Unified algorithms for fluid and kinetic simulations of plasmas

A. H. Hakim   G. W. Hammett

Princeton Plasma Physics Laboratory, Princeton, NJ
ammar@princeton.edu
http://www.ammar-hakim.org/sj

Stability, Energetics, and Turbulent Transport in Astrophysical, Fusion, and Solar Plasmas: Unifying Theoretical and Computational Tools, 2013

Theory and numerics of hyperbolic balance laws provide unifying theme in computational plasma physics

- Hyperbolic balance laws describe wide variety of physics: neutral fluid flow, magnetohydrodynamics, electromagnetism (linear and non-linear dielectrics), shallow-water flows, etc.
- Are building blocks for systems with dissipation, chemical reactions, etc.

Outline

- Definition, examples and properties, of hyperbolic balance laws
- Numerical schemes, in particular discontinuous Galerkin scheme
- Applications: two-fluid magnetic reconnection, FRC formation and jet propagation in vacuum.

Extention of standard theory/numerics provide a framework for solving broad class of kinetic equations

Question

Can one develop accurate and stable schemes for solution of (gyro) kinetic equations 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 better choice of velocity space basis functions.

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 flow

Neutral inviscid flow is described by Euler equations

$$\frac{\partial n}{\partial t} + n\nabla \cdot \mathbf{u} + u \cdot \nabla n = 0$$
$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{mn}\nabla p = \frac{q}{m}(\mathbf{E} + \mathbf{u} \times \mathbf{B})$$
$$\frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p + \gamma p \nabla \cdot \mathbf{u} = 0.$$

This is weakly hyperbolic, isotropic system with eigenvalues $\{u \pm c_s, u, u, u\}$, where $c_s = \sqrt{\gamma p/mn}$.

This system is interesting in itself, and is also a building block for Navier-Stokes equations, two-fluid equations, and MHD equations.

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.
- If a hyperbolic balance law is isotropic, so must be the numerical scheme, i.e. be *grid and coordinate independent*.

Three additional mathematical properties are important

- Schemes must preserve *invariant domains*. For example, $n \geq 0$, $p \geq 0$ and P_{ij} is semi-positive definite.
- Schemes must satisfy *entropy inequalities*. For example, physical entropy should increase across shocks. This is really important as otherwise solutions are no longer unique. I.e if $\eta(U)$ is an entropy and $g_i(U)$ are entropy fluxes, then we must have

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

- *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.

Discontinuous Galerkin algorithms represent state-of-art for solution of hyperbolic partial differential equations

- 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 700 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)
- Certain types of DG have excellent conservation properties for Hamiltonian systems, low noise and low dissipation.
- DG is inherently super-convergent: in FV methods interpolate p points to get pth order accuracy. In DG interpolate p points to get $2p-1$ order accuracy.

What does a typical DG solution look like?

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

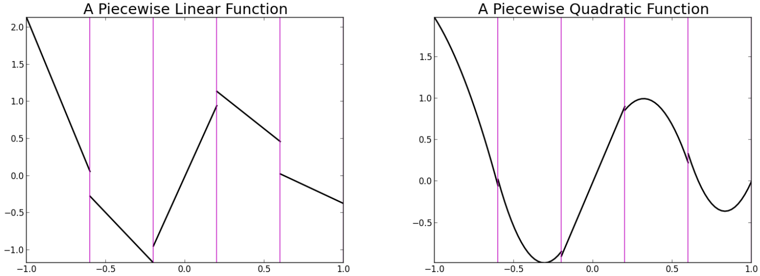


Figure: The best L_2 fit of $x^4 + \sin(5x)$ with piecewise linear (left) and quadratic (right) basis functions.

Discontinuous Galerkin schemes are applicable to phase-space advection equations described as Hamiltonian dynamical system

For example,

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

where $H(z^1, z^2)$ is the Hamiltonian and canonical Poisson bracket is

$$\{g, h\} \equiv \frac{\partial g}{\partial z^1}\frac{\partial h}{\partial z^2} - \frac{\partial g}{\partial z^2}\frac{\partial h}{\partial z^1}.$$

Defining phase-space velocity vector $\boldsymbol{\alpha} = (\dot{z}^1, \dot{z}^2)$, with $\dot{z}^i = \{z^i, H\}$ leads to *phase-space conservation form*

$$\frac{\partial f}{\partial t} + \nabla \cdot (\boldsymbol{\alpha} f) = 0.$$

Example: Incompressible Euler equations in two dimensions serves as a model for $E \times B$ nonlinearities in gyrokinetics

A basic model problem is the *incompressible* 2D Euler equations written in the stream-function (ϕ) vorticity (ζ) formulation. Here the Hamiltonian is simply $H(x, y) = \phi(x, y)$.

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

where $\mathbf{u} = \nabla\phi \times \mathbf{e}_z$. The potential is determined from

$$\nabla^2 \phi = -\zeta.$$

It is important to preserve quadratic invariants

The incompressible Euler equations has two quadratic invariants, *energy*

$$\frac{\partial}{\partial t} \int_K \frac{1}{2} |\nabla \phi|^2 d\Omega = 0$$

and *enstrophy*

$$\frac{\partial}{\partial t} \int_K \frac{1}{2} \zeta^2 d\Omega = 0.$$

Similar invariants can be derived for Vlasov-Poisson and Hasegawa-Wakatani equations. In addition, Vlasov-Poisson also conserves momentum.

Question

Can one design schemes that conserve these invariants?

A DG scheme is used to discretize phase-space advection equation

To discretize the equations introduce a mesh K_j of the domain K. Then the discrete problem is stated as: find ζ_h in the space of discontinuous piecewise polynomials such that for all basis functions w we have

$$\int_{K_j} w \frac{\partial \zeta_h}{\partial t} \, d\Omega + \int_{\partial K_j} w^- \mathbf{n} \cdot \boldsymbol{\alpha}_h \hat{\zeta}_h \, dS - \int_{K_j} \nabla w \cdot \boldsymbol{\alpha}_h \zeta_h \, d\Omega = 0.$$

Here $\hat{\zeta}_h = \hat{\zeta}(\zeta_h^+, \zeta_h^-)$ is the consistent numerical flux on ∂K_j.

A continuous finite element scheme is used to discretize Poisson equation

To discretize the Poisson equation the problem is stated as: find ϕ_h in the space of *continuous* piecewise polynomials such that for all basis functions ψ we have

$$\int_K \psi \nabla^2 \phi_h d\Omega = -\int_K \psi \zeta_h d\Omega$$

Questions

How to pick basis functions for discontinuous and continuous spaces? We also have not specified numerical fluxes to use. How to pick them? Do they effect invariants?

Hybrid DG/CG schemes for Hamiltonian systems have good conservation properties

- With proper choice of function spaces and a *central* flux, both quadratic invariants are exactly conserved by the semi-discrete scheme.
- With upwind fluxes (preferred choice) energy is still conserved, and the scheme is stable in the L_2 norm of the solution.
- For Vlasov-Poisson system, momentum conservation is not exact, but the errors decrease rapidly with spatial resolution, even on a coarse velocity grid.

Questions

Can this scheme be modified to conserve momentum exactly? Can time discretization exactly conserve these invariants? Perhaps try symplectic integrators ...

Only recently conditions for conservation of discrete energy and enstrophy were discovered

Energy Conservation

Liu and Shu (2000) have shown that discrete energy is conserved for 2D incompressible flow if *basis functions for potential are a continuous subset of the basis functions for the vorticity irrespective of numerical flux chosen*! We discovered extension to discontinuous phi for the Vlasov equation.

Enstrophy Conservation

Enstrophy is conserved only if *central fluxes* are used. With upwind fluxes, enstrophy decays and hence the scheme is *stable* in the L_2 norm.

DG with central fluxes like high-order generalization of the well-known *Arakawa* schemes, widely used in climate modeling and recently also in plasma physics.

Under-construction code `Gkeyll` provides unified computational framework for broad class of fluid and kinetic equations

- Gkeyll is written in C++ and scripted using Lua [1].
- Package management and builds are automated via `scimake` and `bilder`, both developed at Tech-X Corporation.
- Linear solvers from Petsc[2] are used for inverting stiffness matrices.
- MPI is used for parallelization via the `txbase` library developed at Tech-X Corporation.

Used presently for reconnection with multi-fluid moment equations and being developed for gyrokinetic simulations of edge turbulence.

[1] http://www.lua.org

[2] http://www.mcs.anl.gov/petsc/

Simulation journal with results is maintained at http://www.ammar-hakim.org/sj

Results are presented for the equation systems.

- Incompressible Euler equations
- Hasegawa-Wakatani equations
- Vlasov-Poisson equations

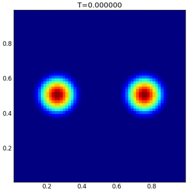


Figure: [Movie] Swirling flow problem. The initial Gaussian pulses distort strongly but regain their shapes after a period of 1.5 seconds.

Two-Fluid magnetic reconnection in a current sheet

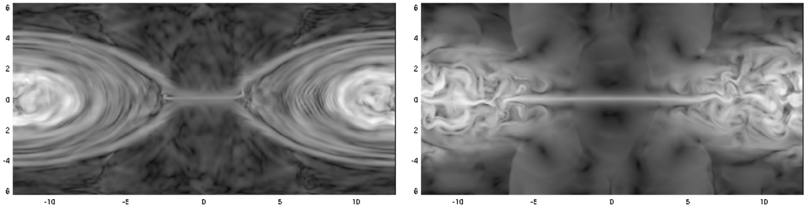


Figure: Electron momentum (left) and ion momentum (right) at $t = 40$. Inward traveling shocks are visible in both the fluids. Thin jets flowing along the X axis are also visible. Ion flow is unstable due to counter flowing fluid jets.

Energy of fluids and fields, reconnection rates can be computed

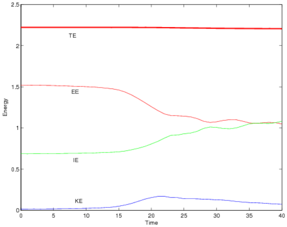


Figure: Electromagnetic energy (EE), fluid thermal energy (IE), fluid kinetic energy (KE) and total energy (TE) as a function of time.

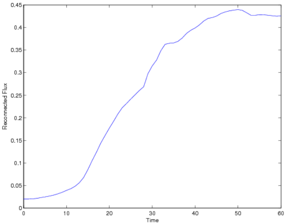
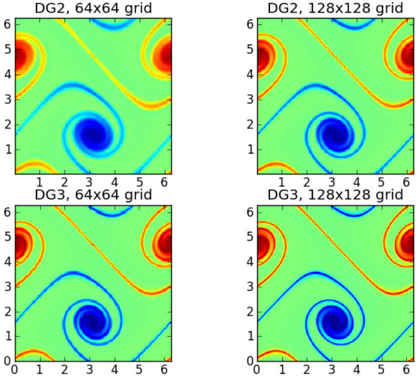


Figure: Reconnected flux verses time. The reconnected flux increases rapidly after the reconnection occurs at about $t = 10$. The flux saturates due to the conducting wall.

Double shear problem is a good test for resolution of vortex shearing in $E \times B$ driven flows

Vorticity at $t = 8$ with different grid resolutions and schemes. Third order DG scheme runs faster and produces better results than DG2 scheme.



Initial studies of Hasegawa-Wakatani drift-wave turbulence are carried out

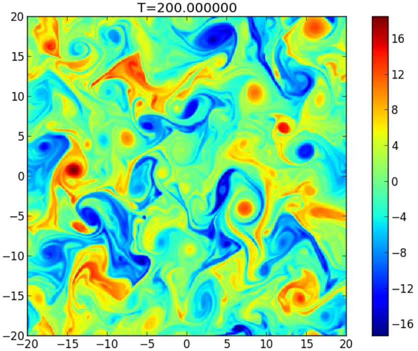


Figure: [Movie] Number density from Hasegawa-Wakatani drift-wave turbulence simulations with adiabacity parameter $D = 0.1$ with (left) and without (right) zonal flow modification.

Algorithms have been tested with nonlinear Landau damping problem

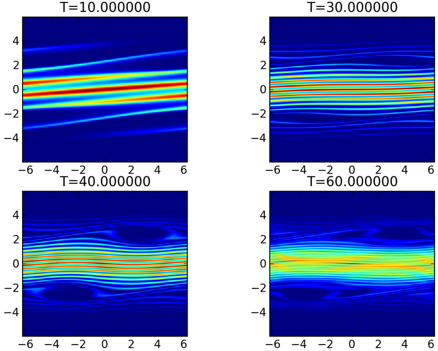


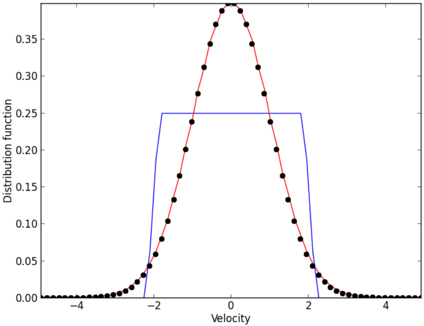
Figure: [Movie] Distribution function from nonlinear Landau damping problem. Hyper-collisions are being implemented for phase-mixing to unresolved scales in velocity.

A particle, momentum and energy conserving Lenard-Bernstein collision operator is implemented

A simple collision operator is implemented:

$$C_{LB}[f] = \frac{\partial}{\partial v}\left(\nu(v-u)f + \nu v_t^2 \frac{\partial f}{\partial v}\right)$$

Figure shows relaxation of an initial step-function distribution function to Maxwellian due to collisions.



Conclusions: DG algorithms are promising for fluid and kinetic problems

- A discontinuous Galerkin scheme to solve a general class of Hamiltonian field equations is presented.
- The Poisson equation is discretized using continuous basis functions.
- With proper choice of basis functions energy is conserved.
- With central fluxes enstrophy is conserved. With upwind fluxes the scheme is L_2 stable.
- Momentum conservation has small errors but is independent of velocity space resolution and converges rapidly with spatial resolution.

Future work: extend scheme to higher dimensions, general geometries and do first physics problems

- The schemes have been extended to higher dimensions and Serendipity basis functions are being explored (with Eric Shi). Testing is in progress.
- Maxwellian weighted basis functions for velocity space discretization will be developed to allow coarse resolution simulations with the option of fine scale resolution when needed.
- A collision model is implemented. It will be tested with standard problems and extended to higher dimensions.
- Extensions will be made to take into account complicated edge geometries using a multi-block structured grid.