Advanced Algorithms for Multi-Moment Fluid and Kinetic Simulations of Plasmas

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Two aims: Present algorithms for Multi-fluid moment equations and continuum kinetic models

Instead of "all particles" we want to use "all fields". Unifying concepts: hyperbolic balance laws and finite-volume/discontinuous Galerkin algorithms.

- Develop unified schemes and software applicable to broad variety of fluid and kinetic problems.
- Explore continuum algorithms for solution of edge gyrokinetic equations in 3D geometries. Question: Can one develop accurate and stable schemes that conserve invariants, maintain positivity and use as few grid points as possible?

Outline

- Definition, examples and properties, of hyperbolic balance laws
- Numerical schemes, in particular discontinuous Galerkin scheme
- Multi-moment multi-fluid models and applications to reconnection and RF wave propagation in plasmas.
- Model problems for kinetic equations and conservative hybrid FE/DG schemes.

Hyperbolic balance laws describe phenomena with finite propagation speeds

Consider the N dimensional system of m balance laws

$$\partial_t U + \sum_{i=1}^{N} \partial_i F_i(U) = S(U, x, t)$$

Here $x \in \mathbb{R}^N$, $U(x,t) \in \mathbb{R}^m$, $F_i(U)$ is the flux $S(U,x,t) \in \mathbb{R}^m$ are source terms.

Informally

If a small perturbation around a equilibrium $U_0(x)$ propagates with *finite speed* then system is hyperbolic.

We can make this formal by looking at eigenstructure of flux Jacobian

Definition (Hyperbolic Equations)

If for any admissible U the flux Jacobian

$$A(U, n) \equiv \sum_{i=0}^{N} n_i DF_i(U)$$

where $[n_1, \ldots, n_N]$ is a unit vector, has real eigenvalues, λ_p and a complete set of right eigenvectors, r_p, $p = 1, \ldots, m$, the system said to be *hyperbolic*.

System is *strictly hyperbolic* if eigenvalues are distinct, *weakly hyperbolic* otherwise, and *isotropic* if eigensystem does not depend on n_i.

Example: Euler equations for neutral fluid dynamics

Euler equations describe neutral, inviscid flows

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho \\ \rho u \\ \rho v \\ \rho w \\ E\end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix}\rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ (E+p)u\end{bmatrix} = 0$$

The eigenvalues are $\{u-c, u, u, u, u+c\}$, where $c = \sqrt{\gamma p/\rho}$ is the speed of sound.

Example: Maxwell equations of electromagnetism

Maxwell equations describe evolution of electric and magnetic fields

$$\frac{\partial}{\partial t}\begin{bmatrix} E_x \\ E_y \\ E_z \\ B_x \\ B_y \\ B_z \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} 0 \\ c^2 B_z \\ -c^2 B_y \\ 0 \\ -E_z \\ E_y \end{bmatrix} = 0.$$

The eigenvalues are $\{0, 0, c, c, -c, -c\}$, where c is the speed of light.

Source terms in plasma physics are often dispersive

Definition (Dispersive Source Terms)

If the ODE

$$\partial_t U = S(U, x, t)$$

has purely oscillatory solutions, then sources are called *dispersive* and lead to dispersive phenomena (non-linear dependence of frequency on wave-number) in the solution.

For example: multi-fluid *ideal* plasma equations have dispersive source terms.

Example: Euler equations with $\lambda \mathbf{u} \times \mathbf{b}$ momentum source terms

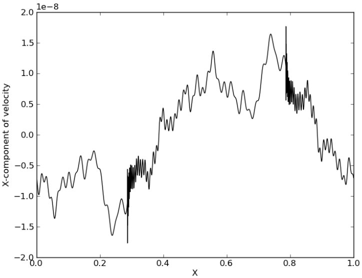


Figure: Solution the linear Euler equations with dispersive sources. Very fine small-scale features are seen which might be mistaken for numerical noise.

Carefully designed software can allow flexible construction of simulations

Example: General implementations in WarpX, Nautilus and Gkeyll, developed in collaboration with University of Washington and Tech-X Corporation.

- A general hyperbolic solver forms the backbone of the framework.
- Different equations can be solved by “plugging in” Riemann solvers.
- Physical modules can be added on as sources and extra terms in equations (general EOS, Lorentz forces, currents, chemical reactions, viscous terms, collisional closures, etc)

Hyperbolic balance laws have number of properties that are important for schemes to satisfy

- Hyperbolic balance laws allow for discontinuous solutions. I.e. shocks, rarefactions and contact discontinuities can develop even from smooth initial conditions. Schemes must be able to handle this, i.e. be *shock capturing*.
- Even if true shocks do not form (due to diffusion), small scale fluctuations and sharp gradients need to be captured.

Additional mathematical properties that are important

- Schemes must preserve *invariant domains*. For example, $\rho \geq 0$, $p \geq 0$.
- Schemes must satisfy *entropy inequalities*. For example, physical entropy should increase across shocks. If $\eta(U)$ is an entropy and $g_i(U)$ are entropy fluxes, then we must have

$$\partial_t \eta(U) + \sum_{i=1}^{N} \partial_i g_i(U) \leq 0$$

- *Involutions* must be satisfied. I.e. constraints like $\nabla \cdot \mathbf{B} = 0$, $\nabla \cdot \mathbf{E} = \varrho_c / \epsilon_0$ etc must be maintained.

Three broad classes of methods exist to solve hyperbolic balance laws

1. Use Taylor series expansion and replace derivatives using the balance law. I.e. $U(x, t + \Delta t) = U(x, t) + \Delta t \partial U / \partial t + \ldots$. Replace $\partial U / \partial t$ using the PDE. Leads to fully discrete schemes. Example, Wave Propagation Scheme of Randy LeVeque (see, for example, LeVeque 2006).
2. Assume we know average solution in each cell. Then, construct a high-order polynomial representation of the solution in each cell using neighbor averages. Leads to semi-discrete schemes which are then integrated using an ODE solver. Example, MUSCL schemes (see Kulikovskii, 2001).
3. Represent solution in each cell using set of basis functions. Leads to *discontinuous* Galerkin schemes.

Moment equations of plasmas form a hyperbolic system with dispersive source terms

For example: ten-moment system

$$\partial_t n + n\partial_j u_j + u_j \partial_j n = 0$$

$$\partial_t u_i + \frac{1}{mn}\partial_j P_{ij} + u_j \partial_j u_i = \frac{q}{m}\left(E_i + \epsilon_{kmi} u_k B_m\right)$$

$$\partial_t P_{ij} + P_{ij}\partial_k u_k + \partial_k u_{[i} P_{j]k} + u_k \partial_k P_{ij} + \partial_k Q_{ijk} = \frac{q}{m} B_m \epsilon_{km[i} P_{jk]}$$

Square brackets around indices represent symmetrization of tensors. Also, n is the number density, u_j is the velocity, P_{ij} the pressure tensor. For a plasma with s species there are total of $10s + 6$ equations to solve. For $P_{ij} \rightarrow p\delta_{ij}$ gives the two-fluid (Euler-Maxwell) system.

What about heat flow and collisions?

In the ten-moment system the full heat tensor Q_{ijk} appears. Also, collision integral needs to be included.

- For heat tensor, initially just set $Q_{ijk} = 0$. Consider closing the system by a perturbative expansion (generalizing Grad) around a multi-variate Gaussian

$$f(x,v,t) = \frac{n}{(2\pi)^{3/2}\triangle^{1/2}} \exp(-\frac{1}{2}\Theta_{ij}^{-1}c_i c_j)\,[1+\chi(x,v,t)]$$

  where $\Theta_{ij} = P_{ij}/mn$, $\triangle = \det\Theta$ and $c_i = v_i - u_i$. Then, expand $\chi(x,v,t)$ in tensor Hermite polynomials. Alternatively, use *non-perturbative* closures (see Levermore, *J. Stat. Phys.*, 1996).
- For collision use a simple two-species BGK collision operator with proper accounting for disparate species masses (see J. Greene, *Phys. Fluids*, 1973).

Some benchmark applications of multi-moment models

Figure: What we *do not* want to do.

Two-fluid magnetic reconnection in a current sheet

- Process by which the topology of the magnetic field lines changes.
- Geospace Environmental Modeling (GEM) Reconnection Challenge project was undertaken to study collisionless reconnection.
- Although an “artificial” problem, GEM Reconnection Challenge serves as important benchmark/application for two-fluid models.

We have performed these simulations with both five-moment (Euler) as well and ten-moment models.

Setup is a Harris current sheet with in-plane fields

Thin current sheet separating oppositely directed magnetic field lines.

$$\mathbf{B}(y) = B_0 \tanh(y/\lambda)\mathbf{e}_x$$
$$\mathbf{J}_e = -\frac{B_0}{\lambda}\mathrm{sech}^2(y/\lambda)\mathbf{e}_z.$$

Domain size is $[-L_x/2, L_x/2] \times [-L_y/2, L_y/2]$. Periodic boundary conditions at $x = \pm L_x/2$, conducting wall boundaries at $y = \pm L_y/2$.

In GEM project reconnected flux

$$\frac{1}{2L_x}\int_{-L_x/2}^{L_x/2} |B_y(x, y = 0, t)| dx$$

computed using various models was measured and compared.

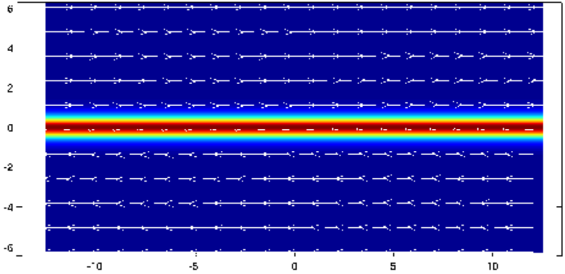


Figure: Electron current and magnetic field lines at $t = 0$. The configuration is in unstable equilibrium.

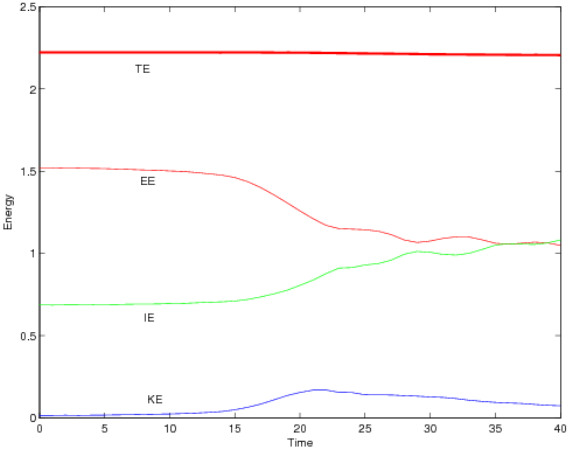


Figure: Electromagnetic energy (EE), fluid thermal energy (IE), fluid kinetic energy (KE) and total energy (TE) as a function of time.

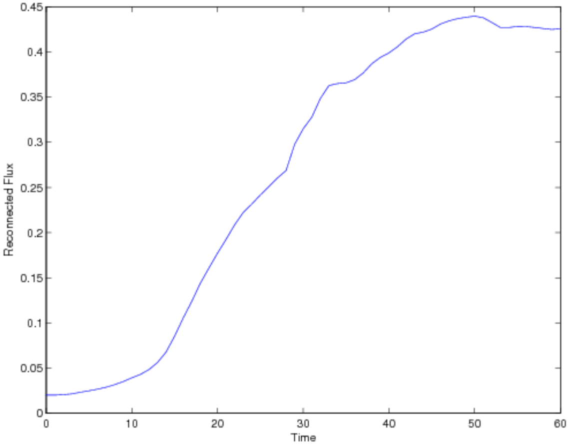


Figure: Reconnected flux verses time. The reconnected flux increases rapidly after the reconnection occurs at about $t = 10$. The flux saturates due to the conducting wall.

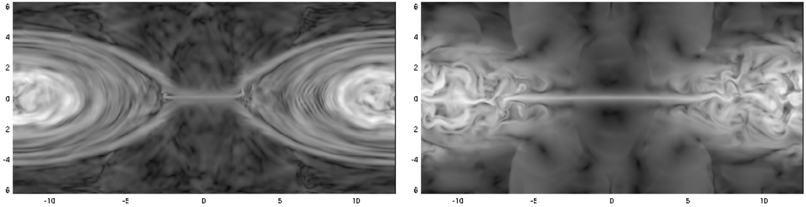
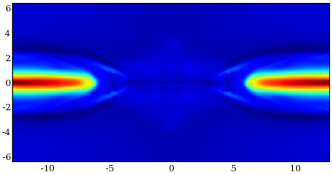


Figure: Electron momentum (left) and ion momentum (right) at $t = 40$. Inward traveling shocks are visible in both the fluids. Thin jets flowing along the X axis are also visible. Ion flow is unstable due to counter flowing fluid jets.

What happens with the ten-moment Maxwell system?[1]



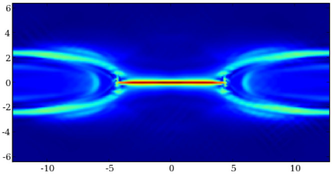


Figure: Electron number density (left) and current density (right) at t=25. (A. Hakim, "Extended MHD Modelling with the Ten-Moment Equations", *Journal of Fusion Energy*, **14**, 055911 (2008))

[1]See E. Alec Johnson thesis for comprehensive study of reconnection with ten-moment model

Although reconnection rates are similar, five- and ten-moment flow details differ

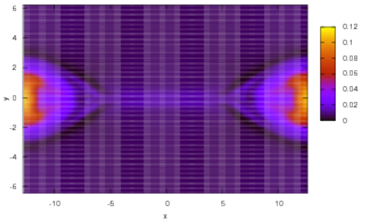


Figure: Electron density for five-moment model (left) and ten-moment model (right) at $t = 30$. Although bulk features are similar the details of the flow are different in the two models.

Ten-moment model with proper heat-flux closure and correction collisional relaxation rates may compare well with kinetic simulations

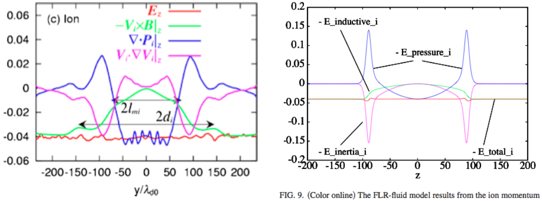


FIG. 7. (Color online) The contributions to the electric field as computed from the ion momentum equation with m_i/m_e=800 in a steady-state simulation by Ishizawa *et al.* (Ref. 3, Fig. 3c). Reprinted with permission from A. Ishizawa and R. Horiuchi, Phys. Rev. Lett. **95**, 045003 (2005). Copyright 2005 American Physical Society.

FIG. 9. (Color online) The FLR-fluid model results from the ion momentum equation with τ_e=0.1 and τ_i=80.0 are better agreement with the simulation results in Fig. 7 than the MHD-fluid results in Fig. 8, especially in the width of the nonideal region.

Figure: Comparison of steady-state 2D PIC (left) reconnection with 1D ten-moment model (right) for various terms in the ion momentum equations. Taken from J. Brackbill, *Phys. Plasmas*, **18**, 032309 (2011).

Multi-moment models can be used for studying high-frequency plasma phenomena

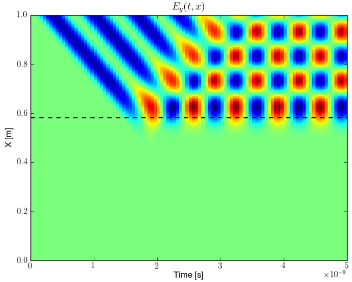


Figure: Electromagnetic wave propagation in a plasma beach driven by a current source in the last cell. Shown here is the electric field Ey as a function of time (increasing towards the right) and space (top of the figure is the right edge). The dashed black line shows the plasma cutoff.

Non-linear phenomena can now be studied: E.g, Parametric decay instability

Basically: PDI belongs to a class of non-linear phenomena that can be described by retaining all quadratic terms in an expansion of the hyperbolic balance laws about an equilibrium solution.

$$\partial_t U_1 + A(U_0)\partial_x U_1 + A'(U_0)U_1\partial_x U_1 = S'(U_0)U_1 + \frac{1}{2}S''(U_0)U_1U_1$$

Notice that Fourier transform of this equation will involve convolutions of all wave-numbers due to the non-linear terms. As far as I am aware there is *no* theory in hyperbolic PDEs literature that study such systems.

First nonlinear simulations of PDI, a possible mechanism for parasitic decay in tokamak RF heating systems

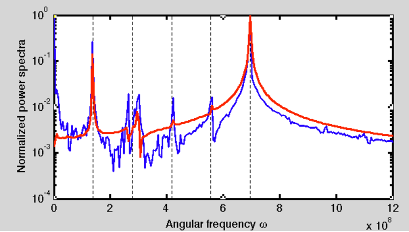


Figure: Wave is excited between 4 and 5 times the local cyclotron frequency results in a complex Parametric Decay scenario involving several sub-harmonic frequencies. A strong 1/5 sub-harmonic signal forms, along with a harmonic cascade of this frequency. The 2/5 sub-harmonic is clearly split, with the upper split peak corresponding closely to the local 2nd harmonic cyclotron frequency. In the figure, the Ex spectrum is the blue line, while the Ey is the red line.


GRAHAM CHAPMAN JOHN CLEESE TERRY GILLIAM
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MONTY PYTHON'S
And Now For Something
COMPLETELY DIFFERENT
DVD
The BEST of Monty Python's Flying Circus

Goal: Accurate and stable continuum schemes for full-F edge gyrokinetics in 3D tokamak/Stellerator geometries

Question: Can one develop accurate and stable schemes that conserve invariants, maintain positivity and use as few grid points as possible?

Proposed Answer

Explore high-order hybrid discontinuous/continuous Galerkin finite-element schemes, enhanced with flux-reconstruction and a clever choice of velocity space basis functions, combined with "conservative" hyper-viscosity operator.

LDRD project at PPPL with Greg Hammett (Caveat: less than four months of work accomplished, so many rough edges.)

Key operator to discretize is the Poisson bracket operator, arising in Hamiltonian formulation of kinetic-theory

A basic model problem is the *incompressible* 2D Euler equations written in the stream-function (ϕ) vorticity (χ) formulation.

$$\frac{\partial \chi}{\partial t} + \nabla \cdot (\mathbf{u}\chi) = 0$$

where $\mathbf{u} = \nabla\psi \times \mathbf{e}_z$ and

$$\nabla^2\psi = -\chi.$$

Incompressibility allows us to write this in "Hamiltonian form"

As the flow is incompressible ($\nabla \cdot \mathbf{u} = 0$) we can rewrite in the form

$$\frac{\partial \chi}{\partial t} + \{\chi, \psi\} = 0$$

where $\{\chi, \psi\}$ is the Poisson bracket operator defined by

$$\{\chi, \psi\} = \frac{\partial \chi}{\partial x}\frac{\partial \psi}{\partial y} - \frac{\partial \chi}{\partial y}\frac{\partial \psi}{\partial x}.$$

Note we can write several plasma kinetic/fluid systems in this form

For example: 1D Vlasov-Poisson system for the distribution function $f(x, p, t)$ can be written as

$$\frac{\partial f}{\partial t} + \{f, H\} = 0$$

where

$$H = \frac{1}{2m}p^2 + q\phi$$

and where p the momentum and ϕ electric potential. Other example: Hasegawa-Wakatani equations for drift-wave turbulence also involves Poisson bracket structure.

Gyrokinetic equation can also be derived from gyro-center Hamiltonian

In the modern gyrokinetic theory the gyrokinetic equation is written using the gyrocentre Hamiltonian (in gyro-center coordinates $(\mathbf{R}, v_\|^2, \mu, \alpha)$

$$H = \frac{1}{2} m_i v_\|^2 + \mu B + e_i \langle \phi \rangle_\alpha$$

where $v_\|$ is the parallel velocity, μ is the magnetic moment, α is gyro-angle and ϕ is the electrostatic potential.
Note: The Poisson bracket in this case is *not canonical* and hence does not have the simple structure shown in the previous slides.

The Hamiltonian structure indicates several invariants of the system that should be preserved by the numerical scheme

For example, for the incompressible Euler equations on periodic (or closed) domain the total energy is conserved

$$\frac{d}{dt}\langle\frac{1}{2}|\nabla\psi|^2\rangle_\Omega \equiv \frac{dE}{dt} = 0$$

Other examples: infinite number of Casimirs of the form $\mathcal{C} = \int_\Omega \mathcal{C}_\alpha(\chi)$ are conserved. An important one is the enstrophy $C_\alpha = \chi^2/2$.

Use a continuous finite-element method to discretize the Poisson equation and discontinuous finite elements to discretize the Poisson bracket operator

The weak-form of the vorticity equation is

$$\langle v_j \frac{\partial \chi}{\partial t} \rangle_{\mathcal{C}_i} + \langle v_j \mathbf{u} \cdot \mathbf{n} \widehat{\chi} \rangle_{\partial \mathcal{C}_i} - \langle \nabla v_j \cdot \mathbf{u} \chi \rangle_{\mathcal{C}_i} = 0.$$

Here, $\widehat{\chi}$ is some sort of "averaged" vorticity at a cell interface.
Typically use upwind or central averages (flux).
On the other hand, the weak-form of the Poisson equation is

$$\langle \varphi_j \nabla \psi \cdot \mathbf{n} \rangle_{\partial \Omega} - \langle \nabla \varphi_j \cdot \nabla \psi \rangle_{\Omega} = -\langle \varphi_j \chi \rangle_{\Omega}$$

Energy and enstrophy conservation properties of the discrete system

We can show that with *proper choice* of basis functions, energy is conserved *even with upwind fluxes*, while enstrophy is conserved with central fluxes. The condition

$$\mathrm{span}\{\varphi_1, \ldots, \varphi_k\} \subseteq \mathrm{span}\{v_1, \ldots, v_k\}$$

I.e. The set of functions representable in the continuous finite-element space must be a subset of that representable in the discontinuous space.

Careful work is needed to extend this result to kinetic systems

- In Vlasov-Poisson system the Poisson equation is on a lower-dimensional space than the Vlasov equation.
- The velocity space range is $[-\infty, \infty]$ so a choice of clever basis and test functions is needed to reduce velocity space resolution and conserve momentum *and* energy. Hermite polynomial basis?
- Hyper-viscosity will be needed to prevent recurrence. However, one needs to ensure selected operator conserves mass, momentum and energy.
- Should one explore some form of symplectic time integrators to eliminate diffusion from standard TV Runge-Kutta schemes?

Example: Merging of two vortices ("vortex waltz")

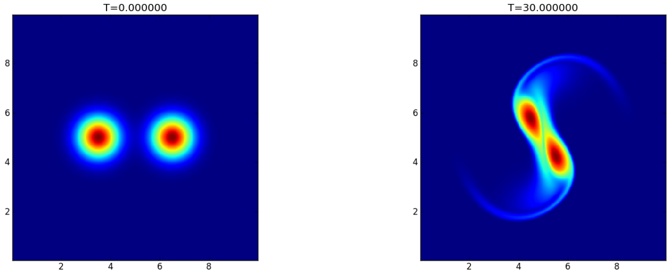

Figure: Drop in energy is 1.82×10^{-4} %. This is greater than machine precision due to diffusion added from TVD Runge-Kutta time-stepping.

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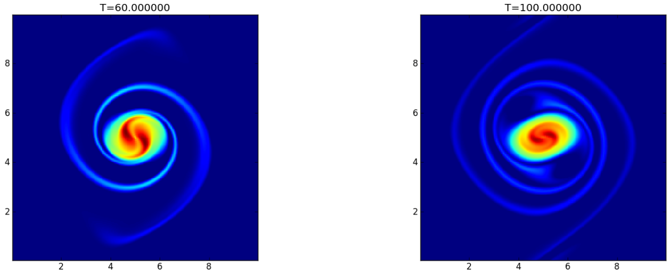

Figure: Drop in energy is 1.82×10^{-4} %. This is greater than machine precision due to diffusion added from TVD Runge-Kutta time-stepping.

Example: Double shear problem

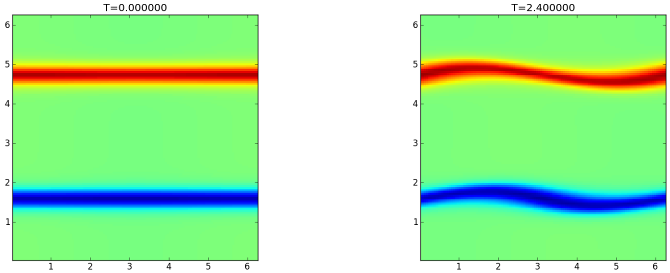

Figure: This problem is harder than “vortex waltz” as aliasing errors can cause scheme to go unstable.

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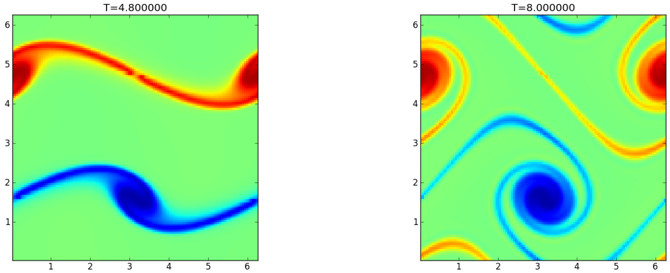

Figure: This problem is harder than "vortex waltz" as aliasing errors can cause scheme to go unstable.

Final thoughts: Hyperbolic balance laws and finite-volume, discontinuous Galerkin schemes form unifying framework

- For long-term production quality reproducible research one needs to translate this unifying mathematical framework into a unified software package.
- The field of continuum algorithms for kinetic equations is extremely rich and can be an efficient and robust compliment to particle methods.
- The plasma physics community needs to adopt advanced schemes to these problems and not be satisfied with existing "state-of-art".