High-order energy conserving, (discontinuous) finite-element algorithms for (gyro) kinetic simulations of plasmas

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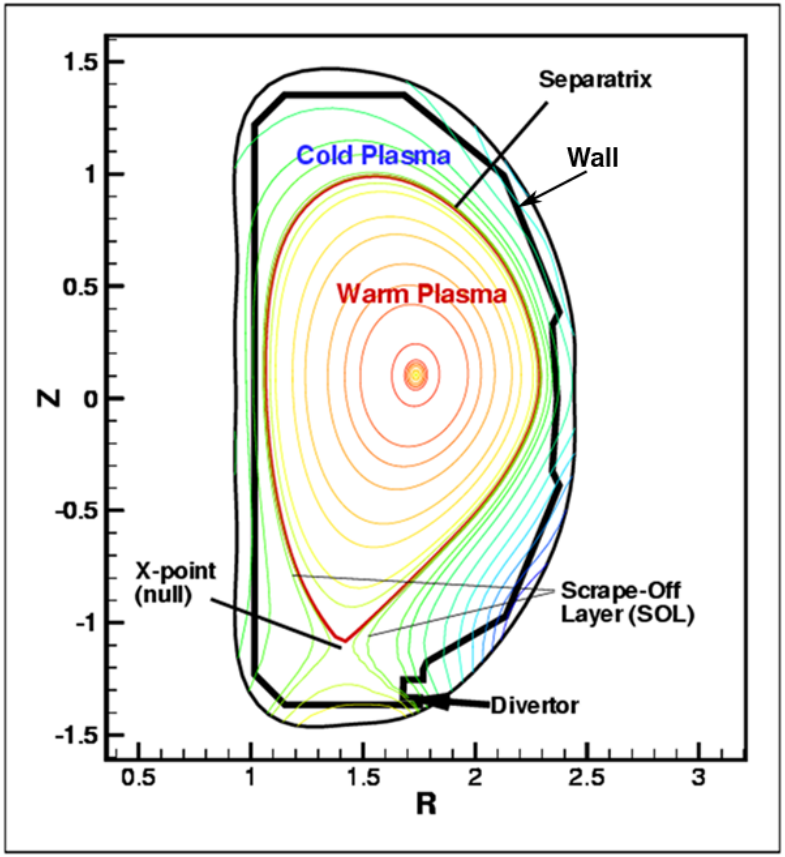
Gkeyll: Robust continuum code for gyrokinetic edge turbulence

- Fusion gain in tokamaks depends sensitively on the edge plasma conditions.
- Edge region is poorly understood and for fundamental understanding requires large-scale kinetic simulations.
- This is difficult due to open *and* closed field line magnetic topology, interaction with tokamak wall and divertor plates, significant interaction with neutrals and large electromagnetic fluctuations.



Gkeyll aims to be a robust code capable of describing gyrokinetic turbulence preserving conservation laws of gyrokinetic equations.

Gkeyll provides a general framework for fluid and kinetic simulation of plasmas

The design of Gkeyll allows one to create solvers for a variety of fluid and kinetic problems, and "plug" them into the generic framework (domain-decomposition, generic grid and data-structures, parallel I/O, and a very powerful scripting facility) to do complex problems in plasma physics.

- At present, we have explicit finite-volume schemes and discontinuous Galerkin schemes for a broad class of hyperbolic and other equations.
- A class of discontinuous/continuous Galerkin schemes are implemented to solve a class of kinetic problems, and used in Vlasov-Poisson/Maxwell solvers, as well as gyrokinetics.
- These are being used to support a number of different plasma projects, both inside PPPL and at other institutions.

Gkeyll being used in projects at PPPL and outside

- At PU/PPPL: Eric Shi, G. Hammett, T. Stoltzfus-Dueck on gyrokinetics, Jonathan Ng, A. Bhattacharjee on advanced fluid closures for multi-fluid moment models, with application to magnetic reconnection. (Latter funded via NSF/NASA grant to Amitava)
- At U. Maryland: James (Jimmy) Juno, Jason TenBarge, B. Dorland on continuum Vlasov-Maxwell solvers for use in solar wind turbulence studies. NSF proposal being submitted to the SHINE program by Jason.
- At Virgina Tech: Petr Cagas, Yang Song and B. Srinivasan on surface physics in Hall thrusters with Vlasov-Poisson models. (This is a new project at PPPL/VT funded by AFOSR, starting Sept. 1 for 4 years).
- At U. New Hampshire: Liang Wang, K. Germaschewski Multi-fluid moment global simulations of magnetosphere. Coupling to community-wide OpenGGCM code.
- At PU/PPPL: Rob Goldston, G. Hammett, M. Jaworski on exploring novel "vapor box" divertor concept to handle heat exhaust in tokamaks.

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 to (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.

Example: Vlasov-Poisson with static magnetic field

The Vlasov equation for charged particles has Hamiltonian

$$H(\mathbf{x}, \mathbf{v}, t) = \frac{1}{2} m v^2 + q\phi(\mathbf{x}, t)$$

where q is species charge and m is species mass and v is particle velocity. The corresponding Poisson bracket is

$$\{f, g\} = \frac{1}{m} \left(\nabla_{\mathbf{x}} f \cdot \nabla_{\mathbf{v}} g - \nabla_{\mathbf{v}} f \cdot \nabla_{\mathbf{x}} g \right) + \frac{q\mathbf{B}_0}{m} \cdot \nabla_{\mathbf{v}} f \times \nabla_{\mathbf{v}} g$$

where $\mathbf{B}_0$ is the *static* magnetic field. The Jacobian is a constant, $\mathcal{J} = m^3$. The fields are determined from

$$\nabla^2_{\mathbf{x}} \phi(\mathbf{x}, t) = -\varrho_c / \epsilon_0$$

The characteristic velocities are

$$\dot{\mathbf{x}} = \{\mathbf{x}, H\} = \mathbf{v}; \quad \dot{\mathbf{v}} = \{\mathbf{v}, H\} = q/m \left(-\nabla_{\mathbf{x}} \phi + \mathbf{v} \times \mathbf{B}_0 \right)$$

For time-dependent electromagnetic fields, the transformation from canonical to noncanonical variables is time-dependent, and care is needed in determining characteristic velocities.

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.

Is it possible to design a scheme that is high-order, robust and conserves total energy?

Answer: Yes, using a version of discontinuous Galerkin schemes. Summary:

- Distribution function is discretized using *discontinuous* basis functions, while Hamiltonian is assumed to be in a continuous subspace
- With these assumptions, our algorithm conserves energy *exactly*, while can optionally conserve the second quadratic invariant *or* decay it monotonically.
- The conservation of total energy is independent of upwinding! This is a surprising result, as upwinding adds diffusion to the system. This diffusion is actually *desirable*, as it gets rid of grid-scale oscillations.
- Momentum conservation is independent of velocity space resolution, and converges rapidly with resolution in configuration space.

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 pair of papers by Cockburn and Shu, JCP 1998. Total of more than 1000 citations.
- DG combines key advantages of finite-elements (low phase error, high accuracy, flexible geometries) with finite-volume schemes (upwinding, limiters to produce positivity/monotonicity, locality). Locality ensures that one can make efficient use of parallel computing, and modern computing architectures which work best when communication is minimized.
- 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 combines best of FV schemes with standard FEM and may lead to optimum algorithms for Hamiltonian PDEs.

There are two key steps in DG: projection and numerical fluxes

In DG one selects a discontinuous approximation space (usually piecewise polynomials). Unlike FV schemes which only evolve cell averages, in DG we also evolve higher moments.

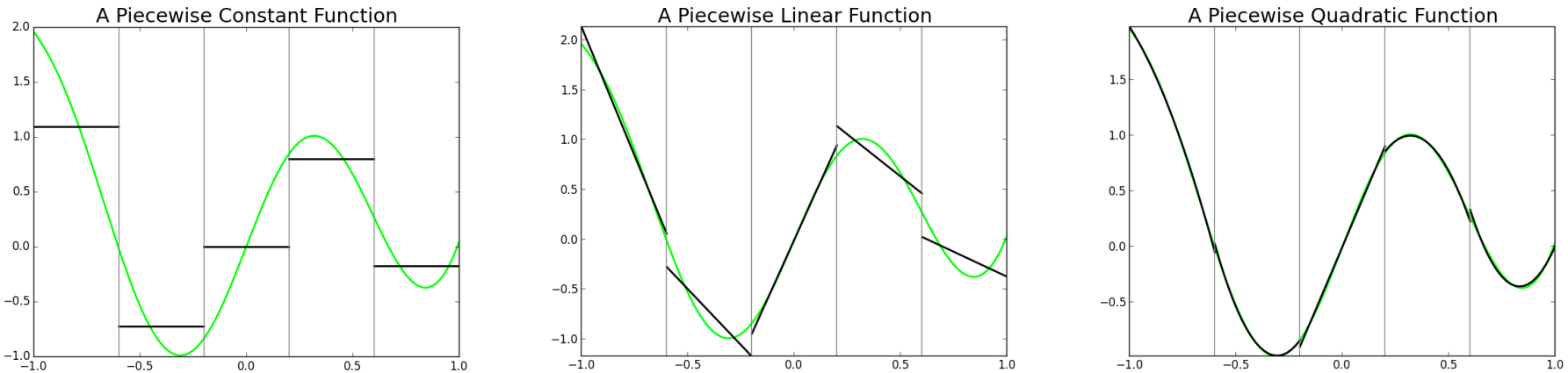


Figure: The projection of $x^4 + \sin(5x)$ onto piecewise constant (left), linear (middle) and quadratic (right) spaces.

Picking a good numerical flux is key to stability, accuracy

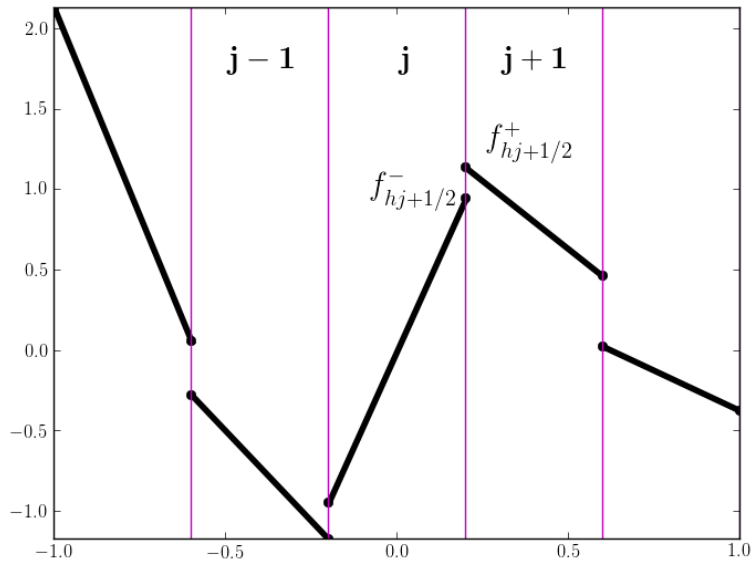
Consider the free-streaming problem $\partial f/\partial t + \partial(vf)/\partial x = 0$. Question: how to compute flux of particles ($\hat{F} \equiv vf$) at cell interface?

- Take averages (central flux)

$$\hat{F}_h(f_h^+, f_h^-) = v(f_h^+ + f_h^-)/2$$

- Use upwinding

$$\begin{aligned} \hat{F}_h(f_h^+, f_h^-) &= vf_h^- \quad v > 0 \\ &= vf_h^+ \quad v < 0 \end{aligned}$$



For system of nonlinear equations (Euler, ideal MHD, etc.) there is cottage industry on choosing numerical fluxes. Google "Riemann solver". Gives about 70K+ hit! The key importance of Riemann solver is that they properly account for the direction in which information propagates, ensuring physically correct numerical fluxes.

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. (Subtle point: normal component of characteristic velocity is continuous).
The discrete Poisson equation is obtained in a similar way (integration by parts), except, the basis set now is global

$$\oint_{\partial\Omega} \psi \nabla_{\mathbf{x}} \phi_h \cdot \mathbf{n} dS - \int_\Omega \nabla\psi \cdot \nabla_{\mathbf{x}} \phi_h\, d\mathbf{x} = -\frac{1}{\epsilon_0} \int_\Omega \psi \varrho_{ch}\, d\mathbf{x}$$

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

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

Integrating out (summing over) the velocity space we get

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

Take time-derivative of discrete Poisson equation and use ϕ_h as test function

$$\int_\Omega \nabla \phi_h \cdot \frac{\partial}{\partial t} \nabla_{\mathbf{x}} \phi_h \, d\mathbf{x} = \frac{1}{\epsilon_0} \int_\Omega \phi_h \frac{\partial \varrho_{ch}}{\partial t} \, d\mathbf{x}$$

in this to show the conservation of total energy

$$\frac{\partial}{\partial t} \int_\Omega \left(\mathcal{E}_h(\mathbf{x}, t) + \frac{\epsilon_0}{2} |\nabla_{\mathbf{x}} \phi_h(\mathbf{x}, t)|^2 \right) d\mathbf{x} = 0,$$

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.

For Vlasov-Poisson momentum conservation is not exact but is *independent of velocity resolution*

- Lack of momentum conservation can be traced to discontinuity in electric field at cell interfaces.
- However, one can show that as electric field depends on *moments* of distribution function (and not distribution function itself), the momentum conservation errors are independent of velocity space resolution.
- One can "fix" this problem by evolving a fluid momentum equation and correcting the distribution function at each step. Corrections will scale as Δx^p. (See Taitano, Chacon, and Simikov, JCP 2014)
- One could construct a momentum conserving scheme, and then energy errors would be independent of velocity space resolution. Could correct for energy errors by solving an energy equation.

We use a different approach for discretizing the Vlasov-Maxwell equations

The Hamiltonian approach is more complicated for the full Vlasov-Maxwell equations. (In fact, first noncanonical Hamiltonian formulation of the system not given till 1980s! Morrison, PRL, 1980, Marsden & Weinstein Physica D, 1982). For now, we are directly discretizing the Vlasov equation, without using the Hamiltonian structure to derive the scheme:

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

where $\mathbf{F}_s = q_s/m_s(\mathbf{E} + \mathbf{v} \times \mathbf{B})$. The EM fields are determined from Maxwell equations (in contrast to evolving the potentials in the Hamiltonian formulation)

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

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 more complicated than in the Hamiltonian case, and requires some careful analysis of the discrete equations (paper is being written up)

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.

There are significant, high-impact, projects for edge gyrokinetics

We are working to demonstrate basic capability of DG to simulate edge turbulence in a numerically robust way, but much work remains. Possible projects that could use help:

- Efficient Gaussian/Maxwellian-weighted basis functions. This is very important, and has the potential to dramatically reduce velocity space resolution requirements.
- Flux limiters to preserve positivity
- Implement local self-adjoint projection operators for efficient energy conservation
- Models (simple ones at first) of neutral recycling, radiation, secondary electron emission, sputtering...
- General geometry (several different ways being investigated)
- Extensive code testing and physics studies: How much does SOL turbulence spread heat flux to divertor plate? How high will pedestal get? How much can performance be improved with lithium?

There are significant, high-impact, projects for the Vlasov-Maxwell system

(Each of the following make good second-year theory projects)

- In general, the divergence relations $\nabla \cdot \mathbf{E} = \varrho_c/\epsilon_0$ and $\nabla \cdot \mathbf{B} = 0$ will not be satisfied numerically. Is there a DG analogy to the classical Yee-scheme for Maxwell equations? Can one do some divergence cleaning?
- It appears like one needs to resolve plasma-frequency and Debye length. Are there efficient *local* schemes that can circumvent this? We may have discovered such an algorithm but it remains to be tested.
- Can one make asymptotic approximations (use a Darwin field model, or impose quasi-neutrality and use an Ohm's law) to relax some constraints from time- and spatial-scales?
- Can one combine various fluid models already present in `Gkeyll` with Vlasov-solver to do efficient hybrid simulations?

One can also imagine a lot of "easy" physics problems (nonlocal heat-transport, particle energization, collisionless shocks, nonlinear RF physics, ...) one can do in lower dimensions (1X/2V or 1X/3V).

There are significant, high-impact, projects for the multi-moment fluid and neutral fluids models

- What are effective closures for ion and electron moment equations, such that key kinetic effects for reconnection and magnetosphere modeling are captured?
- Design more efficient solvers, eliminating uninteresting time and space scales so global, large-scale simulations are possible.
- What are proper boundary conditions for the case in which a vapor is condensing on liquid metals?
- Do automated shape optimization studies for the vapor-box divertor concepts
- Apply the multi-moment fluid models to compact toroids (FRCs in particular. Talk to Sam Cohen for exciting ideas on using `Gkeyll` for FRC edge physics.)

Non-fusion sources of funding (current and future)

- We currently have funding from NASA/NSF (PI Amitava Bhattacharjee) for the multi-fluid work, and AFOSR for surface physics.
- Other potential sources of funding will be pursued, including NSF basic plasma sciences, ASCR for large-scale kinetic solvers, AFOSR Computational Mathematics program, SciDAC ...

Conclusion: We made significant algorithmic advances in Gkeyll project

- Developed DG algorithms for general Hamiltonian systems that conserve energy exactly even with upwinding
- Discovered and fixed a subtle issue with widely-used DG discretizations of second-order operators, needed for collision terms
- Discovered two ways of allowing discontinuous Hamiltonian (original algorithm requires continuous Hamiltonian), removing need for non-local operator in parallel direction. Developed novel local but self-adjoint projection-like operators.
- Discovered and fixed subtle issues with standard algorithm when allowing magnetic fluctuations, which had required tiny time-steps for stability for small $k_\perp \rho_s$. Fixed by noting basis functions for phi need higher order continuity than for $A_\parallel$.
- Studied ELM heat-load problem with gyrokinetics in simplified scrape-off-layer (SOL) geometry, speeding up existing full kinetic (Vlasov and PIC) simulations by many orders of magnitude.
- Flexibility of DG schemes allows used of various basis sets, including "serendipity basis functions", which only very recently have been generalized to 4D and 5D (Arnold, Awanou, F. Comp. Math 2011), which can be further enhanced by using Maxwellian weighted basis functions.