Some New Formulations of DG Methods for Wave Equations

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Collaborators

Galerkin Difference (GD) Methods: Jeff Banks (RPI)

Coupled DG-GD Methods: Jeremy Kozdon and Lucas Wilcox (NPS)

Upwind DG for Second Order Wave Equations: Daniel Appelö (UNM)

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Ideology: Methods should be high order and energy-stable.

As computing power increases the case for higher order methods becomes stronger:

- Harder problems (in terms of number of wavelengths) can be treated - as we'll see below as the propagation distance increases efficiency is optimized at ever higher method orders.
- Higher order methods have increased computation-to-communication ratios and thus should be better positioned to leverage many-core systems.

The simplest case: central difference methods for the scalar wave equation. From the approximate dispersion relation we can directly compute the number of grid points-per-wavelength (PPW) required to propagate a wave a given number of periods with a certain relative accuracy. Here ϵ is the ratio of the error to the propagation time. For example, to propagate a wave 100 wavelengths with a 10% error take $\epsilon = 10^{-3}$ and with a 1% error take $\epsilon = 10^{-4}$.

q	ϵ	PPW	PPW $\times$ $(q+1)$
2	10^{-3}	143.9	432
2	10^{-4}	501.0	1500
4	10^{-3}	13.2	66.0
4	10^{-4}	22.7	114
8	10^{-3}	4.9	44.0
8	10^{-4}	6.2	56.1
12	10^{-3}	3.7	47.7
12	10^{-4}	4.3	55.6
16	10^{-3}	3.2	54.4
16	10^{-4}	3.6	61.0

DG methods: For Friedrichs systems the upwind DG methods popularized by Hesthaven and Warburton (Springer 2008) are a natural choice with a flux based directly on the natural conserved energy - L^2:

$$A_0\frac{\partial u}{\partial t}+\sum_j A_j\frac{\partial u}{\partial x_j}=0,\quad u(x,0)=u_0(x),\quad Bu(x,t)=0,\quad x\in\partial\Omega,$$

$$A_j=A_J^T,\quad A_0>0\ \rightarrow\frac{d}{dt}\int_\Omega u^TA_0u=\text{Boundary Terms}$$

Then the usual formulation is:

$$\int_{\Omega_k}\phi^T\left(A_0u_t+\sum_j A_ju_{x_j}\right)=\int_{\partial\Omega_k}\phi^T\left(\sum_j n_jA_j(u^*-u)\right),$$

Flux splitting:

$$\sum_j n_jA_j=A^+-A^-,\quad A^\pm\ \text{ PDS}$$

$$\sum_j n_jA_ju^*=A^+u^{\text{in}}-A^-u^{\text{out}}$$

then

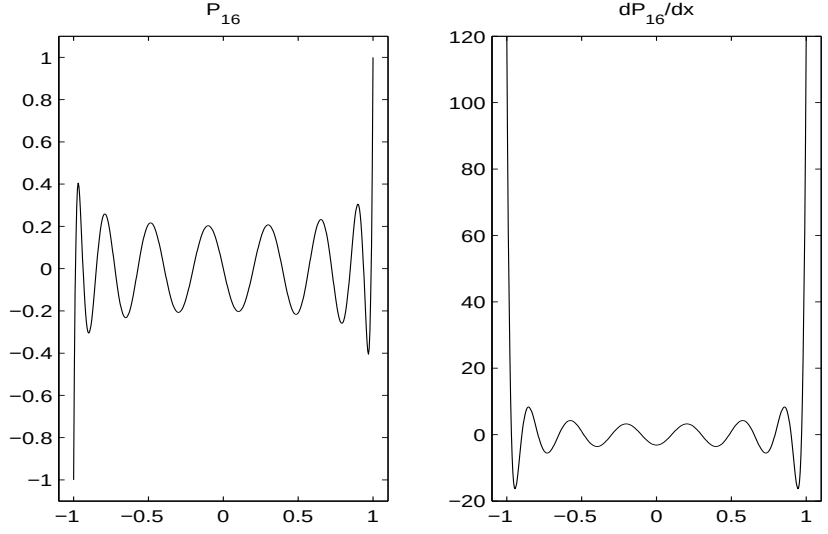
$$\frac{d}{dt}\sum_k\|u\|^2_{L^2(\Omega_k)}\le 0.$$

The downside of high-order element methods is the artificial stiffness induced by one-sided differentiation at the element edges and the possibility of heavy linear algebra within each element. Precisely, the norm of derivative matrices scales like $m^2 h^{-1}$ for degree-m polynomials in width h elements. As a result, practical use typically limits the order to 4 or 5 - well below what we'd like to use. This unfavorable scaling of the derivative matrix is a fundamental property of polynomials - the Markov/Bernstein inequalities. For polynomials of degree m on the standard interval, $[-1, 1]$ we have:

$$\|\frac{dq}{dx}(x)\| \leq \min\left(m^2, \frac{m}{\sqrt{1-x^2}}\right)\|q\|_\infty$$

Linear m-dependence for the derivative requires the use of data outside the interval where the derivative is to be computed - as in difference formulas or the Hermite methods. We believe we can make higher order elements more practical by using **hybrid grids** and more efficient discretizations on structured cells away from boundaries.

We work on two different families of structured grid methods - difference formulas satisfying energy estimates (GD methods) and elements based on Hermite interpolation (also called **jet schemes** - see work by Nave, Seibold, Rosales). For tutorial codes implementing Hermite schemes see **CHIDES** (Charles Hermite Interpolation Differential Equation Solver - www.chides.org)


P_{16}
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1
dP_{16}/dx
120
100
80
60
40
20
0
−20
−1
−0.5
0
0.5
1

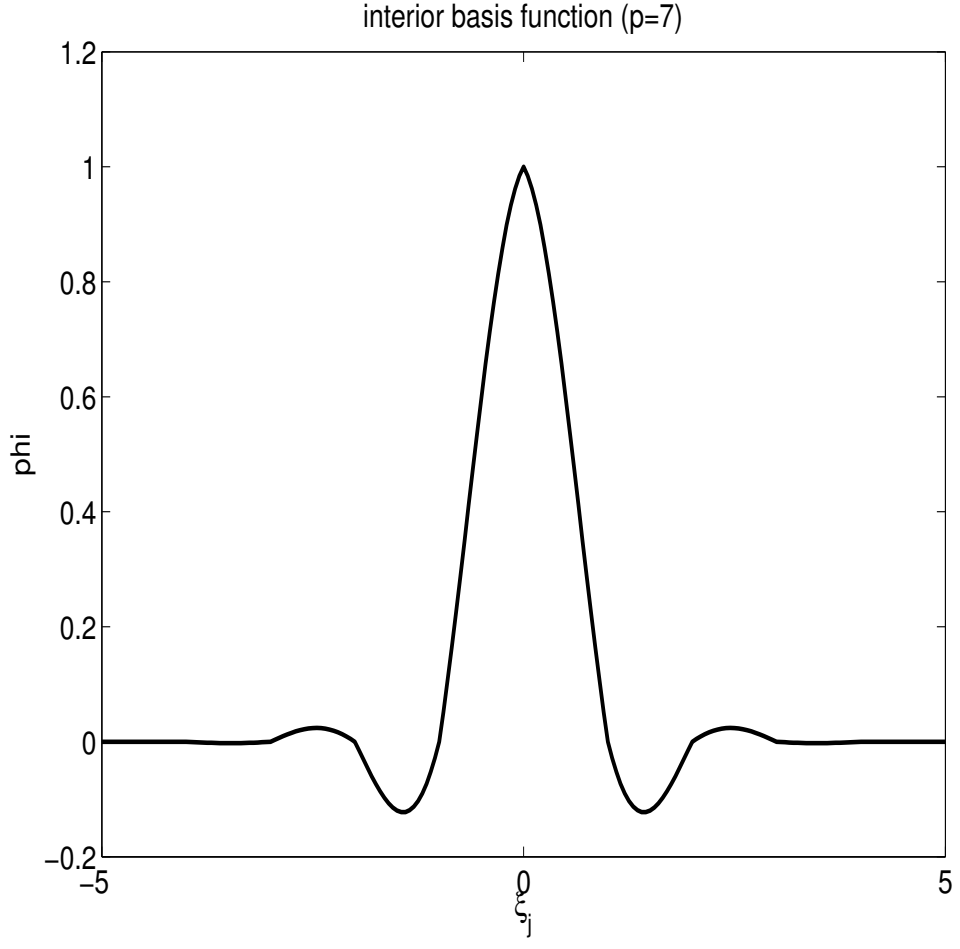
The standard energy-based high order difference methods are the so-called summation-by-parts (SBP) methods - boundary closures of high-order central (or upwind) difference formulas which allow an integration-by-parts formula relative to a quadrature scheme with positive weights.

We are pursing a different approach to the construction of difference methods with energy-stable boundary closures - "global" discontinuous Galerkin method with finite-difference type bases which we call Galerkin differences (GD) (Banks and H., JCP in revision)

- Basis elements extend across multiple elements to avoid the problems caused by differentiating polynomials near element boundaries. For example a typical Lagrange function would be a continuous piecewise polynomial supported on q cells to the right and to the left - see the upcoming picture.
- Boundary closures are obtained either by extrapolation or by allowing basis elements associated with "ghost" nodes to remain in the basis.

Features:

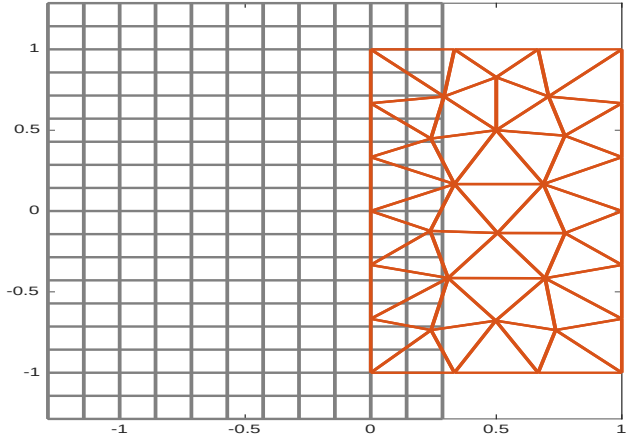
- Tensor-product banded mass matrices - always invertible in linear time. In fact we derive a sort of compact difference scheme.
- Superconvergence away from the boundaries - global order $2q$ but the consistency error of the difference formula away from the boundaries has consistency error of order $4q$ (we could up the accuracy at the boundary to match).
- Stability of the resulting structured-unstructured grid schemes follows automatically from DG theory.

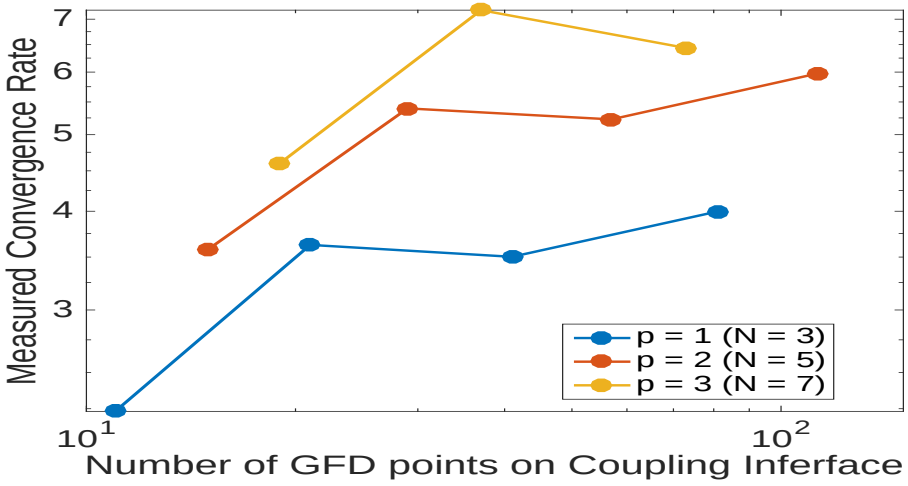

interior basis function (p=7)
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
phi
−5
0
5
ξj

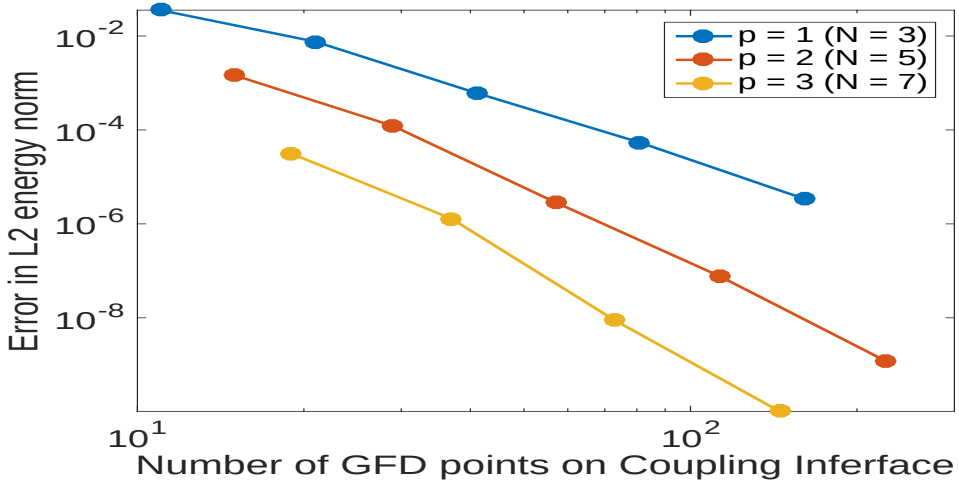
A happy mystery about these methods is that, for Friedrichs systems, **the norm of the derivative matrix is independent of order up through at least thirty-something despite the fact that the boundary basis functions themselves are badly behaved due to the Runge phenomenon** - some magic cancellation is happening due to the bad basis functions appearing in both mass and stiffness matrices. We have yet to analyze this - we have no analytic bounds on the spectrum.

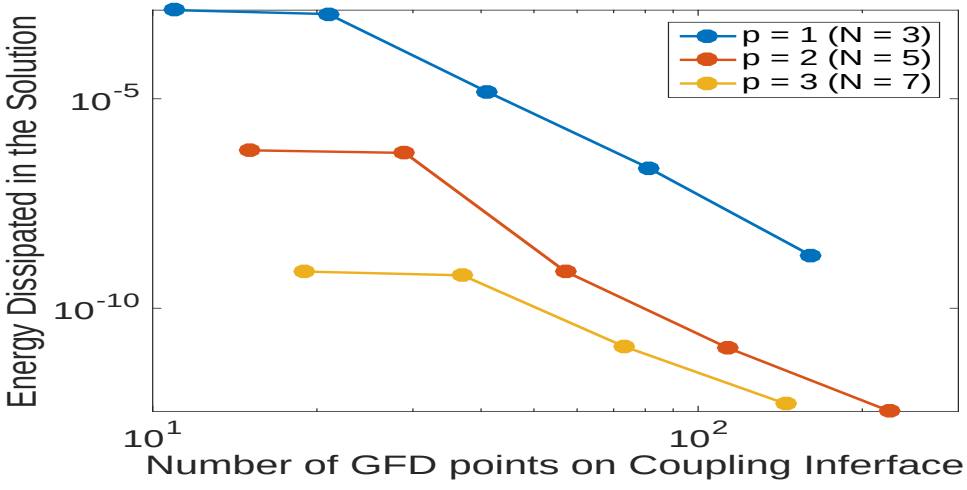
p	3	5	7	9	11	13	15	17
$\Delta x \rho(\left(M^{(p,G)}\right)^{-1} K^{(1,p,G)})$	2.02	2.17	3.41	3.18	3.67	3.81	3.57	3.84
$\Delta x \rho(\left(M^{(p,X)}\right)^{-1} K^{(1,p,X)})$	2.02	2.17	2.27	2.33	2.39	2.43	2.46	2.49

Our first example of DG-GD hybridization (from Saturday!) - acoustic wave equation in a box. No local time stepping yet - has been implemented for the Hermite-DG coupling schemes, where we have more complex examples (Appelö, Chen, H. JCP 257 (2013)) and works - we've had time step ratios as large as $80:1$.


1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1


Measured Convergence Rate
7
6
5
4
3
10^1
10^2
Number of GFD points on Coupling Inferface
p = 1 (N = 3)
p = 2 (N = 5)
p = 3 (N = 7)


p = 1 (N = 3)
p = 2 (N = 5)
p = 3 (N = 7)
Error in L2 energy norm
10^-2
10^-4
10^-6
10^-8
10^1
10^2
Number of GFD points on Coupling Inferface


p = 1 (N = 3)
p = 2 (N = 5)
p = 3 (N = 7)
Energy Dissipated in the Solution
10^-5
10^-10
10^1
10^2
Number of GFD points on Coupling Inferface

Upwind DG methods Lagrange systems (Appelö and H. SINUM (2015)):

$$\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j}\frac{\partial G}{\partial u_{i;j}} - \frac{\partial G}{\partial u_i}, \quad u(x,0) = u_0(x), \quad \frac{\partial u}{\partial t}(x,0) = v_0(x), \quad Bu(x,t) = 0, \quad x \in \partial\Omega,$$

$$G(Du,u) > 0 \ \rightarrow \frac{d}{dt}\int_\Omega \frac{1}{2}\left|\frac{\partial u}{\partial t}\right|^2 + G = \text{Boundary Terms}.$$

Example: standard scalar wave equation $G = \frac{c^2}{2}|\nabla u|^2$.

For second order or higher order systems DG methods have been proposed in a variety of forms:

Nonsymmetric Interior Penalty - (Riviére and Wheeler Contemp. Math. 2003) - dissipative method depending on the choice of an interior penalty parameter.

Symmetric Interior Penalty - (Grote, Schneebeli and Schötzau SINUM 2006) - energy conserving and again depending on the choice of an interior penalty parameter.

Local Discontinuous Galerkin - (Chou, Shu and Xing JCP 2014) - energy conserving based on introducing an approximation to $\mathbf{q} = \nabla u$ as a local variable.

We have been looking at a new formulation based on the energy equality - some similarities to LDG but we introduce an approximation to the time derivative, $v = \frac{\partial u}{\partial t}$, rather than the gradient. In the new formulation the essential idea is to build the weak form and the fluxes directly from the Lagrangian - energy flux:

$$\sum_{i,k} v_i \frac{\partial G}{\partial u_{i,k}} n_k$$

Flux splitting:

$$\sum_k v_i \frac{\partial G}{\partial u_{i,k}} n_k = \frac{1}{4\zeta_i}\left(v_i + \zeta_i \sum_k \frac{\partial G}{\partial u_{i,k}} n_k\right)^2 - \frac{1}{4\zeta_i}\left(v_i - \zeta_i \sum_k \frac{\partial G}{\partial u_{i,k}} n_k\right)^2 \equiv F_i^+ - F_i^-,$$

and choose the boundary states so that F_i^+ is computed using values from outside the element and F_i^- using the values from inside. That is we enforce the equations:

$$v_i^* - \zeta_i \sum_k w_{i,k}^* n_k^{(\ell)} = v_{i,\ell}^h - \zeta_i \sum_k \frac{\partial G}{\partial u_{i,k}}(\mathbf{u}_\ell^h, \nabla \mathbf{u}_\ell^h, \mathbf{x}) n_k^{(\ell)}.$$

This leads to what we call the **Sommerfeld flux**.
For the scalar wave equation - for all $\phi_v \in \Pi^q(\Omega_j)$, $\phi_u \in \Pi^{q+1}(\Omega_j)$

$$\begin{aligned}
\int_{\Omega_j} \nabla^2 \phi_u \left(\frac{\partial u^h}{\partial t} - v^h\right) &= \int_{\partial\Omega_j} \nabla\phi_u \cdot \mathbf{n} \left(\frac{\partial u^h}{\partial t} - v^*\right), \\
\int_{\Omega_j} \phi_v \frac{\partial v^h}{\partial t} + c^2 \nabla\phi_v \cdot \nabla u^h - \phi_v f &= c^2 \int_{\partial\Omega_j} \phi_v \mathbf{w}^* \cdot \mathbf{n}, \\
\int_{\Omega_j} \left(\frac{\partial u^h}{\partial t} - v^h\right) &= 0.
\end{aligned}$$

$$\begin{aligned}
v^* - c\mathbf{w}^* \cdot \mathbf{n}^- &= v^- - c\nabla u^- \cdot \mathbf{n}^-, \\
v^* - c\mathbf{w}^* \cdot \mathbf{n}^+ &= v^+ - c\nabla u^+ \cdot \mathbf{n}^+,
\end{aligned}$$

Energy conserving methods can also be devised based on **central** or **alternating** fluxes.

Energy estimate (note $v^h \neq \frac{\partial u^h}{\partial t}$):

$$E^h(t) = \frac{1}{2} \sum_j \int_{\Omega_j} \left(v^h\right)^2 + c^2 |\nabla u^h|^2,$$

satisfies

$$\frac{dE^h}{dt} - \int_\Omega v^h f = -\sum_k \int_{B_k} \alpha\beta c \left(\left(v^-\right)^2 + c^2 \left(\nabla u^- \cdot \mathbf{n}^-\right)^2 \right) - \mathcal{D},$$

where $\mathcal{D} = 0$ for the central and alternating fluxes and for the upwind flux

$$\mathcal{D} = \frac{c}{2} \sum_k \int_{F_k} |[[v^h]]|^2 + c^2 [[\nabla u^h]]^2 + c \sum_k \int_{B_k} \left(\alpha v^- + \beta c \nabla u^- \cdot \mathbf{n}^-\right)^2.$$

Using the energy estimate and standard arguments adapted from the first-order case we can prove for general grids

$$\|e_v(\cdot,T)\|^2_{L^2(\Omega)} + \|\nabla e_u(\cdot,T)\|^2_{L^2(\Omega)} \leq (C_0 + C_1 T) h^{2\sigma} \max_{t \leq T} \left(|u(\cdot,t)|^2_{H^{q+2}(\Omega)} + |v(\cdot,t)|^2_{H^{q+1}(\Omega)} \right),$$

where

$$\sigma = \begin{cases} q, & \text{Central/alternating flux,} \\ q + \frac{1}{2}, & \text{Upwind flux.} \end{cases}$$

In one space dimension (and probably on Cartesian grids) we can use the upwind projection technique to improve this to $q+1$ for both the upwind and alternating flux. **In our experiments so far we observe L^2-convergence at order $q+2$ for both the central and alternating flux, but we have no proof.** Note that this is a superconvergence phenomenon in that the equation for $\frac{\partial u^h}{\partial t}$ involves v^h which is of degree q.

Rates of convergence for the randomly perturbed quadrilateral grids in 2D.

Degree $q+1$ for approx. of u	1	2	3	4	5	6	7
Rate for u from LS fit S.-flux	1.353	2.123	3.873	5.010	6.078	6.963	7.902
Rate for E from LS fit S.-flux	0.769	1.687	2.867	3.925	4.975	6.045	6.988
Rate for u from LS fit A.-flux	1.399	1.998	3.504	4.723	5.738	6.775	7.803
Rate for E from LS fit A.-flux	0.664	1.773	2.746	4.047	4.984	5.974	6.995
Rate for u from LS fit C.-flux	1.437	1.898	3.441	3.938	5.543	6.044	7.321
Rate for E from LS fit C.-flux	0.618	0.891	2.644	2.996	4.506	4.939	6.340

We also find that the spectral radius of the spatial discretization matrix **grows quadratically with** q - i.e. at the same rate as with first-order formulations.

$$\rho(L_h) \approx .66\frac{q^2}{h}$$

Example: elastic wave equation (isotropic medium - not necessary!)

$$G = \frac{1}{\rho}\left(\lambda\theta^2 + \mu\left(e_{11}^2 + e_{22}^2 + e_{33}^2 + 2e_{12}^2 2 + 2e_{23}^2 + 2e_{13}^2\right)\right)$$

where

$$\theta = \nabla \cdot u, \quad e_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}.$$

Now we need not only additional equations corresponding to constant states (translational symmetries) but also to rotations since now there are nonconstant fields for which $G = 0$.

$$\int_{\Omega_j} \left(\frac{\partial^2 u_1}{\partial x_2 \partial t} - \frac{\partial^2 u_1}{\partial x_1 \partial t}\right) - \left(\frac{\partial v_1}{\partial x_2} - \frac{\partial v_2}{\partial x_1}\right) = 0$$

Some movies - examples with free surface boundary conditions. Due to their small dispersion errors DG schemes do not degrade appreciably in this case as finite difference methods are known to do. We also show scattering from stiff inclusions.

Nonlinear problems: here we must replace the integrals with quadratures. Then again we can prove energy estimates. Note that the mass matrix is still linear.

Nonlinear second order wave equations often form singularities just as nonlinear hyperbolic conservation laws do. **A**n interesting open problem in general is what sort of admissibility conditions are physically correct and what needs to be true for a numerical method to converge to these. Recently Bressan and coworkers have developed uniqueness results for energy conserving weak solutions, but dissipative weak solutions also exist - it is unclear if these are the ones we want. However with our upwind schemes we can certainly run the code and show the pictures!

As an example we consider a model for the dynamics of the director field of a nematic liquid crystal described by a restriction of the Oseen-Frank potential, which follows the general framework with

$$G = \left(\alpha \cos^2 u + \beta \sin^2 u\right) u_x^2.$$

Here the director field is $\cos u e_x + \sin u e_y$.

The model is analyzed by Hunter and Saxton SIAM J. Appl. Math. (1991). They introduce a weakly nonlinear asymptotic model for which there is always breakdown - blowup of derivatives but continuity of u (no shocks) - and suggest simple admissible solutions of it, with explicit constructions of energy-conserving and energy-dissipating weak solutions. We solve as above with $q = 8$ and see what happens as smoothness is lost.