From SOL turbulence to planetary magnetospheres: computational plasma physics at (almost) all scales using the `Gkeyll` code

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December 5th, 2018

What is the Gkeyll Project?

The Gkeyll Project aims to develop a computational plasma physics tool to simulate plasmas at (almost) all scales.

- Group of graduate students, postdocs and senior researchers, spanning multiple institutes (PPPL, PU, Virginia Tech, MIT) working of various aspects of algorithm development and physics applications.
- Started of life as LDRD project. Now funded via multiple SciDACs, NSF/NASA projects and AFOSR
- Group is focused on developing the Gkeyll code[1] and applying it to various physics problems.
- Spans scales from full kinetic (Vlasov-Maxwell), to EM gyrokinetics to muti-fluid moment models
- All solvers share common framework, allowing people to work on different aspects of the code and make an impact on the broader project

[1] See http://gkeyll.rtfd.io

Goal of this talk is to give overview of project

Talk split into four parts:

- Full kinetics with the Vlasov-Maxwell equations
- Progress in implementing electromagnetic gyrokinetics; initial results to NSTX-like SOL turbulence
- Application of multi-fluid models to space plasma problems; in particular to planetary magnetospheres
- Some thoughts on furture of `Gkeyll` Project as well as ideas on building a strong Whole Device Modelling (WDM) focused Advanced Computing group at PPPL.

Part I: The Vlasov-Maxwell System



The core team: **Jason TenBarge**, **Jimmy Juno**, and **Petr Cagas**, **Liang Wang**, **Mana Francisquez**. Funded via NSF grant to J. TenBarge and joint PU-Virgina Tech AFOSR grant.

Kinetic physics from first-principles

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

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

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

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

Can we design an efficient, conservative scheme?

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 by this scheme?

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, **353**, 110-147, 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 by this scheme?

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

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

A simplified collision operator implemented

We have implemented the Lenard-Bernstein operator (LBO) written in the form

$$\left(\frac{\partial f_s}{\partial t}\right)_c = -\frac{\partial}{\partial v_i}\left(\langle \Delta v_i \rangle_s f_s\right) + \frac{1}{2}\frac{\partial^2}{\partial v_i \partial v_j}\left(\langle \Delta v_i \Delta v_j \rangle_s f_s\right).$$

Instead of the full Fokker-Planck operator we use the simplified expressions

$$\begin{aligned} \langle \Delta v_i \rangle_s &= -\nu_s \left(v_i - u_{s,i}\right) \\ \langle \Delta v_i \Delta v_j \rangle_s &= 2\nu_s v_{th,s}^2 \delta_{ij} \end{aligned}$$

where $v_{th,s}^2 = T_s/m_s$. Note that velocity dependent collision frequency is not captured. However, it illustrates most of the difficulties and is a step towards a full Fokker-Planck operator.

Novel version of DG used for LBO

Our first implementation did not conserve energy! Note that as the diffusion terms has two derivatives in it we can perform integration by parts twice. This leads to our Scheme II:

$$
\int_{K_j} d\mathbf{z}\ \psi_k \frac{\partial f}{\partial t} = \int_{\partial K_{j,v_i}} dS_i \ \left(\psi_k F_i - \frac{\partial \psi_k}{\partial v_i} v_{th}^2 f \right) \Bigg|_{v_{i,j-1/2}}^{v_{i,j+1/2}}
$$

$$
- \int_{K_j} d\mathbf{z} \ \left[\frac{\partial \psi_k}{\partial v_i} (v_i - u_i) f - \frac{\partial^2 \psi_k}{\partial v_i \partial v_i} v_{th}^2 f \right]
$$

(Paper with details being written up for publication in JCP)

Density, Momentum and Energy are conserved *if* ...

To ensure that density, momentum and energy are conserved exactly, **one must account for the finite extents in velocity space**. Make computing *moments* tricky.

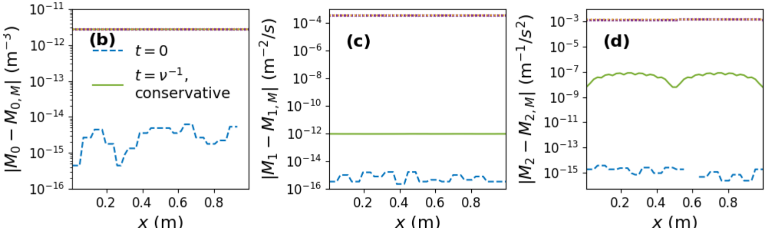


Figure: Error in density (left), momentum (middle) and energy (right) conservation. Green dashed line shows errors in conservative scheme. Dashed blue lines show difference with relaxed Maxwellian.

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?

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 and auto-generated code has reduced cost of our continuum schemes significantly. This is potentially a game-changer as efficiency improves dramatically.

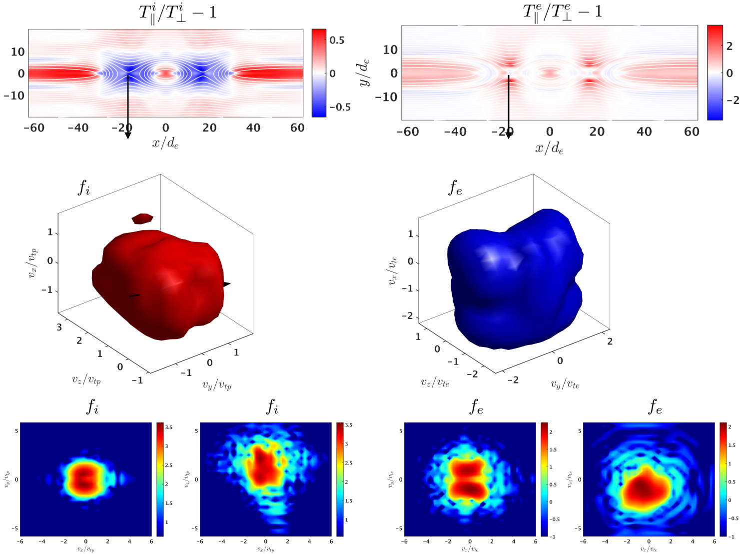
Benchmarking with the GEM Challenge

Extensive, standard non-trivial benchmarks have been performed and documented[2]. The GEM reconnection challenge problem.

$$\mathbf{B} = \delta B \tanh(y/w)\hat{\mathbf{x}} \quad w = 0.5 d_i, L_x = 2 \times L_y = 8\pi d_i$$
$$T_i/T_e = 5, \quad \beta_i = 5/6, \quad m_i/m_e = 25, \quad c/v_{A_e} = 10$$
$$\nu_{ee} = 0.01\Omega_{ci} \quad \rightarrow \quad \lambda^e_{mfp} \sim 1000 d_e \gg L$$
$$(n_x, n_y, n_v^3) = (32, 64, 12^3), \quad p = 2 \quad \rightarrow \quad (96, 192, 36^3)$$

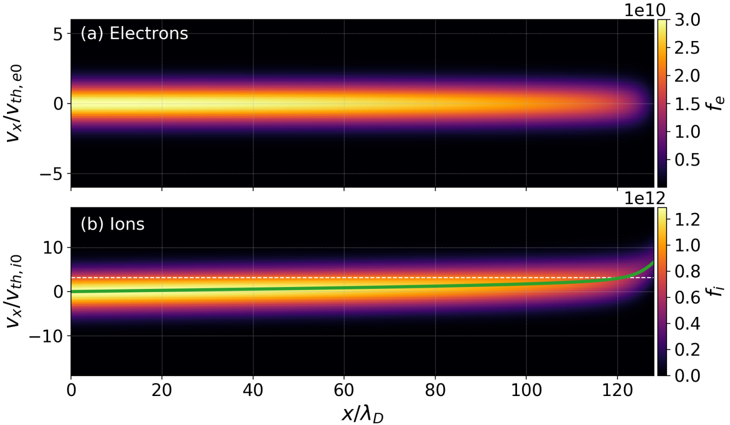
[2] See http://ammar-hakim.org/sj/

Detailed features in distribution functions captured



Simulating plasma sheaths from first principles

As part of AFOSR project and LANL disruption SciDAC we are funded to study plasma-surface interaction using first-principles kinetic models. **See Petr Cagas dissertation linked on `Gkeyll` website.**

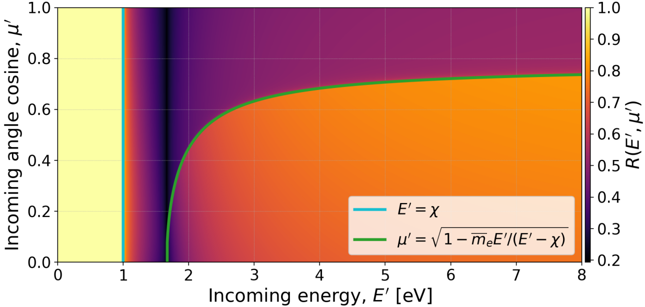


Pushing novel approach to boundary conditions

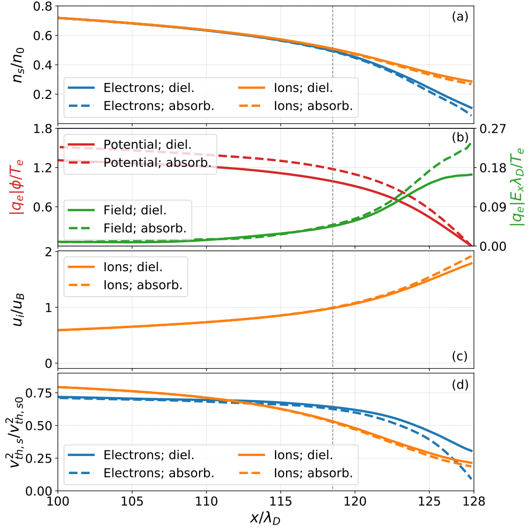
The outgoing distribution function from the wall is described with a reflection function, $R(\boldsymbol{v},\, \boldsymbol{v}')$

$$f_{\text{out}}(t,\, \boldsymbol{x} = \boldsymbol{x}_{\text{wall}},\, \boldsymbol{v}) = \int_{\mathcal{V}^{\text{in}}} R(\boldsymbol{v},\, \boldsymbol{v}') f_{\text{in}}(t,\, \boldsymbol{x} = \boldsymbol{x}_{\text{wall}},\, \boldsymbol{v}')\, d\boldsymbol{v}' \qquad (1)$$

Implementing QM model by *Bronold & Fehske, Phys. Rev. Let., 2015*

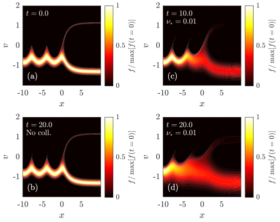


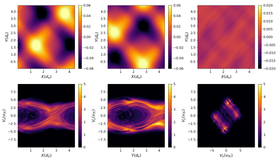
Sheath profiles are modified by the returning electrons

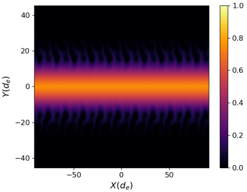


Current physics projects with the Vlasov solver

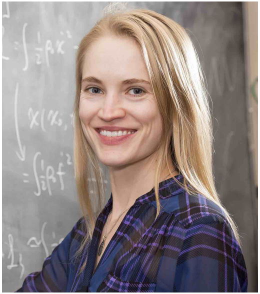
- Electrostatic shocks (with and without collisions)
  - Pustvai *et al.* 2018 PPCF
  - Sundström *et al.* 2018 submitted to JPP
- Weibel instability (in 1D and 2D)
  - Cagas *et al.* 2017 PoP
  - Skoutnev *et al.* in preparation, to be submitted to ApJ letters
- Lower hybrid drift instability
  - Ng *et al.* in preparation, to be submitted to JGR







Part II: Electromagnetic Gyrokinetics


The core team: **Noah Mandell**, **Tess Bernard**, **Mana Francisquez** and **Greg Hammett**. Funded via edge and core SciDACs (C.S Chang, David Hatch).

Status of Gyrokinetics in Gkeyll

- Pioneering work by Eric Shi[3] led to 5D electrostatic full-F GK simulations of LAPD and NSTX-like helical SOL with sheath BCs
- Over past year, we have been rapidly developing a new version of Gkeyll
  - Moving from nodal to modal DG representation $\rightarrow$ orthonormal basis functions, quadrature-free, computer algebra-generated solver kernels (much easier to generalize to higher dimensionality/polynomial order), $\mathcal{O}(10)$ faster
  - Much simpler user interface, details abstracted away
- Have reproduced many of Shi's results with new version of Gkeyll;

What about electromagnetics?

[3] See 2017 thesis; JPP 2017 paper on LAPD; and PoP 2018 paper on Helical SOL

Motivation: electromagnetic effects important in edge

- Electromagnetic effects are especially important in the edge and SOL, where steep gradients can push the plasma close to the ideal-MHD stability threshold and produce stronger turbulence
- Including electromagnetic fluctuations has proved challenging in PIC codes due to sampling noise, which leads to the well-known Ampère cancellation problem
- Continuum gyrokinetic codes for core turbulence have avoided the Ampère cancellation issue
- As `Gkeyll` uses a continuum formulation, we expect that we can handle electromagnetic effects in the edge and SOL in a stable and efficient manner

Hamiltonian ($p_{\|}$) vs. Symplectic ($v_{\|}$) formulations

Two formulations for including electromagnetic fluctuations (see Brizard & Hahm, 2007):

- Hamiltonian formulation: $p_{\|} = mv_{\|} + qA_{\|}$

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

$$H = \frac{1}{2m}p_{\|}^2 + \mu B + q\phi = \frac{1}{2m}(mv_{\|} + qA_{\|})^2 + \mu B + q\phi \qquad \mathbf{B}^* = \mathbf{B_0} + \frac{1}{q}p_{\|}\nabla\times\hat{\mathrm{b}}$$

- Symplectic formulation: $p_{\|} = mv_{\|}$

$$\frac{\partial f}{\partial t} = \{H, f\} + \frac{q}{m}\frac{\partial f}{\partial v_{\|}}\frac{\partial A_{\|}}{\partial t}$$

$$H = \frac{1}{2}mv_{\|}^2 + \mu B + q\phi \qquad \mathbf{B}^* = \mathbf{B_0} + \frac{m}{q}v_{\|}\nabla\times\hat{\mathrm{b}} + \delta\mathbf{B}_{\perp}$$

Poisson bracket:

$$\{F, G\} = \frac{\mathbf{B}^*}{B_{\|}^*}\cdot\left(\nabla F\frac{\partial G}{\partial p_{\|}} - \frac{\partial F}{\partial p_{\|}}\nabla G\right) - \frac{\hat{\mathrm{b}}}{qB_{\|}^*}\times\nabla F\cdot\nabla G$$

Hamiltonian ($p_\|$) vs. Symplectic ($v_\|$) formulations

In Gkeyll's discontinuous Galerkin (DG) scheme, fields can be discontinuous across cell boundaries, but **energy is conserved only if the Hamiltonian is continuous**

- Hamiltonian ($p_\|$) $\Rightarrow$ both ϕ & $A_\|$ must be continuous
- Symplectic ($v_\|$) $\Rightarrow$ ϕ must be continuous, but $A_\|$ (and $\frac{\partial A_\|}{\partial t}$) can be discontinuous in parallel direction

We must evaluate moments (density, momentum) numerically and consistently

- Hamiltonian ($p_\|$) $\Rightarrow$ Integration in $p_\| \sim A_\|$, so integration limits depend on fluctuations.
- Symplectic ($v_\|$) $\Rightarrow$ Integration in $v_\|$, so integration limits not fluctuation-dependent

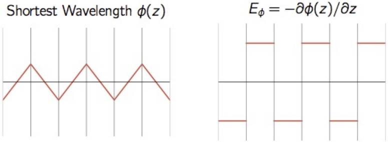
$\partial A_\| / \partial t$ appears explicitly in GK equation in symplectic formulation, but not in Hamiltonian formulation

Challenges with Hamiltonian ($p_{\parallel}$) formulation

Note that in the MHD limit (e.g. for Alfvén waves), we need

$$E_{\parallel} = -\frac{\partial \phi}{\partial z} - \frac{\partial A_{\parallel}}{\partial t} \approx 0$$

Consider the shortest-wavelength mode on the grid with piecewise linear basis functions:



If the system wanted to be in the MHD limit ($E_{\parallel} = 0$), and we required $A_{\parallel}$ to be continuous (as in Hamiltonian formulation), this would result in $A_{\parallel} = 0$

$\Rightarrow$ Effectively an electrostatic Ω_H mode, which requires a very small time step $\Delta t < k_{\parallel,\max} v_{te} / (k_{\perp,\min} \rho_s)$

Would need to require ϕ **and** $\partial\phi/\partial z$ to be continuous! **Symplectic representation does not suffer from this issue. Further, Ampere cancellation issues are not present.**

We choose Symplectic formulation of EMGK

Electromagnetic GK Vlasov equation:

$$\frac{\partial f}{\partial t} = \{H, f\} + \frac{q}{m}\frac{\partial A_\parallel}{\partial t}\frac{\partial f}{\partial v_\parallel} = -\boldsymbol{\alpha}\cdot\nabla_6 f + \frac{q}{m}\frac{\partial A_\parallel}{\partial t}\frac{\partial f}{\partial v_\parallel},$$

or in conservative form,

$$\frac{\partial(\mathcal{J} f)}{\partial t} + \nabla_6\cdot(\boldsymbol{\alpha}\mathcal{J} f) - \frac{\partial}{\partial v_\parallel}\left(\frac{q}{m}\frac{\partial A_\parallel}{\partial t}\mathcal{J} f\right) = 0,$$

with $\mathcal{J} = B_\parallel^*$ the Jacobian (up to some normalization factors). Here

$$\boldsymbol{\alpha} - \frac{q}{m}\frac{\partial A_\parallel}{\partial t}\hat{\mathrm{v}}_\parallel = \{\mathbf{Z}, H\} - \frac{q}{m}\frac{\partial A_\parallel}{\partial t}\hat{\mathrm{v}}_\parallel$$

is the phase-space velocity in the six-dimensional phase space $\mathbf{Z} = (\mathbf{X}, v_\parallel, \mu, \zeta)$.

The Hamiltonian is

$$H = \frac{1}{2}mv_\parallel^2 + \mu B + q\phi,$$

and the Poisson bracket is

$$\{F, G\} = \frac{\mathbf{B}^*}{mB_\parallel^*}\cdot\left(\nabla F\frac{\partial G}{\partial v_\parallel} - \frac{\partial F}{\partial v_\parallel}\nabla G\right) - \frac{c\hat{\mathrm{b}}}{qB_\parallel^*}\times\nabla F\cdot\nabla G.$$

We choose Symplectic formulation of EMGK

Quasineutrality equation (long-wavelength):

$$-\nabla \cdot \sum_s \frac{m}{B^2} \int d^3v \ f \ \nabla_\perp \phi = \sum_s q \int d^3v \ f$$

Parallel Ampère equation:

$$-\nabla_\perp^2 A_\parallel = \mu_0 \sum_s q \int d^3v \ v_\parallel f$$

Parallel Ohm's law:

$$\left(-\nabla_\perp^2 + \sum_s \frac{\mu_0 q^2}{m} \int d^3v \ f \right) \frac{\partial A_\parallel}{\partial t} = \mu_0 \sum_s q \int d^3v \ v_\parallel \{H, f\}$$

Can we design a scheme that 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.

Linear Benchmark: Kinetic Alfvén Waves

In slab geometry, with a uniform Maxwellian background and stationary ions, the linearized GK equation reduces to

$$\frac{\partial f_e}{\partial t} + v_{\|} \frac{\partial f_e}{\partial z} = v_{\|} F_{Me} \left(\frac{\partial \phi}{\partial z} + \frac{\partial A_{\|}}{\partial t} \right).$$

Taking a single Fourier mode with perpendicular wavenumber $k_\perp$ and parallel wavenumber $k_\|$, the field equations become

$$k_\perp^2 \frac{m_i n_0}{B^2} \phi = -e \int dv_\| \; f_e$$

$$k_\perp^2 A_\| = -\mu_0 e \int dv_\| \; v_\| f_e.$$

The KAW dispersion relation is then

$$\omega^2 \left[1 + \frac{\omega}{\sqrt{2} k_\| v_{te}} Z \left(\frac{\omega}{\sqrt{2} k_\| v_{te}} \right) \right] = \frac{k_\|^2 v_{te}^2}{\hat{\beta}} \left[1 + k_\perp^2 \rho_s^2 + \frac{\omega}{\sqrt{2} k_\| v_{te}} Z \left(\frac{\omega}{\sqrt{2} k_\| v_{te}} \right) \right],$$

where $\hat{\beta} = (\beta_e/2) m_i / m_e$, and $Z(x)$ is the usual plasma dispersion function.

Linear Benchmark: Kinetic Alfvén Waves

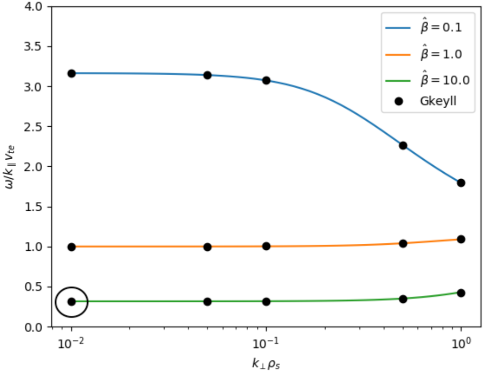


Figure: Alfvén wave dispersion relation computed with `Gkeyll` compared to analytical results.

Linear Benchmark: Kinetic Ballooning Mode

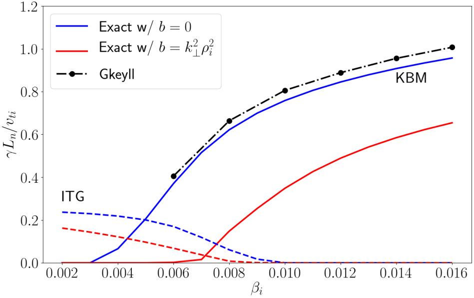
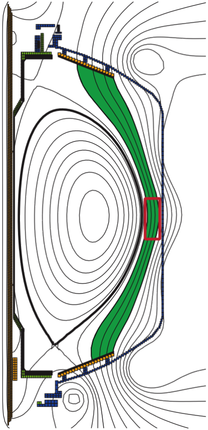


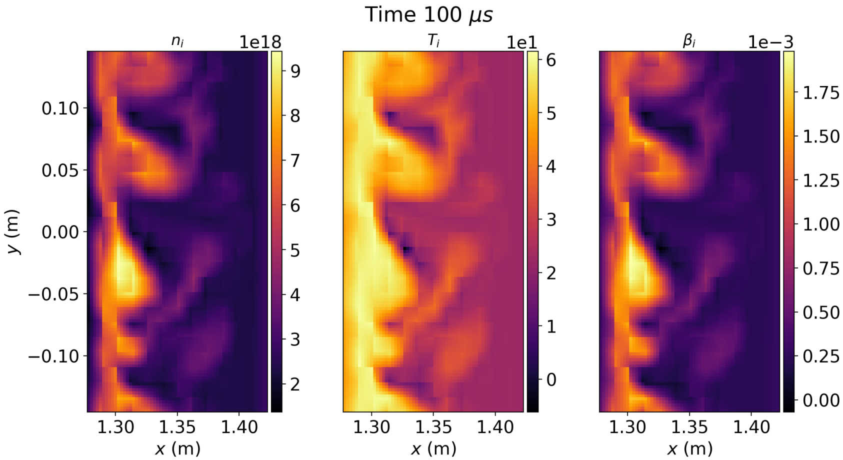
Figure: Kinetic Balloning Mode (KBM) growth rate as function of β_i from `Gkeyll` compared to analytical results.

EM turbulence in NSTX-like helical SOL

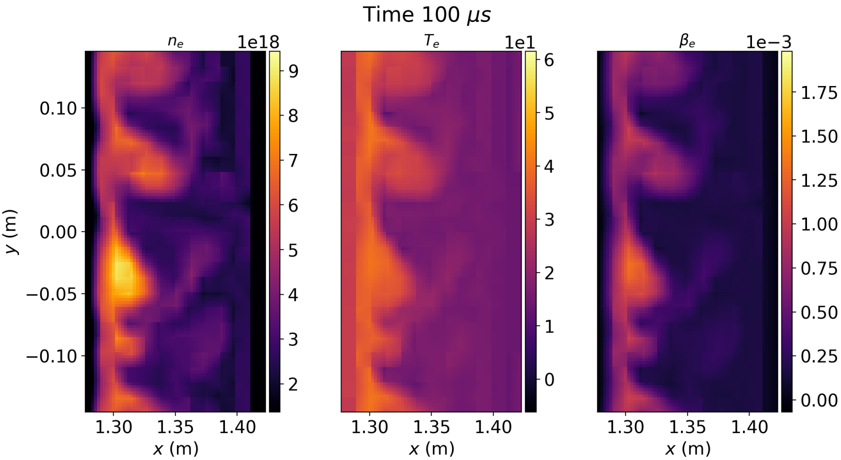


- Simple helical model of tokamak SOL
  - Like the green region, but straightened out to vertical flux surfaces
  - Field-aligned simulation domain that follows field lines from bottom divertor plate, around the torus, to the top divertor plate
  - All bad curvature
- Parameters taken from NSTX SOL measurements
- Conducting sheath boundary conditions at the divertor plates
- Radially-localized source around $x = 1.3$ cm models flux of particles and heat across separatrix from core
- Real deuterium mass ratio, Lenard-Bernstein collisions

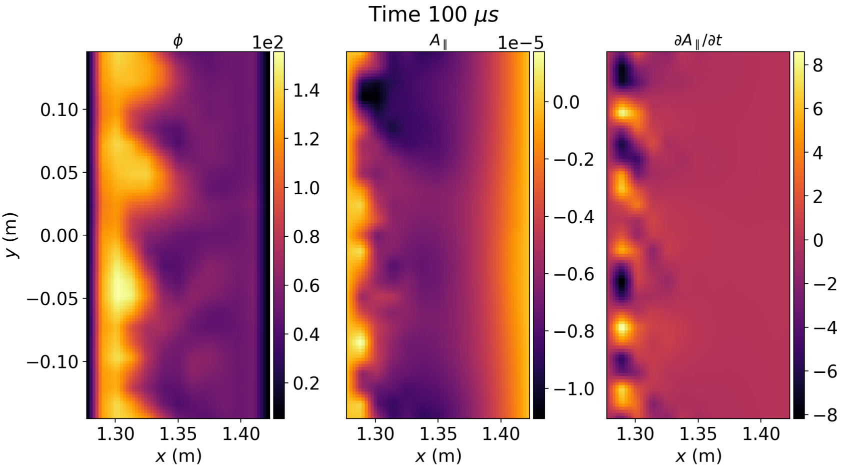
EM turbulence in NSTX-like helical SOL: Ions



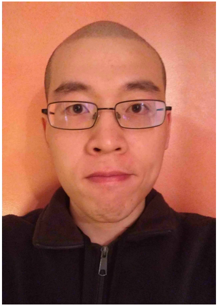
EM turbulence in NSTX-like helical SOL: Electrons



EM turbulence in NSTX-like helical SOL: Fields



Part III: Multi-Fluid Moment Models



The core team: **Jonathan Ng**, **Chaunfei Dong**, **Liang Wang** and **Amitava Bhattacharjee**. Funded via NSF/NASA project (AB) and AFOSR project.

Integrating kinetic effects in fluid models

- For physically accurate simulations of Earth's magnetosphere and space weather modeling, its important to **go beyond resistive and Hall-MHD**.
- Traditional approach has been to use a generalized Ohm's law, adding physics to it in a piecemeal fashion.
- However, this approach has limited success, and in particular, there is no systematic way to add important collisionless kinetic effects in a self-consistent and numerically tractable manner.
- A major challenge in the magnetosphere (and other applications) is that the **plasma is nearly collisionless**, and that the **magnetic fields (planetary dipole, solar wind) add a preferred direction**, adding significant anisotropy to the system.

Alternative is to use multi-fluid moment models

- In this approach we take moments of the Vlasov equation, truncating the moment sequence using a closure.
- The interaction between species is via electromagnetic fields, which are evolved using Maxwell equations (retaining displacement currents)
- This approach allows natural and self-consistent inclusion of **finite electron inertia, Hall currents, anisotropic pressure tensor and heat flux tensor**.
- Even though the multi-fluid moment equations contain physics all the way from light waves and electron dynamics to MHD scales, by use of advanced algorithms very efficient and robust schemes can be developed, **allowing us to treat a sequence of increasing fidelity models in a uniform and consistent manner**.

Sequence of models with 5, 10 and 20 moments

Taking moments of Vlasov equation leads to the *exact* moment equations listed below

$$
\begin{aligned}
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(n u_j) &= 0 \\
m\frac{\partial}{\partial t}(n u_i) + \frac{\partial \mathcal{P}_{ij}}{\partial x_j} &= nq(E_i + \epsilon_{ijk} u_j B_k) \\
\frac{\partial \mathcal{P}_{ij}}{\partial t} + \frac{\partial \mathcal{Q}_{ijk}}{\partial x_k} &= nq u_{[i} E_{j]} + \frac{q}{m}\epsilon_{[ikl}\mathcal{P}_{kj]} B_l \\
\frac{\partial \mathcal{Q}_{ijk}}{\partial t} + \frac{\partial \mathcal{K}_{ijkl}}{\partial x_l} &= \frac{q}{m}(E_{[i}\mathcal{P}_{jk]} + \epsilon_{[ilm}\mathcal{Q}_{ljk]} B_m)
\end{aligned}
$$

In the **five-moment** model, we assume that the pressure is isotropic $P_{ij} = p\delta_{ij}$. For the **ten-moment** model, we include the time-dependent equations for all six components of the pressure tensor, and use a closure for the heat-flux. In the **twenty-moment** model, we evolve all ten components of the heat-flux tensor, closing at the fourth moment.

We need to find a closure for heat-flux tensor

For our current implementation, upon dropping order-unity constants, we have

$$ik_m Q_{ijm}(k) = v_t|k|\tilde{T}_{ij}(k)n_0,$$

where, now, $k = |\mathbf{k}|$, $\tilde{T}_{ij}(k) = (\tilde{P}_{ij}(k) - T_0\tilde{n}\delta_{ij})/n_o$ is the perturbed temperature. Note that this form *does not account for magnetic field direction*, however can be extended easily to do so.
Still a non-local closure! So replace the continuous wave-number, k with a typical wave-number, k_0, which defines a scale over which collisionless damping is thought to occur. Hence, in physical space we can write

$$\partial_m Q_{ijm} \approx v_t|k_0|(P_{ij} - \bar{P}_{ij} - \delta_{ij}(n - \bar{n})\bar{T}).$$

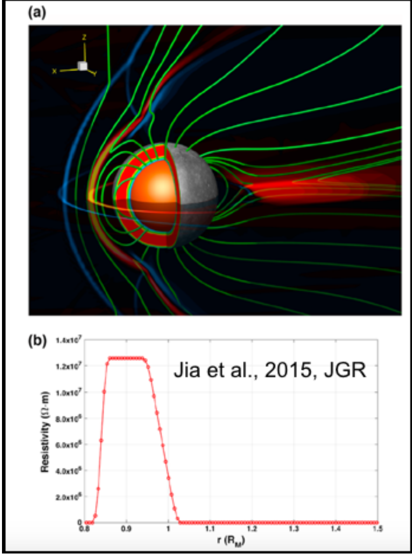
This has the form of a relaxation, driving the pressure tensor towards isotropy (or Chew-Goldberg-Low form) as $v_t|k_0| \to 0$.

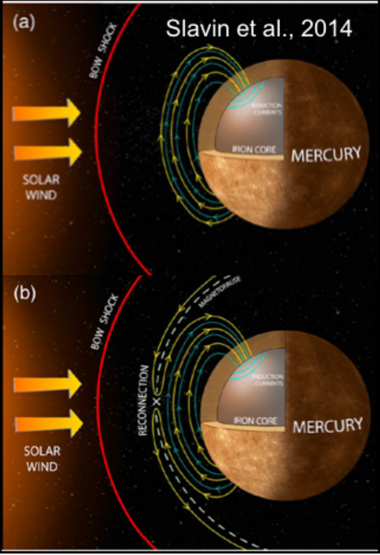
Summary of numerical challenges

Overall implementation relatively straight-forward: we use Riemann solver based finite-volume scheme, with careful handling of source terms.

- There is a **huge set of temporal and spatial scales**, making the models very stiff. We have implemented a **semi-implicit method**, which allows us to step over plasma-frequency and Debye length.
- Maintaining **divergence constraints** in Maxwell equations is difficult: some sort of **divergence cleaning** is required. Note that unlike MHD, we also need to ensure $\nabla \cdot \mathbf{E} = \varrho_c/\epsilon_0$, which is more challenging.
- "Standard" schemes not **asymptotic preserving**: in the situation in which Debye length, electron- or ion-inertial scales are severely under-resolved, the system should asymptote to (Hall-)MHD. This requires reformulation of the equations in **combined fluid-EM** form, with **electric field equation reformulated in curl-curl form**. Implicit methods may be needed.

Overview of 3D Mercury's Magnetosphere Simulation





Overview of 3D Mercury's Magnetosphere Simulation

- Uses realistic ion mass but artificial electron mass ($m_p/m_e=25$) and speed of light ($c=3\times10^6$ m/s). Ion inertial length $d_i=0.2R_M$
- Simulation domain: $-5R_M<x<15R_M$, $-25R_M<y,z<25R_M$
- Smallest resolution: $dx=dy=dz=0.04R_M$
- $k_e = 10/d_e$, $k_i = 10/d_i$
- Include a resistive mantle inside planetary body.
- Boundary conditions are implemented similar to Jia *et al.*, 2015, JGR.

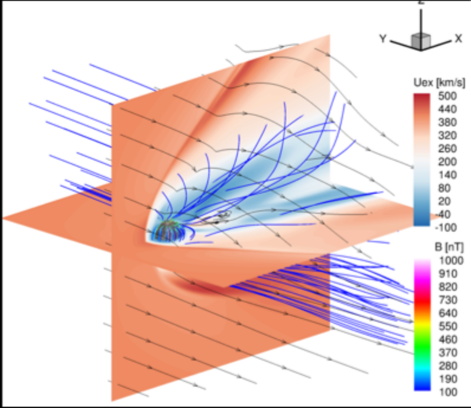
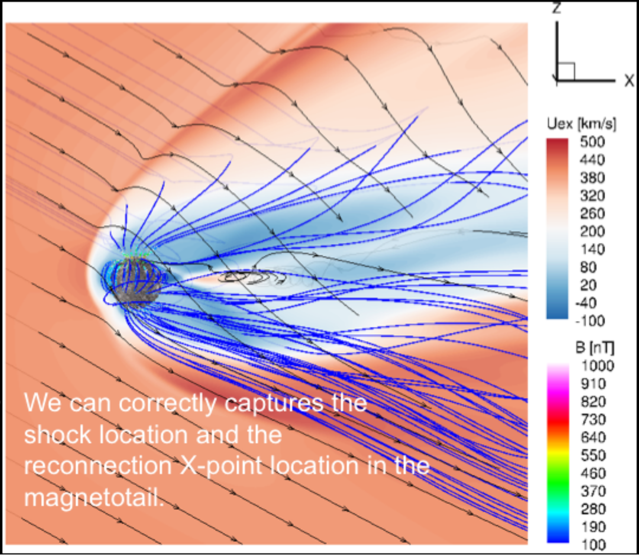


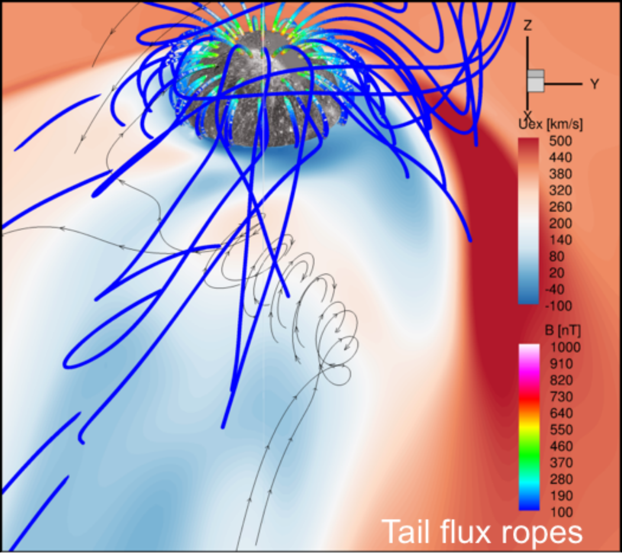
Figure: 3D illustration of solar wind interaction with Mercury. X-axis points from sun to the planet.

Simulated X-Z Plane of Mercury's Magnetosphere

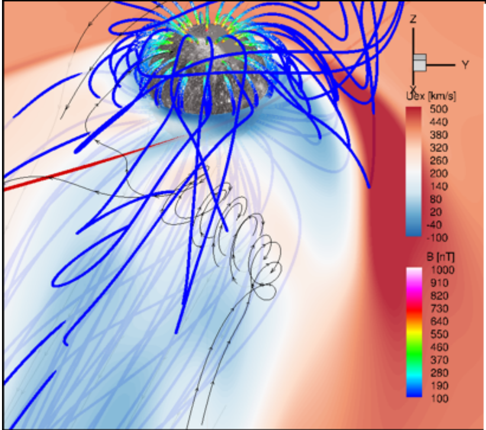


- We can correctly captures the shock location and the reconnection X-point location in the magnetotail.

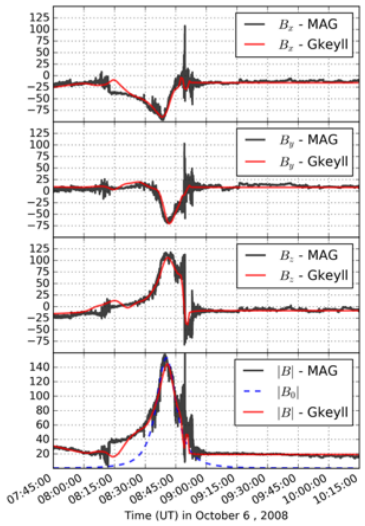
3D View of Mercury's Magnetotail Flux Ropes



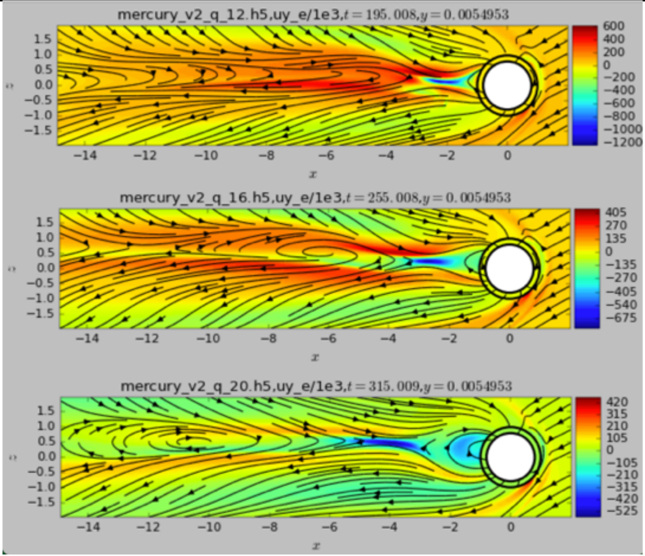
Mercury's Magnetotail Flux Ropes together with MESSENGER's M2 Trajectory



Data-model comparison of magnetic fields along the red spacecraft trajectory (black: spacecraft observation, red: Gkeyll simulations.)



Mercury's Dynamic Magnetotail during a Space Weather Event



Part IV: The Future: `Gkeyll`

`Gkeyll` is in a very exciting phase of development at present. Several major physics studies are underway and significant new development is planned. Hiring two new postdocs.

- Flexible hybrid modeling, e.g. Vlasov ions with 5 or 10 moment electrons coupled to Maxwell's equations (combined with fluid time-stepping)
- More accurate collision operators; possibly nonlinear Fokker-Planck operator; atomic physics; neutrals
- Better geometry. Made a start on mapped grids, need to extend to multiple blocks to do full tokamak geometry; useful also in magnetosphere calculations
- Asymptotic preserving schemes and adaptive mesh refinement
- Longer term add relativistic and radiation reaction to Vlasov solver;

A path to whole device modeling of fusion machines

Prediction of burning plasma state remains a “Grand Challenge” problem.

- How does one model a fusion device? Efforts have focused on reduced models (TRANSP, OMFIT, etc) and first-principles models. The latter are mostly driven by extended MHD and/or major GK codes.
- Reduced models are very useful and used extensively in design and analysis, but often miss key physics.
- In general, first-principle models are at present not in a position to completely model the tokamak (or stellerator) in its entirety.

Whole Device Predictions of Stability and Transport in Burning Plasmas

What are the ingredients needed in this effort?

- Model heating sources (NBI, ICRH, ECRH); Capability to evolve equilibria on transport scales in the core and edge regions; Predict the onset of instabilities; Self-consistent mapping of pedestal stability and inter-ELM simulations; Determine if plasma parameters live within engineering constraints
- This is a highly non-trivial task needing proper mathematical formulation to ensure physics is not violated when various pieces are brought together; multidisciplinary physics, applied math and computer science problem

Whole Device Predictions of Stability and Transport in Burning Plasmas

An "Advanced Computing" research program at PPPL will be ideally poised to address the WDM problem

- What are the "components" needed to model the various physics processes? Do new ones need development?
- Are the equations in each "component" consistent with approximations made in the others? Is time-scale scale separation sufficient to allow multi-scale coupling? What time-stepping is appropriate when each "component" uses its own, potentially incompatible with others, time-stepping scheme?
- What software infrastructure is needed to support a WDM? Adherence to common interfaces and "scriptability" is critical to reuse and flexible composition of "components"; Can one imagine a ITER "App" or a DIII-D "App" that allows user to easily compose WDM simulations? Can "component" software-containers be created that anyone can easily install and use?

Leveraging ECP and other projects a properly defined effort led from PPPL can provide needed leadership to make this happen.