An overview of discontinuous Galerkin algorithms with applications to (gyro) kinetic simulations of plasmas

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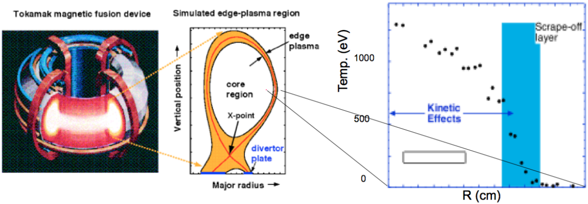
PPPL Theory Seminar, 13^{th} December 2012

Edge region very important but poorly understood



Edge pedestal temperature profile near the edge of an H-mode discharge in the DIII-D tokamak. [Porter2000]. Pedestal is shaded region.

- Need high pedestal temperature for core to get to fusion temperatures
- Need ways to reduce/suppress ELMs than can damage divertor plates
- Is there a way to enhance spontaneous flow to reduce turbulence?
- How much can Lithium improve performance?

Edge region of tokamaks and stellerators is very difficult and efficient numerical methods are needed

Detailed understanding of edge physics relatively poor compared to core of tokamak.

- Tokamak edge physics relatively unexplored: no complete model of self-consistent cross-field transport in open-field line region, very little study of neutral transport, wall effects, etc.
- Large density/amplitude variations, large relative banana width, wide range of collisionalities
  - Stick with full-F simulations
  - Need good algorithms to distinguish physical oscillations from numerical noise (Gibb's phenomena)
- Complicated geometry and magnetic topology, X-points, open field lines, divertor plates ...

Long term goal: Accurate and stable continuum schemes for full-F edge gyrokinetics in 3D 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 proper choice of velocity space basis functions.

Long term goal: Accurate and stable continuum schemes for full-F edge gyrokinetics in 3D geometries

Dream Goal

A robust code capable of running very quickly at coarse velocity space resolution while preserving all conservation laws of gyro-fluid/fluid equations and giving fairly good results. Can occasionally turn up velocity resolution for convergence tests.

To achieve this, exploring combination of techniques

- Efficient, high order, hybrid DG/finite-element scheme with excellent conservation properties.
- Subgrid turbulence models/hypercollision operators and limiters than enable robust results on coarse grids.
- Maxwellian-weighted basis functions.

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.

DG combined with FV schemes can lead to best-in-class explicit algorithms for hyperbolic PDEs.

Discontinuous Galerkin can be a potential "game changer" for (gyro)kinetic plasma simulations

Edge/pedestal gyrokinetic turbulence is very challenging, 5D problem not yet solved. Benefits from all tricks we can find.

- Factor of 2 reduction in resolution would lead to $64\times$ speedup.
- Higher order methods require more FLOPs per data point, but more efficient on modern CPUs where memory bandwidth is the limitation. Combined with data-locality, means modern CPU/GPU optimization can be better (cache optimization, vectorization, fast linear-algebra routines, etc.).

Essential idea of Galerkin methods: L_2 minimization of errors on a finite-dimensional subspace

Consider a general time-dependent problem

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

where $G[f]$ is some operator. To approximate it expand $f(x)$ with a finite set of basis functions $w_k(x)$,

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

This gives discrete system

$$\sum_{k=1}^{N} f'_k w_k(x) = G[f_h]$$

Question

How to determine f'_k in an optimum manner?

Essential idea of Galerkin methods: L_2 minimization of errors on a finite-dimensional subspace

Answer: Do an L_2 minimization of the error, i.e. find f'_k such that

$$E_N = \int \left[\sum_{k=1}^{N} f'_k w_k(x) - G[f_h] \right]^2 dx$$

is minimum. 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

$$\int w_m(x) \left(\sum_{k=1}^{N} f'_k w_k(x) - G[f_h] \right) dx = 0$$

for all $m = 1, \ldots, N$.

Key Idea

Projection of residual on the basis set chosen for expansion leads to minimum errors in the L_2 sense. For this reason DG/CG schemes are constructed by projecting residuals of PDEs on basis sets.

What does a typical L_2 fit look like for discontinuous Galerkin scheme?

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

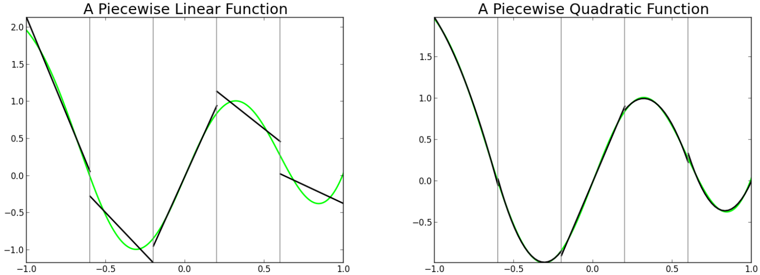


Figure: The best L_2 fit of $x^4 + \sin(5x)$ with piecewise linear (left) and quadratic (right) basis functions.

Passive advection is a good prototype to study DG schemes

Consider the 1D passive advection equation on $I \in [L, R]$

$$\frac{\partial f}{\partial t} + \lambda \frac{\partial f}{\partial x} = 0$$

with λ the constant advection speed. $f(x,t) = f_0(x - \lambda t)$ is the exact solution, where $f_0(x)$ is the initial condition. Designing a good scheme is much harder than it looks.

- Discretize the domain into elements $I_j \in [x_{j-1/2}, x_{j+1/2}]$
- Pick a finite-dimensional function space to represent the solution. For DG we usually pick polynomials in each cell but allow discontinuities across cell boundaries
- Expand $f(x,t) \approx f_h(x,t) = \sum_k f_k(t) w_k(x)$.

Discrete problem can be stated as finding the coefficients that minimize the L_2 norm of the residual

The discrete problem in DG is stated as: find f_h in the function space such that for each basis function φ we have

$$\int_{I_j} \varphi \left(\frac{\partial f_h}{\partial t} + \lambda \frac{\partial f_h}{\partial x} \right) dx = 0.$$

Integrating by parts leads to the discrete *weak-form*

$$\int_{I_j} \varphi \frac{\partial f_h}{\partial t}\, dx + \lambda \varphi_{j+1/2} \hat{f}_{hj+1/2} - \lambda \varphi_{j-1/2} \hat{f}_{hj-1/2} - \int_{I_j} \frac{d\varphi}{dx} \lambda f_h \, dx = 0.$$

Here $\hat{f}_h = \hat{f}(f_h^+, f_h^-)$ is the consistent *numerical flux* on the cell boundary. Integrals are performed using high-order quadrature schemes.

Picking a good numerical flux is key to stability, accuracy

- Take averages

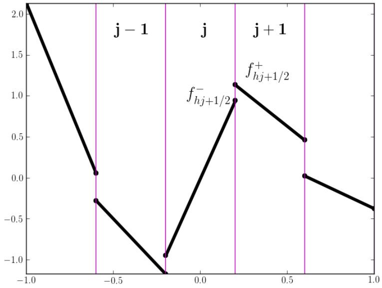
$$\hat{f}_h(f_h^+, f_h^-) = \frac{1}{2}(f_h^+ + f_h^-)$$

- Use upwinding

$$\begin{aligned} \hat{f}_h(f_h^+, f_h^-) &= f_h^- \quad \lambda > 0 \\ &= f_h^+ \quad \lambda < 0 \end{aligned}$$

- Or some combination

$$\begin{aligned} \hat{f}_h(f_h^+, f_h^-) &= \frac{1}{2}(f_h^+ + f_h^-) \\ &+ \frac{c}{2}(f_h^+ - f_h^-) \end{aligned}$$



For system of nonlinear equations (Euler, ideal MHD, etc.) there is cottage industry on choosing numerical fluxes. Google "Riemann solvers"

Example: Piecewise constant basis functions lead to familiar difference equations

- A central flux with piecewise constant basis functions leads to the familiar central difference scheme

$$\frac{\partial f_j}{\partial t} + \lambda \frac{f_{j+1} - f_{j-1}}{2\Delta x} = 0$$

- An upwind flux with piecewise constant basis functions leads to the familiar upwind difference scheme (for $\lambda > 0$)

$$\frac{\partial f_j}{\partial t} + \lambda \frac{f_j - f_{j-1}}{\Delta x} = 0$$

Solution is advanced in time using a suitable ODE solver, usually strong-stability preserving Runge-Kutta methods.

Example: Piecewise constant basis functions with central flux leads to dispersive errors

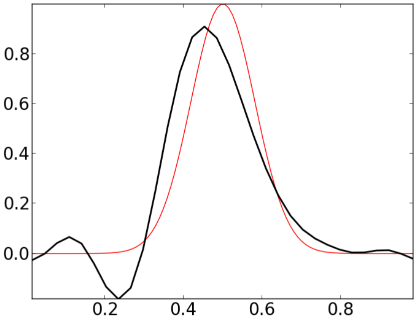


Figure: Advection equation solution (black) compared to exact solution (red) with central fluxes and piecewise constant basis functions.

Example: Piecewise constant basis functions with upwind flux is very diffusive

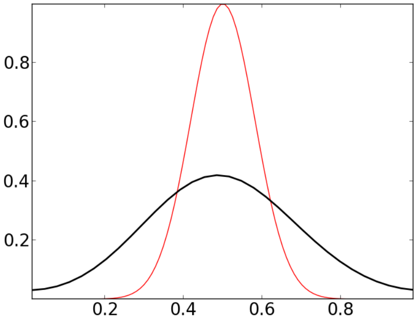


Figure: Advection equation solution (black) compared to exact solution (red) with upwind fluxes and piecewise constant basis functions.

Example: Piecewise linear space with upwind flux leads to good results

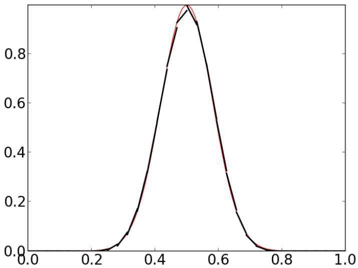


Figure: Advection equation solution (black) compared to exact solution (red) with upwind fluxes and piecewise linear basis functions.

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

Summary of DG schemes

- Pick basis functions. These are usually piecewise polynomials, but could be other suitable functions.
- Construct discrete weak-form using integration by parts.
- Pick suitable numerical fluxes (Riemann solvers) for the surface integrals.
- Pick a suitable quadrature scheme to perform surface and volume integrals.
- Use Runge-Kutta (or other suitable) schemes for evolving the equations in time.

Other major topics in DG: limiters for positivity/monotonicity, nodal vs. modal basis functions, Serendipity basis functions, diffusion terms, general geometry, error and accuracy analysis, hp-refinement, etc.

Several fluid and kinetic problems can be written with Poisson bracket structure leading to phase-space advection equation

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

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

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

Example: Hasegawa-Wakatani equations serve as a model for drift-wave turbulence in tokamak edge

The Hasegawa-Wakatani equations describe $E \times B$ driven flows in certain limits:

$$
\begin{aligned}
\frac{\partial n}{\partial t} + \{\phi, n + N\} &= D(\phi - n) \\
\frac{\partial \zeta}{\partial t} + \{\phi, \zeta\} &= D(\phi - n)
\end{aligned}
$$

with $\nabla^2 \phi = \zeta$. Here n is the number density fluctuations, ζ the $E \times B$ vorticity, ϕ is the potential, D is an adiabacity parameter and $N(x)$ is the fixed background density profile.

Example: Vlasov equation for electrostatic plasmas

The Vlasov-Poisson system has the Hamiltonian

$$H(x,p) = \frac{1}{2m}p^2 + q\phi(x)$$

where q is species charge and m is species mass and $p = mv$ is momentum. With this $\dot{x} = v$ and $\dot{v} = -q\partial\phi/\partial x$ leading to

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \frac{q}{m}\frac{\partial \phi}{\partial x}\frac{\partial f}{\partial v} = 0$$

It is important to preserve quadratic invariants of these systems

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?

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.

For Vlasov-Poisson momentum conservation is not exact but is *independent of velocity resolution*

For electrostatic problems the condition for conservation of discrete momentum reduces to vanishing of the average force. However we can show that

$$\int n_h E_h \, dx \neq 0$$

Hence momentum is not exactly conserved.
One can imagine smoothing E_h or solving the Poisson equation with higher order continuity. However, we have not yet been able to construct a direct scheme that conserves momentum and energy simultaneously.

Small errors in momentum conservation, independent of velocity space resolution and converging rapidly with spatial resolution

N_x	Error P1	Order
8	1.3332×10^{-3}	
16	3.9308×10^{-4}	1.76
32	8.5969×10^{-5}	2.19
64	1.5254×10^{-5}	2.49
128	2.3105×10^{-6}	2.72

N_x	Error P2	Order
8	1.9399×10^{-5}	
16	4.0001×10^{-7}	5.60
32	5.1175×10^{-8}	2.97
64	2.2289×10^{-9}	4.52
128	8.9154×10^{-11}	4.64

Summary of hybrid DG/CG schemes for Hamiltonian systems

- 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 there are small errors in momentum conservation even on a coarse velocity grid, and decrease rapidly with spatial resolution.

Questions

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

Prototype code named Gkeyll is being developed

- Gkeyll is written in C++ and is inspired by framework efforts like Facets, VORPAL (Tech-X Corporation) and WarpX (U. Washington). Uses structured grids with arbitrary dimension/order nodal basis functions.
- Package management and builds are automated via `scimake` and `bilder`, both developed at Tech-X Corporation.
- Linear solvers from Petsc[1] are used for inverting stiffness matrices.
- Programming language Lua[2], used in widely played games like World of Warcraft, is used as an embedded scripting language to drive simulations.
- MPI is used for parallelization via the `txbase` library developed at Tech-X Corporation.

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

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

Results are presented for each of the equation systems described above.

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

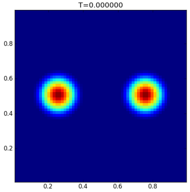


Figure: [Movie] Swirling flow problem. The initial Gaussian pulses distort strongly but regain their shapes after a period of 1.5 seconds.

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

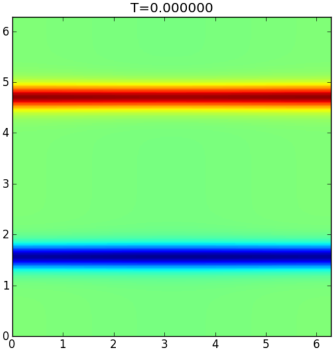
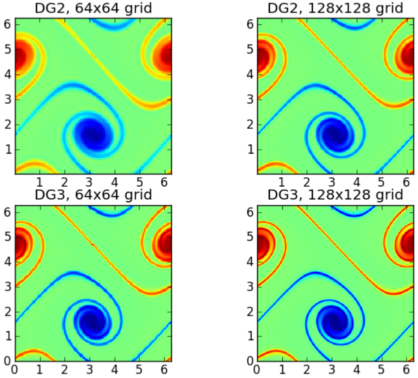


Figure: [Movie] Vorticity from double shear problem with piecewise quadratic DG scheme on 128×128 grid.

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.



Vortex waltz problem tests resolution of small-scale vortex features

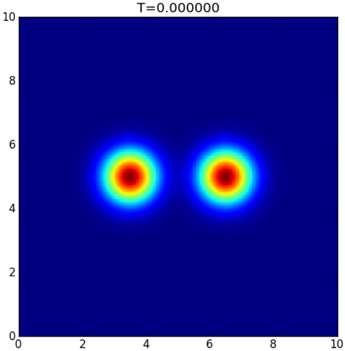


Figure: [Movie] Vorticity from vortex waltz problem with piecewise quadratic DG scheme on 128×128 grid.

Vortex waltz problem tests resolution of small-scale vortex features and energy and enstrophy conservation

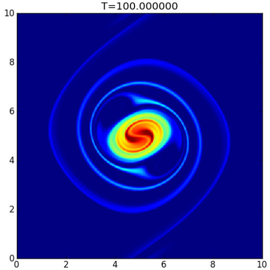


Figure: Vorticity for the vortex waltz problem with the piecewise quadratic scheme on a 128×128. *Upwind fluxes* were used for this calculation.

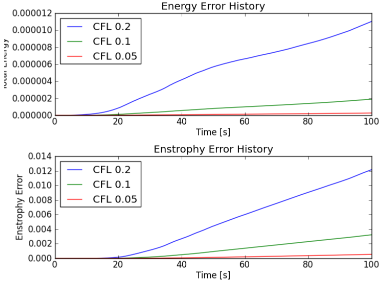


Figure: Energy and enstrophy error for vortex waltz problem. *Central fluxes* were used and show $O(\Delta t)^3$ convergence on a fixed 64×64 grid.

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

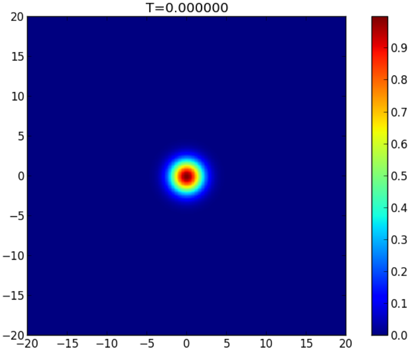


Figure: [Movie] Number density from Hasegawa-Wakatani drift-wave turbulence simulations with adiabacity parameter $D = 0.1$.

Initial scans of turbulent structures were performed with varying adiabacity parameter

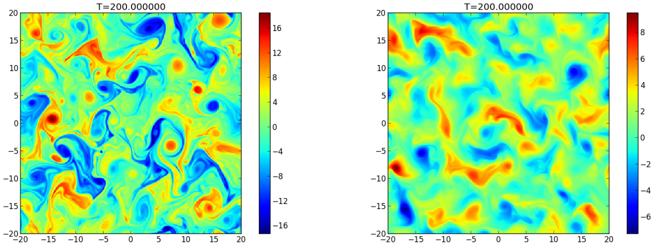
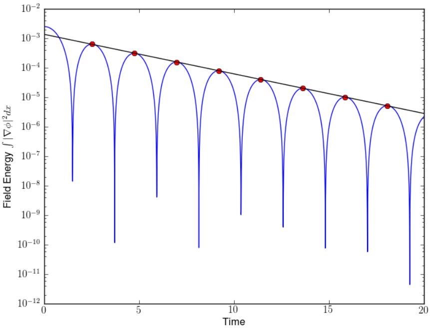


Figure: Number density from Hasegawa-Wakatani drift-wave turbulence simulations with adiabacity parameter $D = 0.1$ (left) and $D = 1.0$.

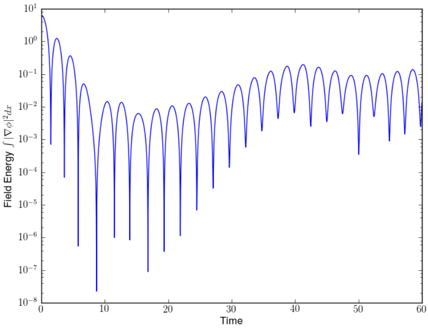
Linear Landau damping simulations were compared with exact solutions of dispersion relations

Field energy (blue) as a function of time for linear Landau damping problem with $k = 0.5$ and $Te = 1.0$. The red dots represent the maxima in the field energy which are used to compute a linear least-square fit. The slope of the black line gives the damping rate.



Nonlinear Landau damping simulations show particle trapping and phase-space hole formation

Field energy as a function of time for nonlinear Landau damping problem with k=0.5, $Te = 1.0$ and $\alpha = 0.5$. The initial perturbation decays at a rate of $\gamma = 0.2916$, after which the damping is halted from particle trapping. The growth rate of this phase is $\gamma = 0.0879$.



DG scheme can efficiently capture fine-scale features in phase-space

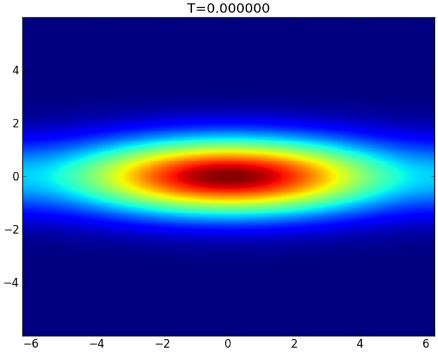
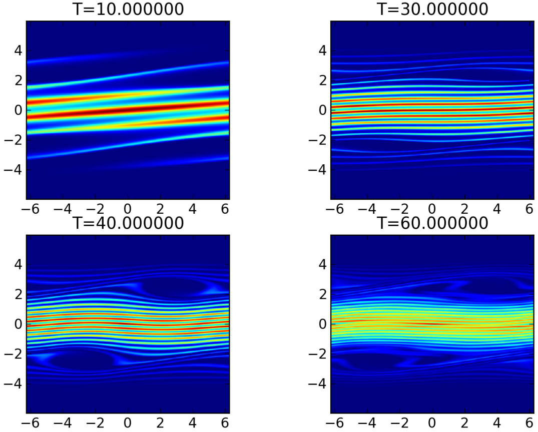


Figure: [Movie] Distribution function from nonlinear Landau damping problem.

DG scheme can efficiently capture fine-scale features in phase-space

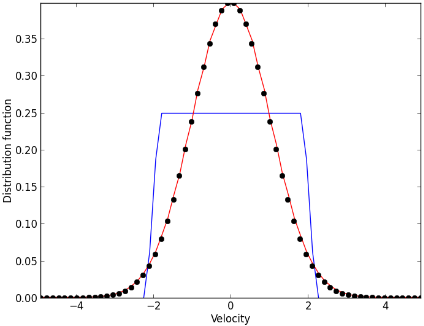


A particle, momentum and energy conserving Lenard-Bernstein collision operator is implemented

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: Our tests confirm that DG algorithms are promising for 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.