psi \varrho_{gc}\, d\mathbf{x}$$

Requirement of energy conservation put constraints on discrete Hamiltonian

To check if energy is conserved, use discrete Hamiltonian H_h in the discrete weak-form to get

$$\int_{K_j} H_h \frac{\partial f_h}{\partial t}\, d\mathbf{z} + \int_{\partial K_j} H_h^- \mathbf{n}\cdot\boldsymbol{\alpha}_h \hat{F}\, dS - \int_{K_j} \underbrace{\nabla H_h \cdot \boldsymbol{\alpha}_h}_{=0 \text{ from } \{f,f\}=0} f_h\, d\mathbf{z} = 0$$

On summation over all cells the second term will vanish only if H_h is *continuous*. I.e. we get the required identity

$$\sum_j \int_{K_j} H_h \frac{\partial f_h}{\partial t}\, d\mathbf{z} = 0$$

Hence: H_h must lie in the *continuous sub-set* of the space use to define f_h.

This results, combined with field equation can be used to prove conservation of *total* energy

Use Hamiltonian and sum over species to get

$$\sum_s \sum_{K_j \in \mathcal{T}} \int_{K_j} \left(\frac{1}{2} m v_{\parallel h}^2 + \mu B + q\phi_h(\mathbf{x}, t) \right) \frac{\partial f_h}{\partial t} d\mathbf{z} = 0.$$

Integrating out (summing over) the velocity space we get

$$\sum_{\Omega_j \in \mathcal{T}_\mathbf{x}} \int_{\Omega_j} \left(\frac{\partial \mathcal{E}_h}{\partial t} + \phi_h(\mathbf{x}, t) \frac{\partial \varrho_{gc}}{\partial t} \right) d\mathbf{x} = 0,$$

Take time-derivative of discrete Poisson equation and use ϕ_h as test function to show the conservation of total energy

$$\frac{\partial}{\partial t} \int_\Omega \left(\mathcal{E}_h(\mathbf{x}, t) + \frac{\epsilon_\perp}{8\pi} |\nabla_\perp \phi_h(\mathbf{x}, t)|^2 \right) d\mathbf{x} = 0,$$

Summary of conservation properties of scheme

The hybrid discontinuous/continuous Galerkin scheme has the following provable properties

Proposition

Total number of particles are conserved exactly.

Proposition

The spatial scheme conserves total energy exactly.

Proposition

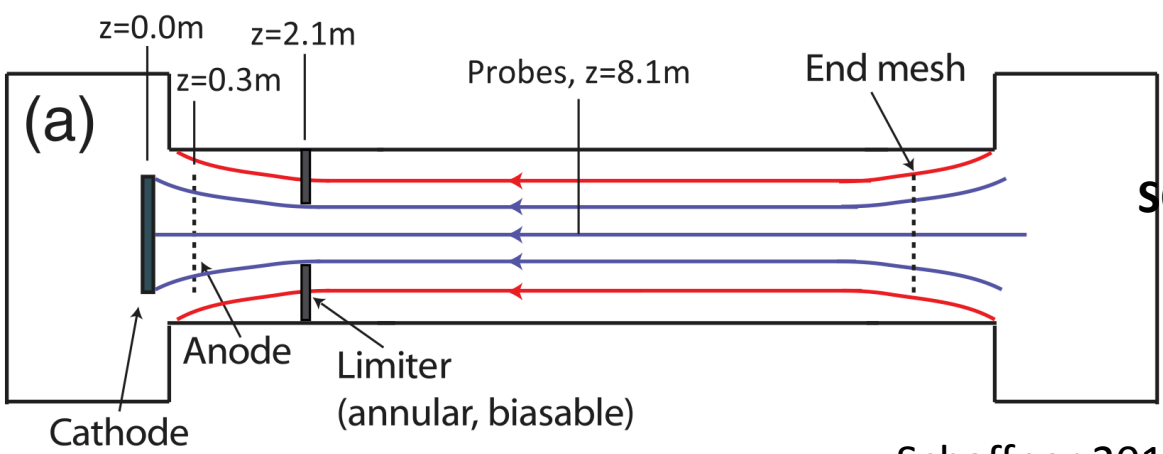
The spatial scheme exactly conserves the second quadratic invariant of the distribution function when using a central flux, while monotonically decaying it when using an upwind flux.

We were first to note a version of DG used by Liu & Shu (2000) for 2D hydro can be extended to conserve energy for general Hamiltonian systems.

Gkeyll can solve 5D gyrokinetic equations on open field-lines

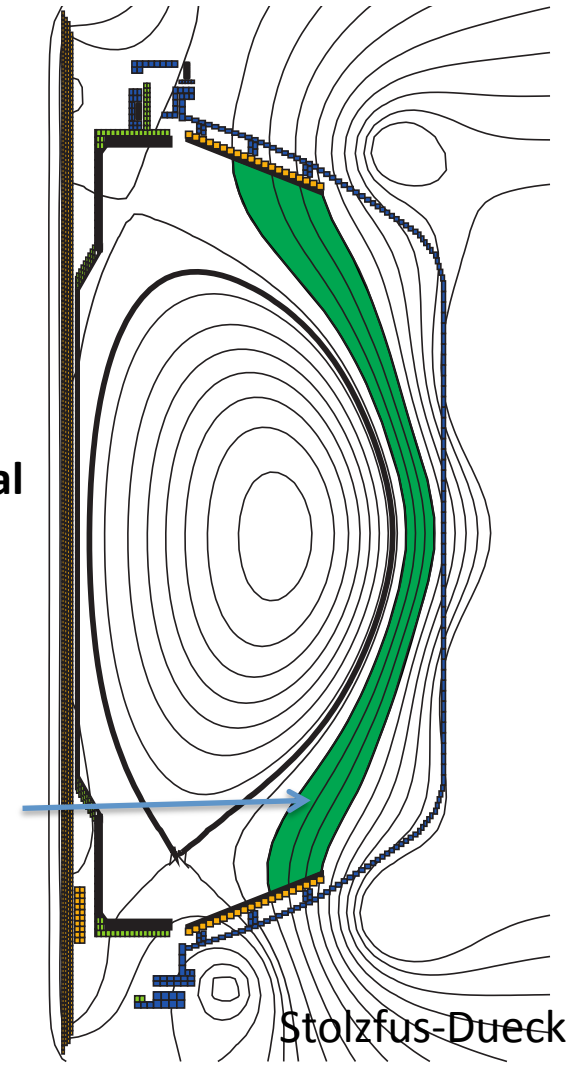
$$\frac{\partial(\mathcal{J}f)}{\partial t} + \nabla\cdot(\mathcal{J}\{\mathbf{z}, H\}f) = 0$$

LAPD linear device



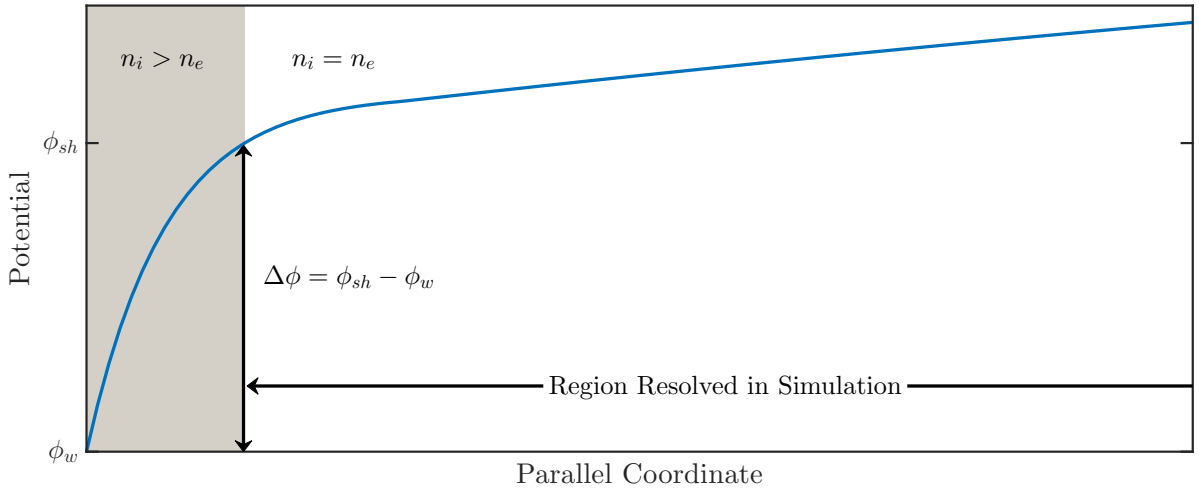
Schaffner 2012

Cross-section of typical NSTX plasma



Stolzfus-Dueck

A plasma sheath forms when plasma touches wall



- Need to model sheath using BCs due to GK quasineutrality condition
- Get ϕ_{sh} from solving GK Poisson equation, then use $\Delta\phi = \phi_{sh} - \phi_w$ to reflect low $v_{\|}$ electrons entering sheath
  - Kinetic version of sheath boundary conditions used in some fluid models that determined $v_{\|,e}$ BC from ϕ [5,6]
- Allows currents in and out of the wall
- Currently exploring possible improvements to the sheath boundary conditions

Goal: Understand kinetic physics in plasma from first-principles

We would like to solve the Vlasov-Maxwell system, treating it as a partial-differential equation (PDE) in 6D:

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f_s) + \nabla_{\mathbf{v}} \cdot (\mathbf{F}_s f_s) = 0$$

where $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. The EM fields are determined from Maxwell equations

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$
$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{B} = -\mu_0 \mathbf{J}$$

Question: Can we solve the VM system *efficiently* while conserving important invariants?

We know that the Vlasov-Maxwell system conserves, total number of particles; total (field + particle) momentum; total (field + particle) energy; other invariants. Can a numerical scheme be designed that retains (some or all) of these properties?

For understanding solar-wind turbulence and other problems, we would like a noise-free algorithm that allows studying phase-space cascades correctly, in a noise-free manner.

We use DG for both Vlasov and Maxwell equations

Start from Vlasov equation written as advection equation in phase-space:

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{z}} \cdot (\boldsymbol{\alpha} f_s) = 0$$

where advection velocity is given by $\boldsymbol{\alpha} = (\mathbf{v}, q/m(\mathbf{E} + \mathbf{v} \times \mathbf{B}))$.

To derive the semi-discrete Vlasov equation using a discontinuous Galerkin algorithm, we introduce phase-space basis functions $w(\mathbf{z})$, and derive the discrete scheme:

$$\int_{K_j} w \frac{\partial f_h}{\partial t}\, d\mathbf{z} + \oint_{\partial K_j} w^- \mathbf{n} \cdot \hat{\mathbf{F}}\, dS - \int_{K_j} \nabla_{\mathbf{z}} w \cdot \boldsymbol{\alpha}_h f_h\, d\mathbf{z} = 0$$

We use DG for both Vlasov and Maxwell equations

Multiply Maxwell equations by basis φ and integrate over a cell. We have terms like

$$\int_{\Omega_j} \underbrace{\varphi \nabla \times \mathbf{E}}_{\nabla\times(\varphi\mathbf{E})-\nabla\varphi\times\mathbf{E}} \, d^3\mathbf{x}.$$

Gauss law can be used to convert one volume integral into a surface integral

$$\int_{\Omega_j} \nabla \times (\varphi \mathbf{E}) \, d^3\mathbf{x} = \oint_{\partial\Omega_j} d\mathbf{s} \times (\varphi \mathbf{E})$$

Using these expressions we can now write the discrete weak-form of Maxwell equations as

$$\int_{\Omega_j} \varphi \frac{\partial \mathbf{B}_h}{\partial t} \, d^3\mathbf{x} + \oint_{\partial\Omega_j} d\mathbf{s} \times (\varphi^- \hat{\mathbf{E}}_h) - \int_{\Omega_j} \nabla\varphi \times \mathbf{E}_h \, d^3\mathbf{x} = 0$$

$$\epsilon_0\mu_0 \int_{\Omega_j} \varphi \frac{\partial \mathbf{E}_h}{\partial t} \, d^3\mathbf{x} - \oint_{\partial\Omega_j} d\mathbf{s} \times (\varphi^- \hat{\mathbf{B}}_h) + \int_{\Omega_j} \nabla\varphi \times \mathbf{B}_h \, d^3\mathbf{x} = -\mu_0 \int_{\Omega_j} \varphi \mathbf{J}_h \, d^3\mathbf{x}.$$

Is energy conserved? Are there any constraints on basis functions/numerical fluxes?

Answer: Yes! If one is careful. We want to check if

$$\frac{d}{dt}\sum_j\sum_s\int_{K_j}\frac{1}{2}m|\mathbf{v}|^2 f_h\,d\mathbf{z}+\frac{d}{dt}\sum_j\int_{\Omega_j}\left(\frac{\epsilon_0}{2}|\mathbf{E}_h|^2+\frac{1}{2\mu_0}|\mathbf{B}_h|^2\right)d^3\mathbf{x}=0$$

Proposition

If central-fluxes are used for Maxwell equations, and if $|\mathbf{v}|^2$ is projected to the approximation space, the semi-discrete scheme conserves total (particles plus field) energy exactly.

The proof is rather complicated, and needs careful analysis of the discrete equations (See Juno et. al. JCP 2018)

Remark

If upwind fluxes are used for Maxwell equations, the total energy will decay monotonically. Note that the energy conservation does not depend on the fluxes used to evolve Vlasov equation.

Is momentum conserved?

Answer: No. Errors in momentum come about due to discontinuity in electric field at cell interfaces. However, *momentum conservation errors are independent of velocity space discretization, and drop rapidly with increasing configuration space resolution*.

Entropy increases monotonically

In order to correctly understand entropy production, one needs to ensure that discrete scheme either maintains or increase entropy in the collisionless case. We can show

Proposition

If the discrete distribution function f_h remains positive definite, then the discrete scheme grows the discrete entropy monotonically

$$\sum_j \frac{d}{dt} \int_{K_j} -f_h \ln(f_h) \geq 0$$

To give and not to count the cost ...

Question: Are continuum schemes competitive compared to PIC schemes in terms of cost for a given accuracy?

I am not completely sure and it probably depends on what you are looking for.

In general, if one is interested in detailed phase-space structure of distribution function, then continuum scheme can be very efficient as the lack of noise allows interpretation of data (for turbulence, for example) easier.

Our recent algorithmic innovations in constructing special basis sets has reduced cost of out continuum schemes significantly. This is potentially a game-changer as efficiency improves dramatically (at the cost of (probably incomprehensible) auto-generated code).

Application: 2D turbulence in magnetized plasmas

We have performed 2X/3V simulations of 2D turbulence in a magnetized plasma

Orszag-Tang initial conditions. Widely used to benchmark MHD codes and study physics of turbulence in 2D. We add a guide field of 5. $40 \times 40 \times 8^3$ mesh, with 112 nodes per cell. (90 million DOFs)

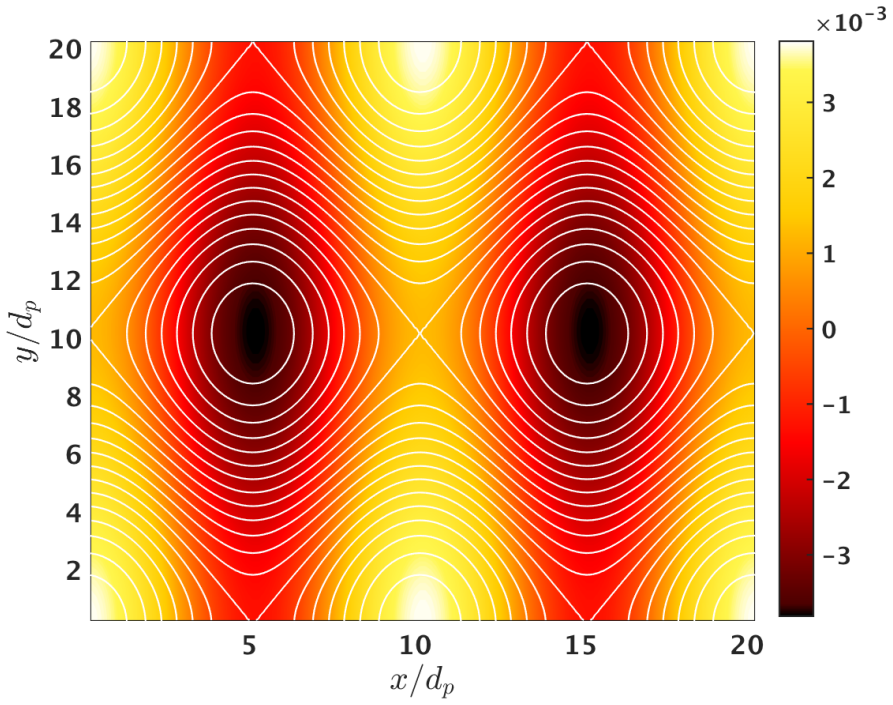


Figure: The out of plane current J_z with magnetic field contours superimposed

Energy spectrum of turbulence

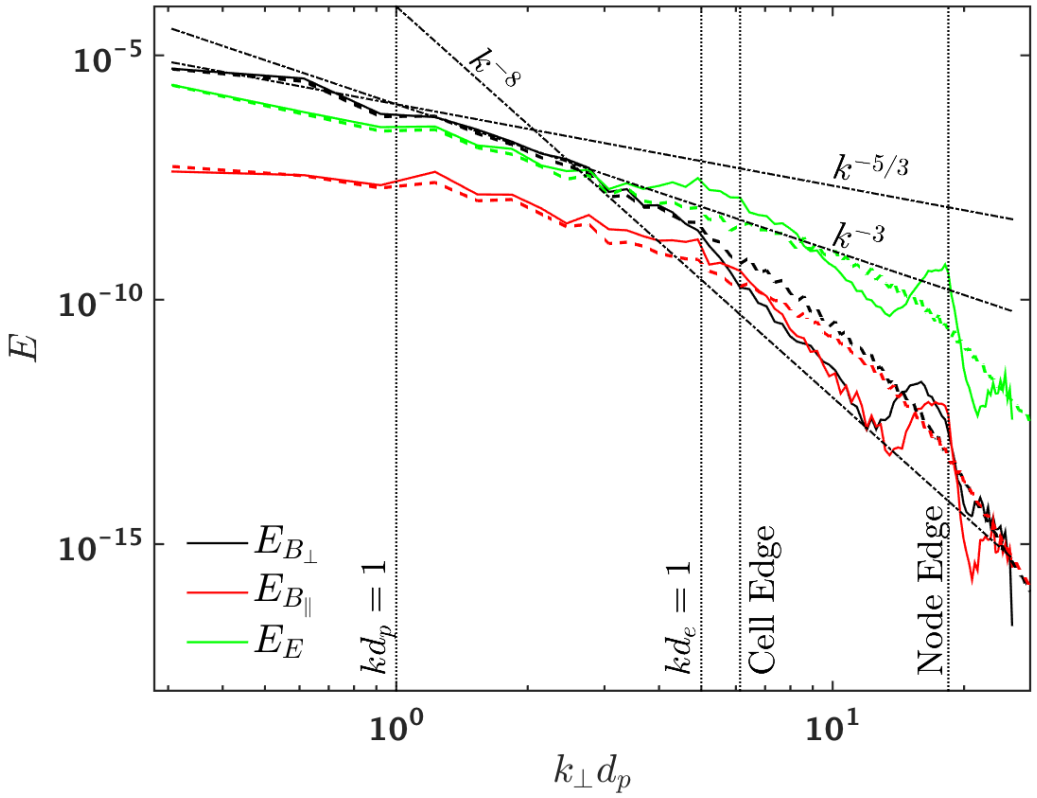


Figure: The energy spectra for Vlasov (solid lines) and 10 moment two fluid (dashed lines) at $t = 35\Omega_{cp}^{-1}$ of the Orszag-Tang vortex simulation. The perpendicular and parallel magnetic energy spectra are directions with respect to the magnetic field. The various slopes denote the fitted spectra at each of the spectral breaks. These compare well with previous results which suggest that at scales $kd_p < 1$, the spectra in $k_\perp$ is fitted by a -5/3 slope, before steepening at $kd_p > 1, kd_e < 1$, and steepening further at $kd_e > 1$.

Conclusion: The Gkeyll Project has developed robust schemes for various plasma equations

- We have implemented finite-volume schemes for multi-fluid equations, and high-order discontinuous Galerkin algorithm for the solution of gyrokinetic and Vlasov-Maxwell equations
- Our algorithm conserves particles and energy exactly; momentum conservation is not exact, but is independent of velocity space resolution
- We have performed extensive benchmarks simulating basic plasma physics problems
- We have performed initial studies of sheath bounded turbulence in straight-field line machines, as well as tokamak SOL with simplified geometry.
- We have applied our algorithms to study physics of plasma shocks, Weibel instability and 2D plasma turbulence
- Current work is aimed towards improving performance via algorithmic improvements and code optimization