Efficient Continuum Schemes for the Vlasov-Maxwell Equations with Applications to Phase-Space Dynamics in Collisionless Plasmas

Ammar Hakim **Jimmy Juno** **Noah Mandell** and the `Gkeyll` Team

Princeton Plasma Physics Laboratory

September 11th, 2019

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 , kinetic wall-bounded plasmas 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

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

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

Hamiltonian systems: gyrokinetics, self-gravitating systems

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.

Solve VM system *efficiently* and conserve invariants

We know that the Vlasov-Maxwell (and Hamiltonian) 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?

Important to realize that conservation properties are indirect: don't evolve total energy or total momentum equation.

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 kinetics systems as a PDE in phase-space.

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.

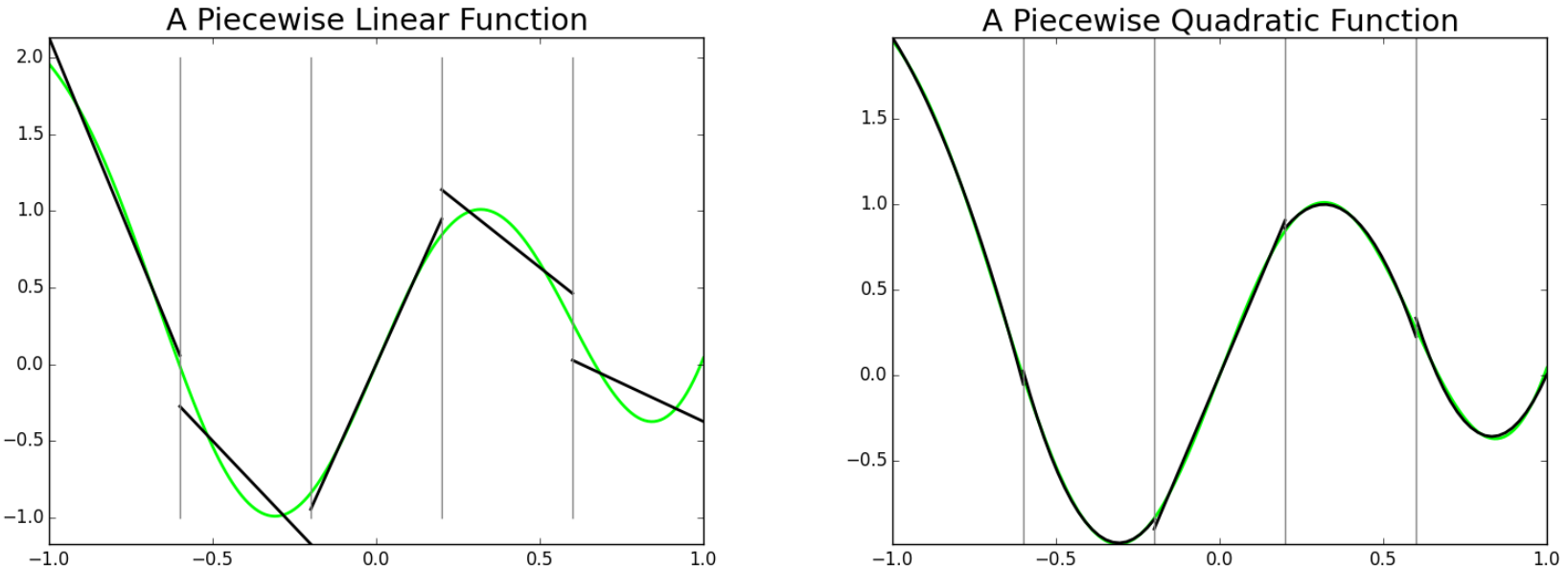

Figure: The best L_2 fit of $x^4 + \sin(5x)$ with piecewise linear (left) and quadratic (right) basis functions.

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.

Example of recovery: Exponential recovery in a cell

- Consider we have a linear representation of the particle distribution function $f_h(x) = f_0 + xf_1$ in a cell.
- We can use this to *reconstruct* an exponential function that has the desirable property that it is *positive* everywhere in the cell. That is, we want to find

$$\exp(g_0 + g_1 x) \doteq f_0 + xf_1$$

- This will lead to a coupled set of nonlinear equations to determine g_0 and g_1
- Note that this process is not always possible: we need $f_0 > 0$ as well as the condition $|f_1| \leq 3f_0$. Otherwise, the f_h is not realizable (i.e. there is no positive distribution function with the same moments as f_h).

Example of recovery: Exponential recovery in a cell

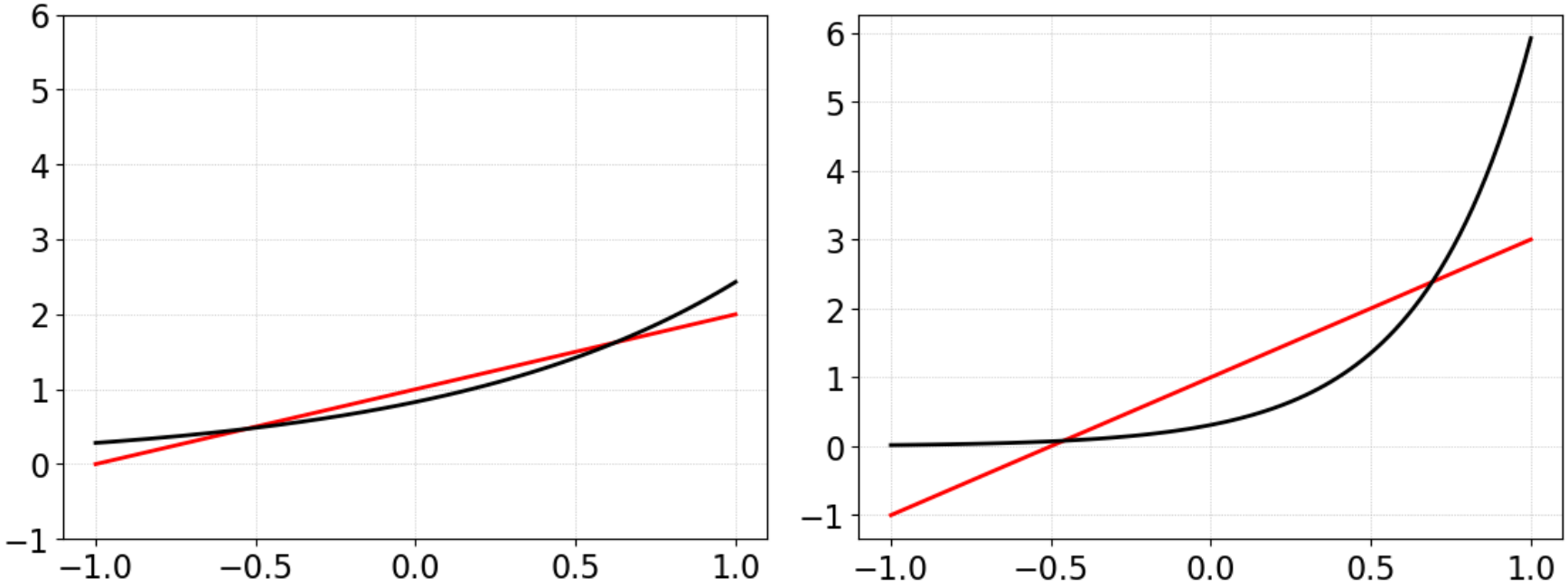

Figure: Recovery of exponential function (black) from linear function (red). Left plot is for $f_0 = 1$, $f_1 = 1$ and right for $f_0 = 1$ and $f_1 = 2$.

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.

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

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

This is a simple corollary of the conservation/decay of f_h^2.

Discretizing full-F Fokker-Planck operators

We have implemented a full-F nonlinear Fokker-Planck operator written in the Rosenbluth form

$$\left(\frac{\partial f}{\partial t}\right)_c = -\nabla\cdot(\mathbf{a}f) + \frac{1}{2}\nabla\cdot[\nabla\cdot(\mathbf{D}f)]\,.$$

Here $\mathbf{a} = \nabla h$ is the *drag velocity* and $\mathbf{D} = \nabla\nabla g$ the (symmetric) diffusion tensor.

- The *Rosenbluth potentials* h and g are determined from $\nabla^2 h = f$ and $\nabla^2 g = h$.
- Often, one can avoid the Poisson solves and approximate the potentials directly as

$$h = -\nu\left(\frac{1}{2}\mathbf{v}^2 - \mathbf{v}\cdot\mathbf{u}\right)$$
$$g = \nu v_{th}^2\mathbf{v}^2$$

  This leads to the Dougherty or Lenard-Bernstein operator (D-LBO). See H. et. al. arxiv:1903.08062.
- Other approximations are also possible: solve Poisson equations for Rosenbluth potentials using spherical harmonics, retaining only a few (even one) term.

Full-F Fokker-Planck operators: conservation

We can show that momentum and energy conservation is obtained (as for any good collision operator) if the following relations are satisfied

$$\int_{-\infty}^{\infty} \mathbf{a} f \, d^3\mathbf{v} = 0.$$

for momentum conservation, and

$$\int_{-\infty}^{\infty} \left(\mathbf{a} \cdot \mathbf{v} + \frac{1}{2} \mathrm{Tr}(\mathbf{D}) \right) f \, d^3\mathbf{v} = 0.$$

for energy conservation.

We must ensure that the discrete scheme satisfies these relations to ensure discrete momentum and energy conservation. In general, **we must directly incorporate these relations in constructing the scheme**. They can't be automatically satisfied otherwise.

Full-F Fokker-Planck operators: DG scheme

Two key tricks to ensure momentum and energy conservation:

- To derive weak-form of FPO we must to *integrate by parts twice for the diffusion term*
- To solve for the Rosenbluth potentials we must use a *DG representation to solve a constrained form of Poisson equations*. (Not sure of this. Perhaps there is a way to use standard FEM based Poisson solvers too).

The weak-form is

$$\int_{K_j} w\frac{\partial f}{\partial t}\,d\mathbf{v}^3 = -\oint_{\partial K_j} w^-(\mathbf{a}f)\cdot d\mathbf{s} + \int_{K_j}\nabla w\cdot\mathbf{a}f\,d\mathbf{v}^3 + \frac{1}{2}\oint_{\partial K_j}\left[w^-\nabla\cdot(\mathbf{D}f) - \nabla w^-\cdot\mathbf{D}f\right]\cdot d\mathbf{s} + \frac{1}{2}\int_{K_j}(\nabla\nabla w):\mathbf{D}f\,d\mathbf{v}^3$$

We need to evaluate first *and* second derivatives of discontinuous functions at cell interfaces. How to do this?

Lets revisit weak-equality and recovery

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

$$f \doteq g.$$

Recall that the DG solution is only a *representation* of the solution and not the solution itself. Hence, we can consider the following "inverse" problem: given a discontinuous solution across two cells, is it possible to *recover* a *continuous representation* that can then be used in the above weak-form?

Use weak-equality to *recover* continuous function

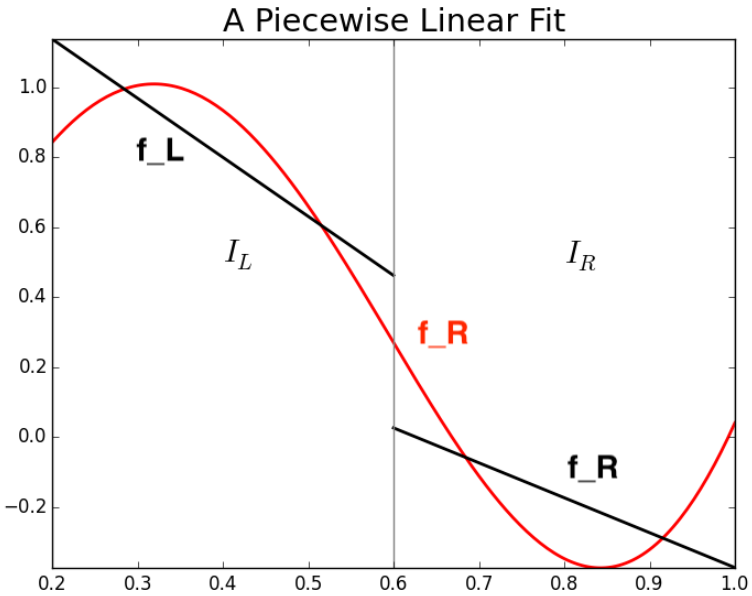

Figure: Given piecewise linear representation (black) we want to recover the continuous function (red) such that **moments of recovered and linear representation are the same in the respective cells**.

Use weak-equality to *recover* continuous function

- Consider recovering $\hat{f}$ on the interval $I = [-1, 1]$, from a function, f, which has a single discontinuity at $x = 0$.
- Choose some function spaces $\mathcal{P}_L$ and $\mathcal{P}_R$ on the interval $I_L = [-1, 0]$ and $I_R = [0, 1]$ respectively.
- Reconstruct a continuous function $\hat{f}$ such that

$$\hat{f} \doteq f_L \quad x \in I_L \quad \text{on } \mathcal{P}_L$$
$$\hat{f} \doteq f_R \quad x \in I_R \quad \text{on } \mathcal{P}_R.$$

  where $f = f_L$ for $x \in I_L$ and $f = f_R$ for $x \in I_R$.
- To determine $\hat{f}$, use the fact that given $2N$ pieces of information, where N is the number of basis functions in $\mathcal{P}_{L,R}$, we can construct a polynomial of maximum order $2N - 1$. We can hence write

$$\hat{f}(x) = \sum_{m=0}^{2N-1} \hat{f}_m x^m.$$

  Plugging this into the weak-equality relations gives a *linear* system for $\hat{f}_m$.

Use recovered function in weak-form

Once we have determined $\hat{f}$ we can use this in the discrete weak-form of the diffusion equation:

$$\int_{I_j} \varphi f_t \, dx = \varphi \hat{f}_x \Big|_{x_{j-1/2}}^{x_{j+1/2}} - \int_{I_j} \varphi_x f_x \, dx.$$

Note that now as $\hat{f}$ is continuous at the cell interface there is no issue in computing its derivative. We can, in fact, do a second integration by parts to get another discrete weak-form

$$\int_{I_j} \varphi f_t \, dx = (\varphi \hat{f}_x - \varphi_x \hat{f}) \Big|_{x_{j-1/2}}^{x_{j+1/2}} + \int_{I_j} \varphi_{xx} f \, dx.$$

Recall the second integration by parts is needed to get momentum and energy conservation for the FPO. **Use recovery also to solve Poisson equations**: Rosenbluth potentials need a discontinuous representation!

Another look at computing numerical fluxes

- To design a scheme for the diffusion equation we used a recovery procedure to compute the edge values and slopes
- Can this process be used to compute numerical fluxes for use in updating advection equations? Instead of using upwinding or central fluxes, we can use recovered polynomial at each cell interface to compute numerical fluxes.

This leads to a *differential* form of the DG scheme that is very simply written as (for the linear advection equation)

$$\left(\psi_k, f_t\right) = -\left(\psi_k, \hat{f}_x\right).$$

Potentially much more accurate scheme for smooth solution. Likely leads to the *most accurate possible DG scheme using a three-point stencil*.

Recovery based DG scheme is surprisingly accurate

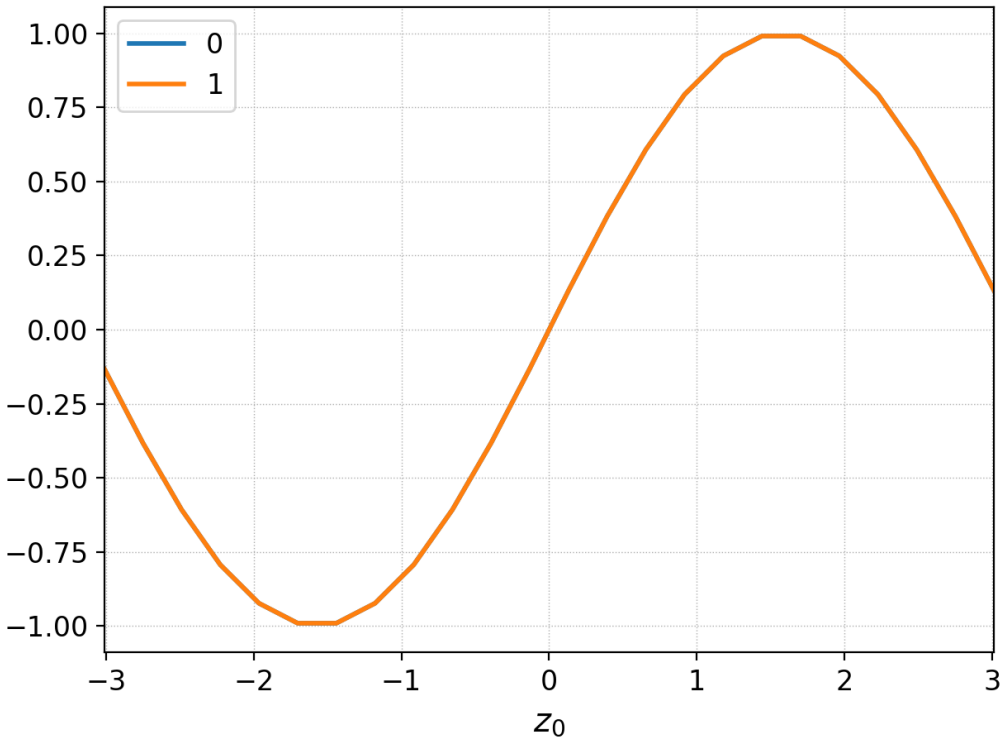

Figure: An EM wave propagated 10 periods using recovery DG scheme

Recovery based DG scheme is surprisingly accurate

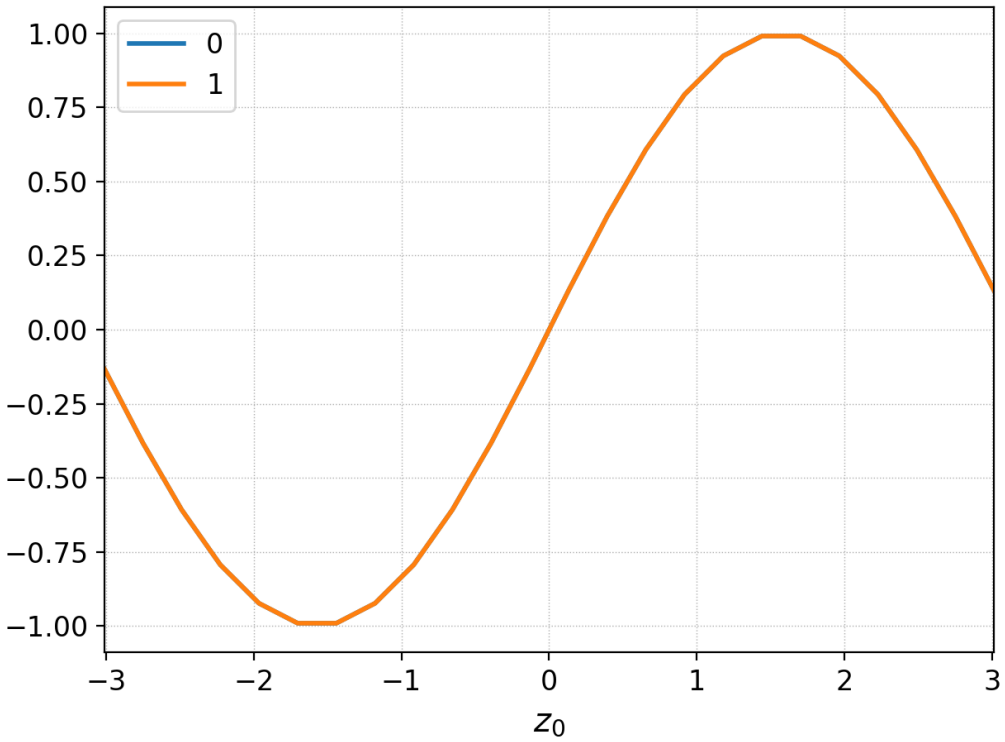

Figure: An EM wave propagated 100 periods using recovery DG scheme

Recovery based DG scheme is surprisingly accurate

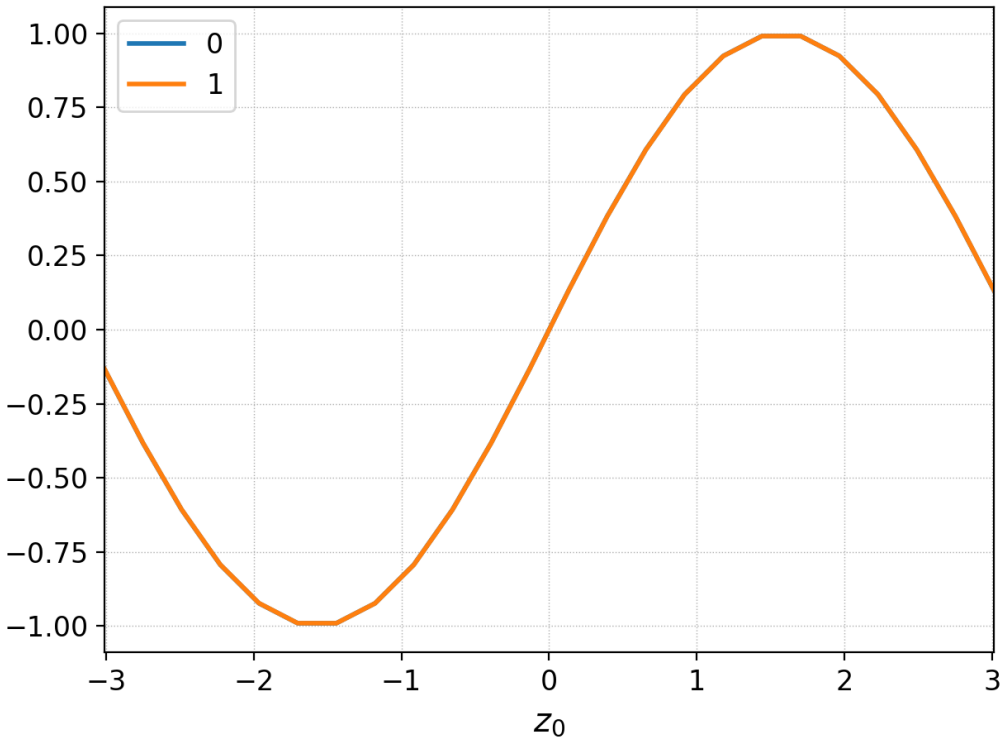

Figure: An EM wave propagated 1000 periods using recovery DG scheme

Recovery based DG scheme is surprisingly accurate

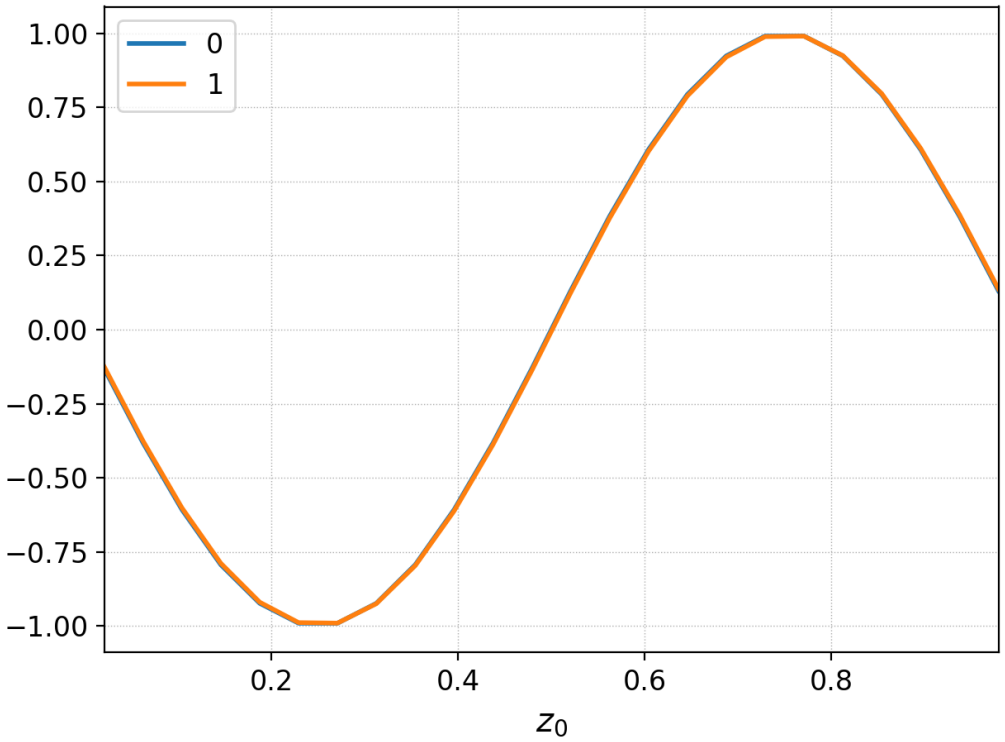

Figure: An EM wave propagated 10000 periods using recovery DG scheme

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!)).

Conclusion and Future Work

- We have developed a continuum scheme to directly discretize the Vlasov-Maxwell equations as a PDE in phase-space using the discontinuous Galerkin scheme
- Our scheme conserves total energy exactly, and has the correct sign for entropy production. Very delicate features in the solutions (like Landau resonances) can be recovered.
- A scheme that conserves momentum and energy for collision terms has been developed. Extensions to full nonlinear Fokker-Planck operator is underway
- The concept of recovery can potentially lead to even more accurate schemes; perhaps the optimium DG scheme with a three-cell stencil?
- Present algorithmic work is focussed on moving to GPUs, improving parallel performance; using recovery for collisionless terms, ...
- A large number of physics studies are underway.