Aspects of Discontinuous Galerkin Schemes for Fluid and Kinetic Simulations of Plasmas

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Outline: Present scheme for a class of fluid and kinetic problems

Long term goal: Accurate and stable schemes fluid/kinetic turbulence simulations of plasmas.

- Present discontinuous/continuous Galerkin schemes for solution of a class of fluid and kinetic problems in plasmas.
- Discuss use on non-polynomial basis functions to optimize capturing known physical features.
- Outline some subtle issues in discretization of second-order derivatives operators using various DG approaches.

Significant prior work exists on Vlasov-Poisson, Vlasov-Maxwell

A lot of work is from Institute of Fusion Studies (IFS) and ICES studies here in U. Texas. See series of papers by Cheng, Morrison, Gamba and co-workers

- Y. Cheng, I. M. Gamba, F. Li, and P. J. Morrison, "Discontinuous Galerkin Methods for the Vlasov-Maxwell Equations," submitted (2013).
- Y. Cheng, I. M. Gamba, and P. J. Morrison, "Study of Conservation and Recurrence of Runge-Kutta Discontinuous Galerkin Schemes for Vlasov-Poisson Systems," Journal of Scientific Computing (2012)
- R. E. Heath, I. M. Gamba, P. J. Morrison, and C. Michler, "A Discontinuous Galerkin Method for the Vlasov-Poisson System," Journal of Computational Physics 231, 11401174 (2012).

Other efforts by C.W. Shu (Brown), J. Rossmanith (Iowa State), David Seal (Michigan State) etc.

A basic model of a class of problems in plasma physics is nonlinear advection in phase space

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

Here $f(z^1, z^2, \ldots, t)$ is a scalar "distribution function" and $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots)$ is advection velocity vector in phase space.

These models can be derived from a Hamiltonian and a Poisson Bracket structure

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

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 $\alpha_i = \{z^i, H\}$ 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 prototype model for a class of turbulence fluid problems

Incompressible 2D Euler equations written in the stream-function (ϕ) vorticity (ζ) formulation. Here the Hamiltonian is simply

$$H(x, y) = \phi(x, y)$$

Advection speed is $u_x = \{x, H\}$ and $u_y = \{y, h\}$ or $\mathbf{u} = \nabla\phi \times \mathbf{e}_z$

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

The potential is determined from

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

Example: Vlasov equation for electrostatic plasmas

The Vlasov-Poisson system has the Hamiltonian

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

where q is species charge and m is species mass and v is velocity. Poisson bracket is *noncanonical*

$$\{g, h\} = \frac{1}{m}\left(\frac{\partial g}{\partial x}\frac{\partial h}{\partial x} - \frac{\partial g}{\partial v}\frac{\partial h}{\partial x}\right)$$

With this $\dot{x} = v$ and $\dot{v} = -q/m\partial\phi/\partial x$ leading to

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

Example: For Valsov equation two methods to determine potential

For non-neutral plasmas solve a Poission equation

$$\frac{\partial^2 \phi}{\partial x^2} = -\frac{\rho_c}{\epsilon_0}$$

where

$$\rho_c = |e| \left(Z n_{io}(x) - \int_{-\infty}^{\infty} f(x,v,t) dv \right)$$

OR, For a quasi-neutral plasma in certain limits

$$\int_{-\infty}^{\infty} f(x,v,t) dv = n_{eo} \left(1 + \frac{|e|\phi}{T_e} \right)$$

It is important to preserve quadratic invariants of these systems

One can show that

$$\int H \frac{\partial f}{\partial t} d\mathbf{Z} = 0$$

$$\int f \frac{\partial f}{\partial t} d\mathbf{Z} = 0$$

In deriving these one can use the identity $\boldsymbol{\alpha} \cdot \nabla H = 0$.
Many other invariants might exist, some of which may be important to conserve. Example: momentum in electrostatic Vlasov equations.

Example: For incompressible Euler these are called energy and enstrophy

The energy is defined as

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

and *enstrophy* is defined as

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

Often diffusive processes need to be included

Diffusion (from vicous effects or collisions) might be needed. For example, the collisional Vlasov equation in some approximation is

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} - \frac{q}{m}\frac{\partial \phi}{\partial x}\frac{\partial f}{\partial v} = \frac{\partial}{\partial v}\left(\nu(v-u)f + \nu v_t^2\frac{\partial f}{\partial v}\right)$$

where ν is a collision frequency.

In summary: we need to descretize advection equation coupled to elliptic equation

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 and a proper choice of velocity space basis functions.

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 if *space spanned by potential basis functions are a continuous subset of the space spanned by the vorticity basis functions*.

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.

However, conservation needs Hamiltonian (fields) to be *continuous*

Look at the a quasi-neutral plasma (or parallel dynamics in gyrokinetics)

$$\int_{-\infty}^{\infty} f(x,v,t)dv = n_{eo}\left(1 + \frac{|e|\phi}{T_e}\right)$$

This *can not* be true point-wise, but must be enforced only in a *weak-sense*.
Problem: This leads to a global solve to determine $\phi(x)$, even though the point-wise expression is local. Is there a way to conserve energy even in this case?

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.

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

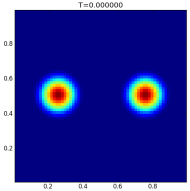

Figure: [Movie] Swirling flow problem. The initial Gaussian pulses distort strongly but regain their shapes after a period of 1.5 seconds.

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

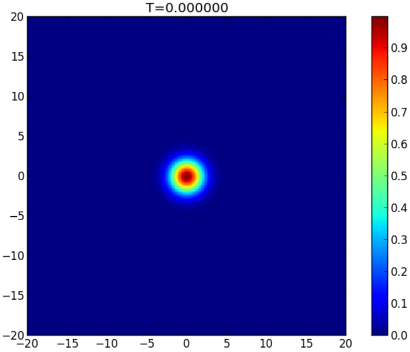

Figure: [Movie] Number density from Hasegawa-Wakatani drift-wave turbulence simulations with adiabacity parameter $D = 0.1$.

Modified Hasegawa-Wakatani equations are used to study zonal flow formation

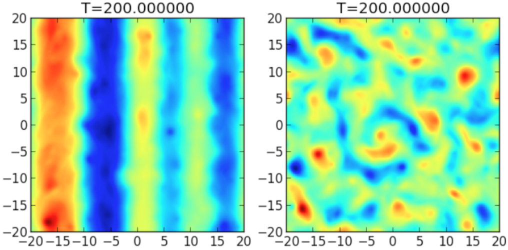

Figure: [Movie] Number density from Hasegawa-Wakatani drift-wave turbulence simulations with adiabacity parameter $D = 0.1$ with (left) and without (right) zonal flow modification.

How to handle second-order derivatives with DG?

Numerical Methods 101: How to discretize

$$g(x) = \frac{d^2 f}{dx^2}$$

Simplest finite difference scheme

$$g_j = \frac{1}{\Delta x^2}(T - 2 + T^{-1}) f_j$$

The shift operators are used

$$T(j) = f_{j+1}$$
$$T^{-1}u(j) = f_{j-1}.$$

A whole zoo of schemes have been developed to handle such terms in DG

But: Are they *consistent*?

What is consistency?

Write the expansion in a cell using Taylor series basis functions centered around $x = x_j$

$$f_{jh}(x) = \sum_{n=0}^{N} f_j^{(n)} (x - x_j)^n / n!$$

Given a function $f(x)$, we call a discrete representation f_{jh} *consistent* if

$$\lim_{\Delta x \to 0} f_j^{(n)} = \left. \frac{d^n f}{dx^n} \right|_{x_j}.$$

For example, the standard Galerkin procedure of minimization of the error in each cell, $\int_{I_j} \left[f(x) - f_{jh}(x) \right]^2 dx$, leads to a consistent representation.

What is consistency?

Consistency for operators. Consider

$$g(x) = f_{xx}(x) \tag{1}$$

Given a domain $I \in [a, b]$ divided into uniform cells I_j

$$g(x) = f_{xx}(x) \approx g_{jh}(x) = \sum_{n=0}^{N} g_j^n P_n(\eta_j(x)) \tag{2}$$

in each cell I_j. We define a discretization to be *consistent in the mean* as follows

Definition (Consistency in the mean)

A discrete DG representation, $g_{jh}(x)$, of f_{xx} said to be *consistent in the mean*, if

$$\lim_{\Delta x \to 0} g_j^0 = f_{xx}|_{x_j}.$$

What is consistency?

Consistency in the mean is required if the discrete operator is to be represented correctly. *But what about other terms in expansion?* We define a discretization to be *fully consistent* as follows

Definition (Full consistency)

A discrete DG representation, $g_{jh}(x)$, of f_{xx} said to be *fully consistent*, if

$$\lim_{\Delta x \to 0} \frac{d^n g_{jh}}{dx^n} = \left. \frac{d^n f_{xx}}{dx^n} \right|_{x_j}$$

for all $n = 0, \ldots, N$.

A whole zoo of schemes have been developed to handle such terms in DG

Example: Local DG schemes. Rewrite the system as system of first order equations

$$\frac{\partial w}{\partial x} + f = 0,\ \frac{\partial g}{\partial x} + w = 0$$

For piecewise linear basis functions

$$u_h(x,t) = u_0 + \frac{x - x_j}{\Delta x/2} u_1$$

A whole zoo of schemes have been developed to handle such terms in DG

Claim

Many popular DG schemes for such terms are not fully consistent.

Example: Local DG scheme for piece-wise linear basis functions

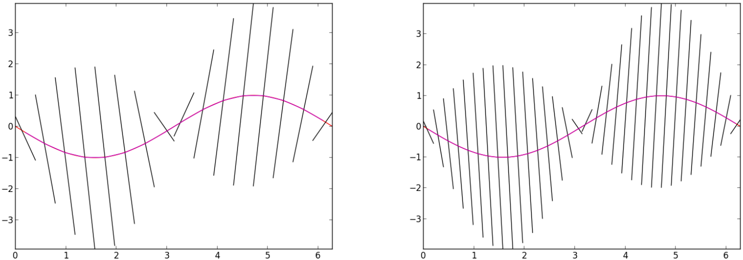

Figure: Derivatives of $\sin(x)$ computed using LDG scheme with 16 cells (left) and 32 cells (right). Notice slopes are completely mispredicted, showing scheme is inconsistent.

Example: Local DG scheme for piece-wise linear basis functions

For piecewise linear basis functions we can write update formula as

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \frac{1}{\Delta x^2} \begin{pmatrix} 4T^{-1} - 8 + 4T & 2T^{-1} + 2 - 4T \\ -12T^{-1} + 6 + 6T & -6T^{-1} - 24 - 6T \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}$$

General procedure to check consistency: perform Taylor series expansion and plug into above expression and take limit as $\Delta x \to 0$

Example: Local DG scheme for piece-wise linear basis functions

Taylor series analysis, confirmed numerically, shows that

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \begin{pmatrix} f_{xx} + \Delta x(\ldots) \\ -6 f_{xx}/\Delta x + \Delta x(\ldots) \end{pmatrix}$$

Notice: not only the slopes are incorrect, but they blow up as $\Delta x \to 0$!

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Example: What if use a symmetric form of local DG scheme?

For piecewise linear basis functions we can write update formula as

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \frac{1}{\Delta x^2} \begin{pmatrix} 4T^{-1} - 8 + 4T & 3T^{-1} - 3T \\ -9T^{-1} + 9T & -6T^{-1} - 24 - 6T \end{pmatrix}$$

Example: What if use a symmetric form of local DG scheme? Also inconsistent.

Taylor series analysis, confirmed numerically, shows that

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \begin{pmatrix} f_{xx} + \Delta x(\ldots) \\ 3f_{xxx}/5 + \Delta x(\ldots) \end{pmatrix}$$

Notice: slopes are incorrect.

Many other popular schemes, including popular pentalty methods are inconsistent

A philosophical problem: we are trying to use ideas from traditional FEM toolbox to construct the discrete operators.

Instead, lets use ideas from finite volume toolbox, in particular the idea of *recovery* widely used in finite-volume Navier-Stokes solvers.

Basic idea: recover a continous solution in two cells sharing edge (van Leer AIAA 2005, Huynh AIAA 2009)

Let $R(\zeta)$, $\zeta = x_{j-1/2} - x \in [-\Delta x, \Delta x]$, be a *reconstructed* poynomial that extends across two cells and defined as

$$R(\zeta) = f_0 + \zeta f' + \frac{1}{2}\zeta^2 f'' + \ldots$$

over $\zeta = x_{j-1/2} - x \in [-\Delta x, \Delta x]$.

Determine $R(\zeta)$ by L2 minimization over each of the neigboring cells

$$\int_{I_{j-1}} vR\mathrm{d}x = \int_{I_{j-1}} vf\mathrm{d}x$$

$$\int_{I_j} vR\mathrm{d}x = \int_{I_j} vf\mathrm{d}x$$

for all $v(x)$ being the basis functions.

Basic idea: recover a continous solution in two cells sharing edge

For piecewise linear basis function this leads to

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \frac{1}{4\Delta x^2} \begin{pmatrix} 9T - 18 + 9T^{-1} & -5T + 5T^{-1} \\ 15T - 15T^{-1} & -7T - 46 - 7T^{-1} \end{pmatrix}$$

Basic idea: recover a continuous solution in two cells sharing edge

Taylor series analysis, confirmed numerically, shows that

$$\begin{pmatrix} g_0 \\ g_1 \end{pmatrix} = \begin{pmatrix} f_{xx} + \Delta x(\ldots) \\ f_{xxx} + \Delta x(\ldots) \end{pmatrix}$$

Notice: *fully consistent scheme!*

Lesson

The fact that the solution is discontinous is actually just a cartoon or reality. Advection equations do not mind these discontinuties, but diffusion operators do. So for the latter use *recovery* and for the former *upwinding*. Upwinding does not make sense for diffusion.

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.