Full-stack (gyro)kinetics: novel algorithms and some results

Ammar Hakim and the `Gkeyll` Team

Princeton Plasma Physics Laboratory

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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.
- 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

Part I: The Vlasov-Maxwell System



The core team: **Jason TenBarge**, **Jimmy Juno**, and **Petr Cagas**, **Mana Francisquez**.

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

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

Solve VM system *efficiently* and conserve 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 kinetic turbulence and other problems, we would like a noise-free algorithm that allows studying phase-space structures correctly, in a noise-free manner.

Explore high-order discontinuous Galerkin algorithms to directly discretize the Vlasov-Maxwell system.

DG represents state-of-art for hyperbolic PDEs

DG algorithms hot topic in CFD and applied mathematics.

- First introduced by Reed and Hill in 1973 as a conference paper to solve steady-state neutron transport equations. More than 2100 citations.
- Some earlier work on solving *elliptic* equations by Nitsche in 1971 (original paper in German). Introduced the idea of "interior penalty". Usually, though, DG is not used for elliptic problems. Paradoxically, perhaps DG may be even better for certain elliptic/parabolic problems.
- Key paper for nonlinear systems in multiple dimensions is by Cockburn and Shu (JCP, **141**, 199-224, 1998). More than 1700 citations.
- Almost continuous stream of papers in DG, both for fundamental formulations and applications to physics and engineering problems. This continues to be an active area of research, and at present *DG is under-utilized in plasma physics*.

What are discontinuous Galerkin schemes?

Discontinuous Galerkin schemes are a class of *Galerkin* schemes in which the solution is represented using *piecewise discontinuous* functions.

- *Galerkin* minimization
- Piecewise *discontinuous* representation

Essential ideas

Consider a general time-dependent problem on $x \in [-1, 1]$:

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

where $G[f]$ is some operator. To approximate it expand $f(x)$ with our basis functions $P_k(x)$,

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

This gives discrete system

$$\sum_{k=1}^{N} f_k' P_k(x) = G[f_h]$$

Question

How to determine f_k' in an optimum manner?

Essential idea

Answer: Do an L_2 minimization of the error, i.e. find f_k' such that the error as *defined by our selected norm* is minimized.

$$E_N = \left\| \sum_{k=1}^{N} f_k' P_k(x) - G[f_h] \right\|_2 = \int_{-1}^{1} \left[\sum_{k=1}^{N} f_k' P_k(x) - G[f_h] \right]^2 dx$$

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'

$$\int_{-1}^{1} P_m(x) \left(\sum_{k=1}^{N} f_k' P_k(x) - G[f_h] \right) dx = 0$$

for all $m = 1, \ldots, N$. This will give

$$f_k' = \frac{2k+1}{2} \int_{-1}^{1} P_k(x) G[f_h] \, dx$$

What does a typical L_2 fit look like?

In discontinuous Galerkin schemes we split interval into cells and use Galerkin scheme in each cell. This will naturally lead to *discontinuities* across cell boundaries.

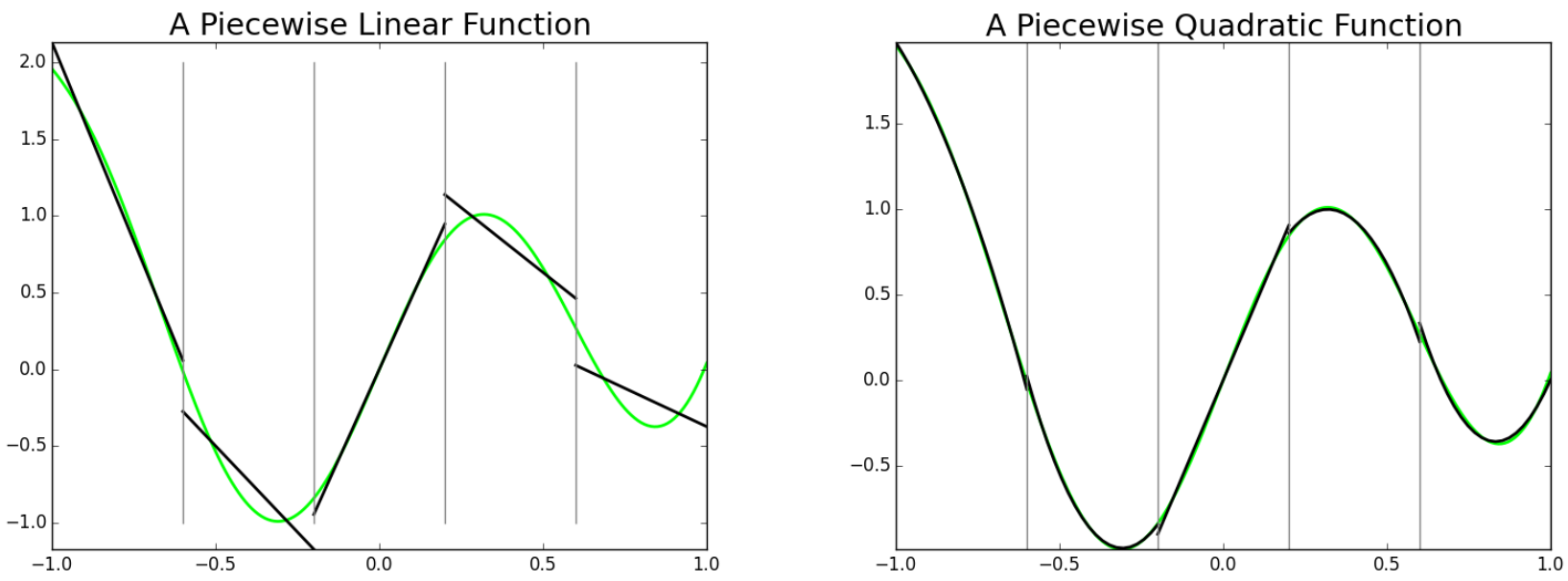


Figure: The best L_2 fit of $x^4 + \sin(5x)$ with piecewise linear (left) and quadratic (right) basis functions.

Weak-equality and recovery

- It is important to remember that the discontinuous Galerkin solution is a *representation* of the solution and not the solution itself.
- Notice that even a continuous function will, in general, have a discontinuous *representation* in DG.

We can formalize this idea using the concept of *weak-equality*. Choose an inner product, for example

$$(f, g) \equiv \int_I f(x)g(x)\,dx.$$

Definition (Weak equality)

Two functions, f and g are said to be *weakly equal* if

$$(\psi_k, f - g) = 0$$

for all $k = 1, \ldots, N$. We denote weak equality by

$$f \doteq g.$$

Weak-equality and recovery

- Notice that weak-equality depends on the function space as well as the inner-product we selected.
- The Galerkin L_2 minimization is equivalent to, for example, restating that

$$f'(x,t) \doteq G[f]$$

  This implies

$$\left(\psi_k, f'(x,t) - G[f]\right) = 0$$

  which is exactly what we obtained by minimizing the error defined using the L_2 norm.
- Hence, we can say that the *DG scheme only determines the solution in the weak-sense*, that is, all functions that are weakly equal to DG representation can be potentially interpreted as the actual solution.
- This allows a powerful way to construct schemes with desirable properties by *recovering* weakly-equal functions using the DG representations.

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?

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.

A model Fokker-Planck operator implemented

We have implemented the Dougherty Lenard-Bernstein operator (DLBO) 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.

To give and not to count the cost ...

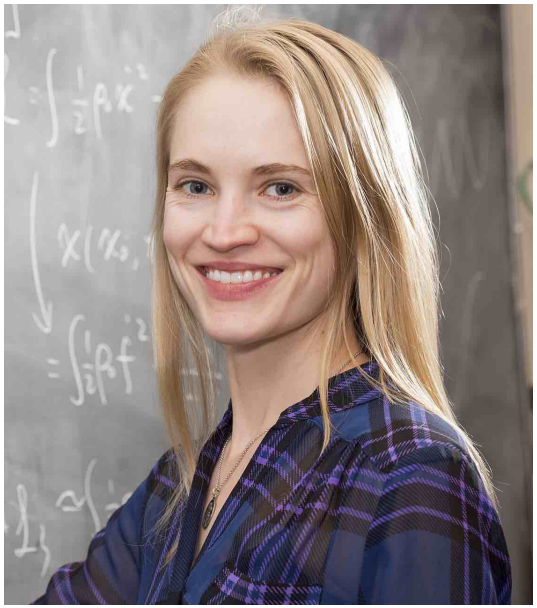
Question: Are continuum schemes competitive compared to PIC schemes in terms of cost for a given accuracy?

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 and using CAS generated code has shown that continuum schemes can be made to scale as number of basis functions in phase-space. (In standard DG, the schemes usually scale quadratically or cubially with number of basis functions!). This is potentially a game-changer as efficiency improves dramatically (at the cost of more complex code (however, no one really needs to read the code!)).

Part II: Electromagnetic Gyrokinetics


The core team: **Noah Mandell**, **Tess Bernard**, **Mana Francisquez** and **Greg Hammett**.

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, straight **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.

Important to preserve quadratic invariants

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.

Can one construct conservative schemes?

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.

Status of Gyrokinetics in Gkeyll

- Initial ES-GK work by Eric Shi[2] led to 5D electrostatic full-F GK simulations of LAPD and NSTX-like helical SOL with sheath BCs. More recently, Tess Bernard (PoP 2019) performed simulations of Texas Helimak and compared to experiments.
- 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; added geometry (but no X-point yet)

<u>What about electromagnetics?</u> See G. Hammett talk.

[2] See 2017 thesis; JPP 2017 paper on LAPD; and PoP 2019 paper on Helical NSTX-like SOL