Energy Conserving Discontinuous Galerkin Algorithms for Continuum (Gyro)Kinetic Simulations of Turbulence

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PPPL

Goal: Understand plasma turbulence from first-principle (Gyro)kinetics

- For weakly collisional (or collisionless) plasmas, kinetic effects are required to capture the physics of micro-turbulence.
- By treating both the Vlasov and gyrokinetic equations as PDEs in phase-space we can use the same infrastructure to solve both equations
- We use a version of discontinuous Galerkin scheme that conserves particle and energy exactly.
- We have implemented solvers for kinetic and gyrokinetic equations in the computational plasma physics framework, Gkeyll.
- Gkeyll also contains solvers for multi-fluid equations, allowing fluid-kinetic hybrid simulations, with some species of the plasma treated with fluids while others are treated fully kinetically.

(Gyro)kinetic equation as PDE in phase-space

Instead of using particles, we solve the (gryo)kinetic equation as a partial differential equation in phase-space:

$$\frac{\partial f}{\partial t} + \nabla_z \cdot (\alpha f) = C[f]$$

Here α is the phase-space velocity vector and $C[f]$ are collision terms.

- For the full Vlasov system the phase-space velocity is given by

$$\alpha = (\mathbf{v}, q/m(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

- For gyrokinetics, the phase-space velocity is determined from the Hamiltonian and the Poisson-bracket:

$$\alpha = \{\mathbf{z}, H\}$$

where $H(\mathbf{z})$ is the Hamiltonian and $\{f, g\}$ is the (potentially noncanonical) Poisson bracket operator.

Fields that go into α or the Hamiltonian are determined by field solves in configuration space. These can be either hyperbolic (Maxwell equations) or parabolic (gyrokinetic Poisson/Ampere equations).

Can we conserve important invariants?

- We know that the (gyro)kinetic system conserves total number of particles; total (field + particle) momentum; total (field + particle) energy; enstrophy and other invariants.
- Conserving particles and energy is particularly important to develop trust in simulations run over long plasma time-scales
- Maintaining positivity of the distribution, $f(\mathbf{z}, t) > 0$, is also important to obtain physically realizable solutions.
- Can a numerical scheme be designed that retains (some or all) of these properties, *while continuing to maintain conservation properties*?

We use novel versions of the *discontinuous Galerkin* method to construct efficient, high-order schemes that maintain positivity and conserve particles and total energy.

Discontinuous Galerkin algorithm

- 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 1000 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)

DG combined with FV schemes may lead to excellent algorithms for kinetic PDEs.

DG achieves locality with discontinuous solutions

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

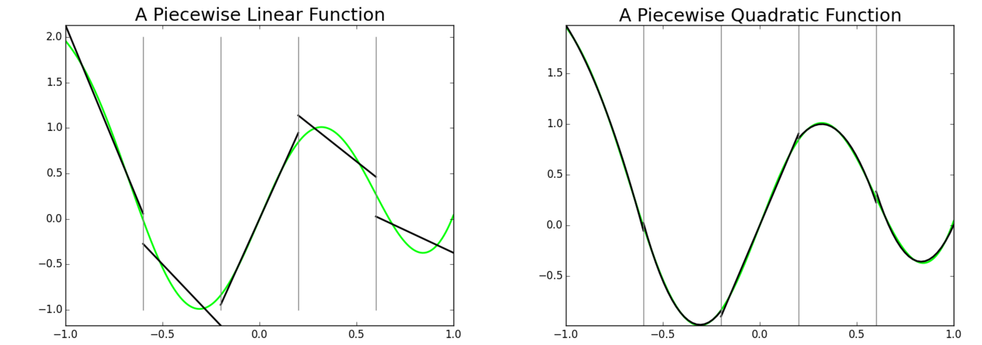

Figure 1: The best L_2 fit of $x^4 + \sin(5x)$ with piecewise linear (left) and quadratic (right) basis functions.

Example: constant and linear basis with upwinding

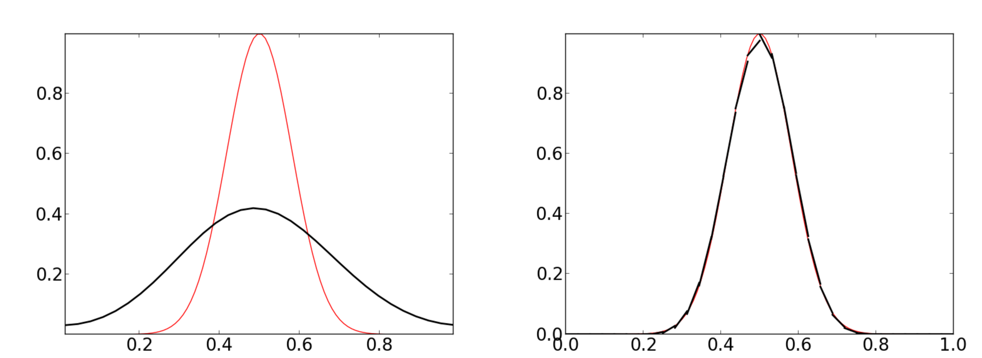

Figure 2: Advection equation solution (black) compared to exact solution (red) with upwind fluxes and constant (left) piecewise linear (right) basis functions.

In general, with upwind fluxes and linear basis functions numerical diffusion goes like $|\lambda|\Delta x^3 \partial^4 f/\partial x^4$.

Particles and energy are conserved

From the semi-discrete scheme we can prove the following propositions.

- The discrete scheme conserves total number of particles.
- The semi-discrete scheme conserves total (particles plus field) energy exactly, independent of upwinding of Vlasov equation.
- The L_2 norm of the distribution function decays monotonically.
- The total entropy of the system increases monotonically.

See Juno et al. [2017] for detailed proofs of these and other properties.

We have performed first 3X/2V gyrokinetic simulations of turbulence in open-field line devices

Using our gyrokinetic code, we have performed the first GK simulations of LAPD. See Shi et al. [2017], NSTX (See Eric Shi's thesis arXiv:1708.07283).

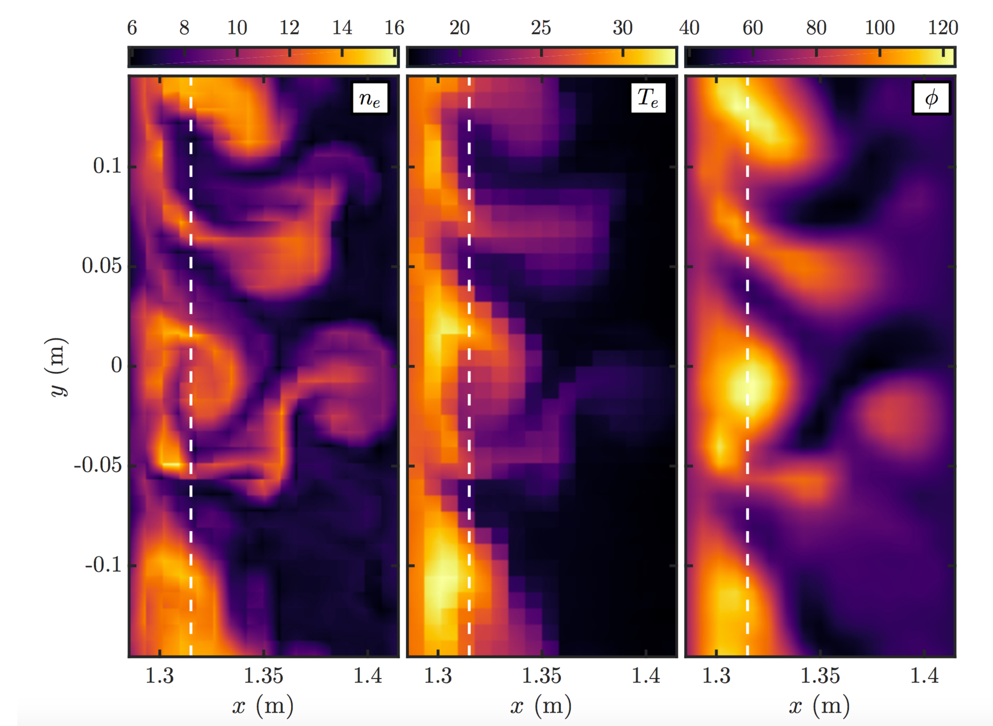

Figure 3: Snapshots of the electron density (in 10^{18} m^{-3}), electron temperature (in eV), and electrostatic potential (in V) in the plane perpendicular to the magnetic field at $z = 0$m. Parameters are for a "NSTX" like case, with bad-curvature driving drift-wave turbulence.

We have performed first *fully kinetic* turbulence simulations in 2X/3V in periodic domains

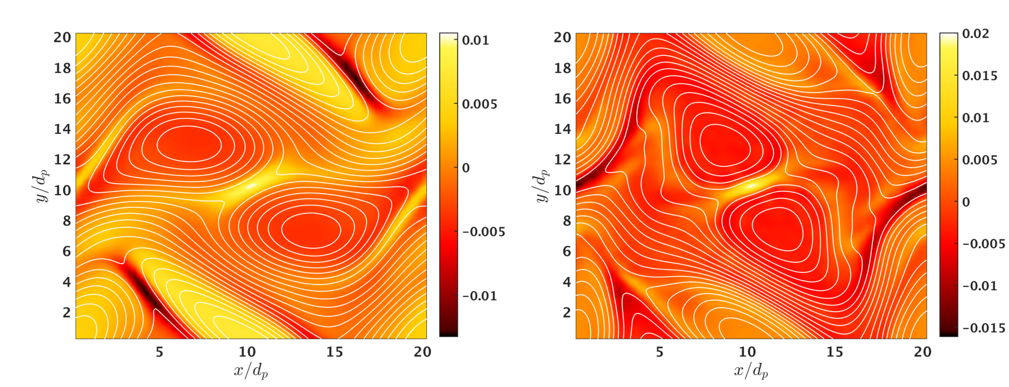

Figure 4: The out of plane current J_z with magnetic field contours superimposed at 20 and 40 Ω_{cp}^{-1} for Orsag-Tang turbulence simulation using fully kinetic 5D Vlasov-Maxwell equations.

How to maintain positivity without changing energy?

- The distribution function of particles is a non-negative scalar function. That is $f(\mathbf{x}, \mathbf{v}, t) \geq 0$. However, there is no guarantee that a numerical scheme will preserve this property.
- Standard positivity Zhang and Shu, can't be used for evolution of kinetic equations, as it involved modifying moments of the solution, leading to errors in energy conservations.
- Algorithms that change the moments of the distribution function (while maintaining cell averages) will change the particle energy. (The energy conservation in kinetic system is indirect, unlike fluid systems in which one evolves an explicit energy equation). Hence, use of such "sub-cell diffusion" based positivity schemes should be minimized or avoided altogether, if possible.

Designing a positivity preserving scheme that in addition maintains total energy conservation is non-trivial.

Perform exponential reconstruction in each cell

- The DG scheme, in a sense, does not tell us the solution, but only the *moments* of the solution in each cell.
- However, we can construct infinite number of functions can be constructed from given set of moments.
- For problems in plasma physics we know that locally, the solution should be well approximated by a exponential function, which, by definition, is positive.

Given a set of moments, is it always possible to reconstruct an exponential? Or, are there some bounds on the moments that permit the construction of an exponential?

Consider a distribution function $f(x) = f_0 + f_1 x$, for $x \in [-1, 1]$. Now, consider finding a new function $g(x) = \exp(g_0 + g_1 x)$ such that the moments match. We will write this as

$$f(x) \doteq g(x)$$

(Note this is not strict equality, only equality in the L_2 sense, that the projection of both sides on a set of basis functions are the same). Taking moments we get

$$2f_0 = \frac{1}{g_1}(g_R - g_L)$$
$$\frac{2}{3}f_1 = \frac{1}{g_1^2}[(g_1 - 1)g_R + (g_1 + 1)g_L]$$

where $g_R = e^{g_0 + g_1}$ and $g_L = e^{g_0 - g_1}$.

To gain some insight use the first equation to express g_1 and substitute this in the second equation to solve for g_R, for example, to get

$$g_R = \frac{6f_0^2 - (3f_0 + f_1)g_L}{3f_0 - f_1}.$$

This shows that as $f_1 \to 3f_0$, $g_R \to \infty$. Similarly, we can show that as $f_1 \to -3f_0$, $g_L \to \infty$, hence showing that we must have the bound

$$|f_1| \leq 3f_0.$$

Defining $r \equiv f_1/f_0$ we see that for a exponential reconstruction to exist, we must have $|r| \leq 3$. Hence, in 1D for piecewise linear basis functions, we say that the scheme is positivity preserving if $f_0 > 0$ and $|f_1|/f_0 \leq 3$.

Use exponential reconstructions for numerical fluxes

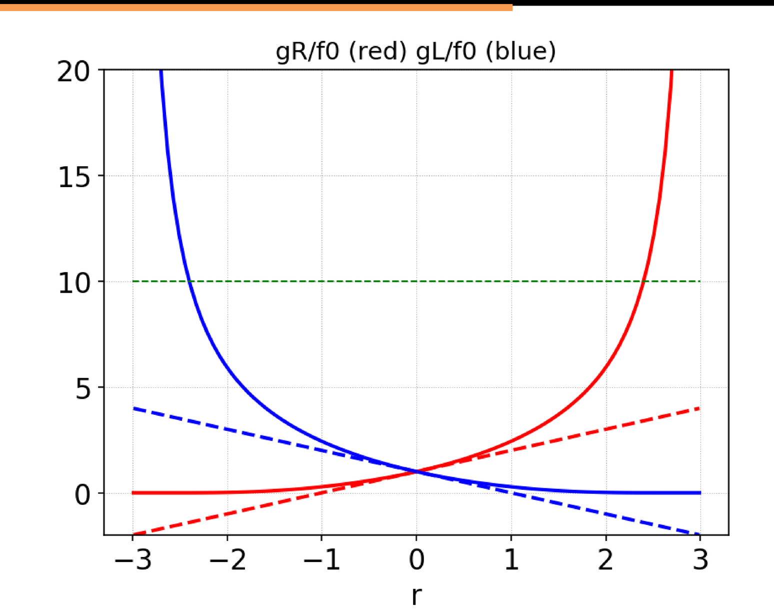

Figure 5: Exact nonlinear fits of g_R/f_0 (solid red), g_L/f_0 (solid blue) as a function of $r = f_1/f_0$. Also shown are the cell edge values computed from $f_0(1 \pm r)$ (dashed red/blue). The exponential fit, even though has the same moments as the linear function, always gives larger edge values than those computed from the linear function.

Extension of exponential reconstruction to multiple dimension is a hard problem, and hence we use a dimension-by-dimension reconstruction along specially selected 1D slices.

With exponential reconstruction positivity is maintained!

Consider a 2D advection of a square top-hat distribution function. With standard DG method there are very severe positivity errors. Exponential reconstruction completely eliminates this!

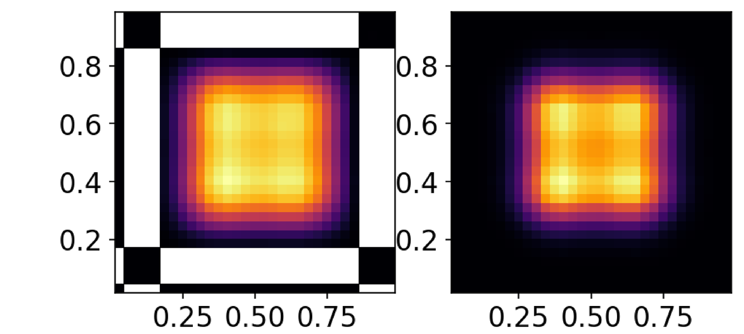

Figure 6: Comparison of distribution function for square-top-hat initial conditions with standard DG (left) and exponential DG (right). Regions where the distribution function goes negative are masked out and appear as white patches. Note the huge regions in which the standard DG shows positivity violation.

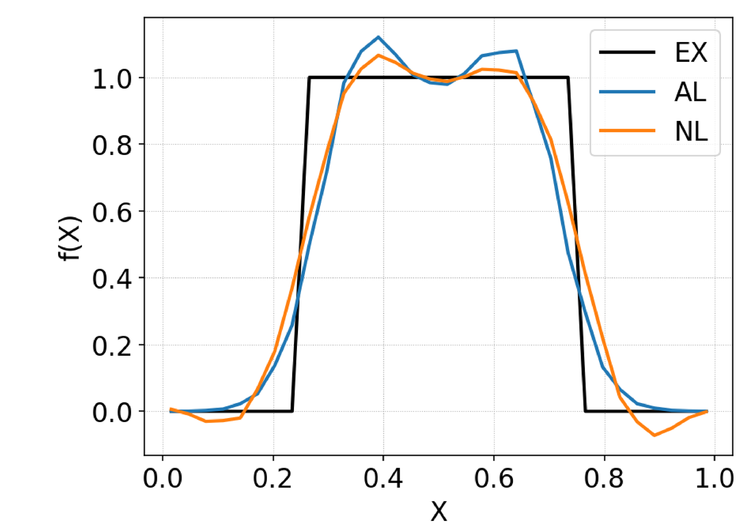

Figure 7: Lineout of standard DG (orange line) and anti-limiter based DG (blue line), for square-top-hat initial condition

Collaboration Opportunities

- Extension of exponential reconstruction to higher-order remains a challenge: With piece-wise quadratic (or higher) basis it is not clear how to construct a exponential reconstruction: however, this will allow "exact" representation of "local Maxwellian" in each cell.
- Develop efficient, conservative discretization of non-linear Fokker-Planck collision operator.
- Implicit schemes for collisions will be eventually required. Developing these in 5D remains an outstanding challenge.
- Developing scalable IO at large processor counts; in-situ visualization from running simulations
- Porting key kernels to GPUs and implementing hybrid MPI/GPU messaging system for gyrokinetic equations
- Developing special grid systems for divertor geometries with X-points is highly challenging due to anisotropic nature of plasma flows.

Reference

J. Juno, A. Hakim, J. TenBarge, E. Shi, and W. Dorland. Discontinuous galerkin algorithms for fully kinetic plasmas. *Journal of Computational Physics*, 2017. ISSN 0021-9991. doi: https://doi.org/10.1016/j.jcp.2017.10.009.

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