Discontinuous Galerkin methods and applications in computational fluid dynamics: survey and recent developments

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Outline

- Introduction to DG methods and CFD applications
- Positivity-preserving high order DG methods: explicit and implicit time discretizations
- Concluding remarks

Introduction to DG methods and CFD applications

The original discontinuous Galerkin (DG) methods were designed to solve hyperbolic conservation laws. We concentrate on time-dependent partial differential equations (PDEs) in this lecture. In 1D the conservation law is

$$u_t + f(u)_x = 0$$

and in the system case u is a vector, and the Jacobian $f'(u)$ is diagonalizable with real eigenvalues.

In 2D the equation is

$$u_t + f(u)_x + g(u)_y = 0.$$

Several properties of the solutions to hyperbolic conservation laws:

- The solution u may become discontinuous regardless of the smoothness of the initial condition.
- Weak solutions are not unique. The unique, physically relevant entropy solution satisfies additional entropy inequalities

$$U(u)_t + F(u)_x \leq 0$$

in the distribution sense, where $U(u)$ is a convex scalar function of u and the entropy flux $F(u)$ satisfies $F'(u) = U'(u)f'(u)$.

To solve the hyperbolic conservation law:

$$u_t + f(u)_x = 0, \tag{1}$$

we multiply the equation with a test function v, integrate over a cell $I_j = [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$, and integrate by parts:

$$\int_{I_j} u_t v dx - \int_{I_j} f(u) v_x dx + f(u_{j+\frac{1}{2}}) v_{j+\frac{1}{2}} - f(u_{j-\frac{1}{2}}) v_{j-\frac{1}{2}} = 0$$

Now assume both the solution u and the test function v come from a finite dimensional approximation space V_h, which is usually taken as the space of piecewise polynomials of degree up to k:

$$V_h = \left\{ v : v|_{I_j} \in P^k(I_j),\ j = 1, \cdots, N \right\}$$

However, the boundary terms $f\left(u_{j+\frac{1}{2}}\right)$, $v_{j+\frac{1}{2}}$ etc. are not well defined when u and v are in this space, as they are discontinuous at the cell interfaces.

From the conservation and stability (upwinding) considerations, we take

- A single valued monotone numerical flux to replace $f\left(u_{j+\frac{1}{2}}\right)$:

$$\hat{f}_{j+\frac{1}{2}} = \hat{f}(u^-_{j+\frac{1}{2}}, u^+_{j+\frac{1}{2}})$$

  where $\hat{f}(u,u) = f(u)$ (consistency); $\hat{f}(\uparrow,\downarrow)$ (monotonicity) and $\hat{f}$ is Lipschitz continuous with respect to both arguments.

- Values from inside I_j for the test function v

$$v^-_{j+\frac{1}{2}}, \qquad v^+_{j-\frac{1}{2}}$$

Hence the DG scheme is: find $u \in V_h$ such that

$$\int_{I_j} u_t v dx - \int_{I_j} f(u) v_x dx + \hat{f}_{j+\frac{1}{2}} v^-_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} v^+_{j-\frac{1}{2}} = 0 \qquad (2)$$

for all $v \in V_h$.

Time discretization could be by the TVD Runge-Kutta method (Shu and Osher, JCP 88). For the semi-discrete scheme:

$$\frac{du}{dt} = L(u)$$

where $L(u)$ is a discretization of the spatial operator, the third order TVD Runge-Kutta is simply:

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n) \\ u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}) \\ u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}) \end{aligned}$$

Properties and advantages of the DG method:

- Easy handling of complicated geometry and boundary conditions (common to all finite element methods). Allowing hanging nodes in the mesh (unique to DG).
- Compact. Communication only with immediate neighbors, regardless of the order of the scheme.
- Explicit. Because of the discontinuous basis, the mass matrix is local to the cell, resulting in explicit time stepping (no systems to solve).

- Parallel efficiency. Achieves 99% parallel efficiency for static mesh and over 80% parallel efficiency for dynamic load balancing with adaptive meshes (Biswas, Devine and Flaherty, ANM 94; Remacle, Flaherty and Shephard, SIAM Rev 03; Beck, Bolemann, Flad, Frank, Gassner, Hindenlang and Munz, IJNMF 14; Atak, Beck, Bolemann, Flad, Frank, Hindenlang and Munz, High Performance Computing in Science and Engineering 14, Springer 15). Also friendly to GPU (Klockner et al, JCP10).

- Provable cell entropy inequality and L^2 stability, for arbitrary nonlinear equations in any spatial dimension and any triangulation, for any polynomial degrees, without limiters or assumption on solution regularity (Jiang and Shu, Math. Comp. 94 (scalar case); Hou and Liu, JSC 07 (symmetric systems)). For $U(u) = \frac{u^2}{2}$:

$$\frac{d}{dt}\int_{I_j} U(u)dx + \hat{F}_{j+1/2} - \hat{F}_{j-1/2} \leq 0$$

Summing over j: $\frac{d}{dt}\int_a^b u^2 dx \leq 0.$

This also holds for fully discrete RKDG methods with third order TVD Runge-Kutta time discretization, for linear equations (Zhang and Shu, SINUM 10). Also for other entropy (Chen and Shu, JCP 17; Liu, Shu and Zhang, JCP18).

- Optimal or near optimal error estimates for smooth solutions, or in smooth regions for piecewise smooth solutions, also various superconvergence results.
- For strong shocks, nonlinear limiters are needed to control spurious oscillations. Recently, a particularly simple weighted essentially non-oscillatory (WENO) limiter has been designed, which uses information only from immediate neighboring cells and hence does not destroy the local property of the original DG schemes. See Zhong and Shu, JCP13 (structured meshes); Zhu, Zhong, Shu and Qiu, JCP 13 (unstructured meshes); Zhu, Zhong, Shu and Qiu, CiCP 16 (improved); Zhu, Zhong, Shu and Qiu, CiCP 17 (improved, unstructured).

- Bound preserving limiters, which can preserve strict maximum principle for scalar equations and positivity of relevant physical quantities (e.g. density and pressure for Euler systems for gas dynamics and water height for shallow water equations) while maintaining the original high order accuracy of the DG schemes, have been designed in a series of papers (Zhang and Shu, SINUM 10 (TVD); JCP 10 (scalar); JCP 11 (Euler), JCP 11b (source term); Proc Roy Soc A 11 (survey); Num Math 12 (entropy); Xing, Zhang and Shu, Adv Water Res 10 (shallow water); Zhang, Xia and Shu, JSC 12 (unstructured mesh); Wang et al, JCP 12 (detonations); Qin, Shu and Yang, JCP 16 (relativistic hydrodynamics); Vila, Shu and Maire, JCP 16, JCP 16b (Lagrangian multi-material flows); Yuan, Cheng and Shu, SISC 16 (radiative transfer); Qin and Shu, SISC to appear (implicit time discretization)).

- Easy h-p adaptivity.
- Stable and convergent DG methods are now available for many nonlinear PDEs containing higher derivatives: convection diffusion equations, KdV equations, ...

Examples

We show a couple of examples to demonstrate the excellent performance of the DG method.

The first example is a variable coefficient scalar equation for the front propagation problem (level set equation). The solution u at $t = 0$ has a 0-level set which is the x axis. The front evolves up to time $t = T/2$ then it comes back to the initial data at time $t = T$. $T/2$ represents the number of turns. Computations have been done up to time $T = 10$, using P^4 and a coarse 24×24 mesh cells. See Bokanowski, Cheng and Shu, SISC 11.

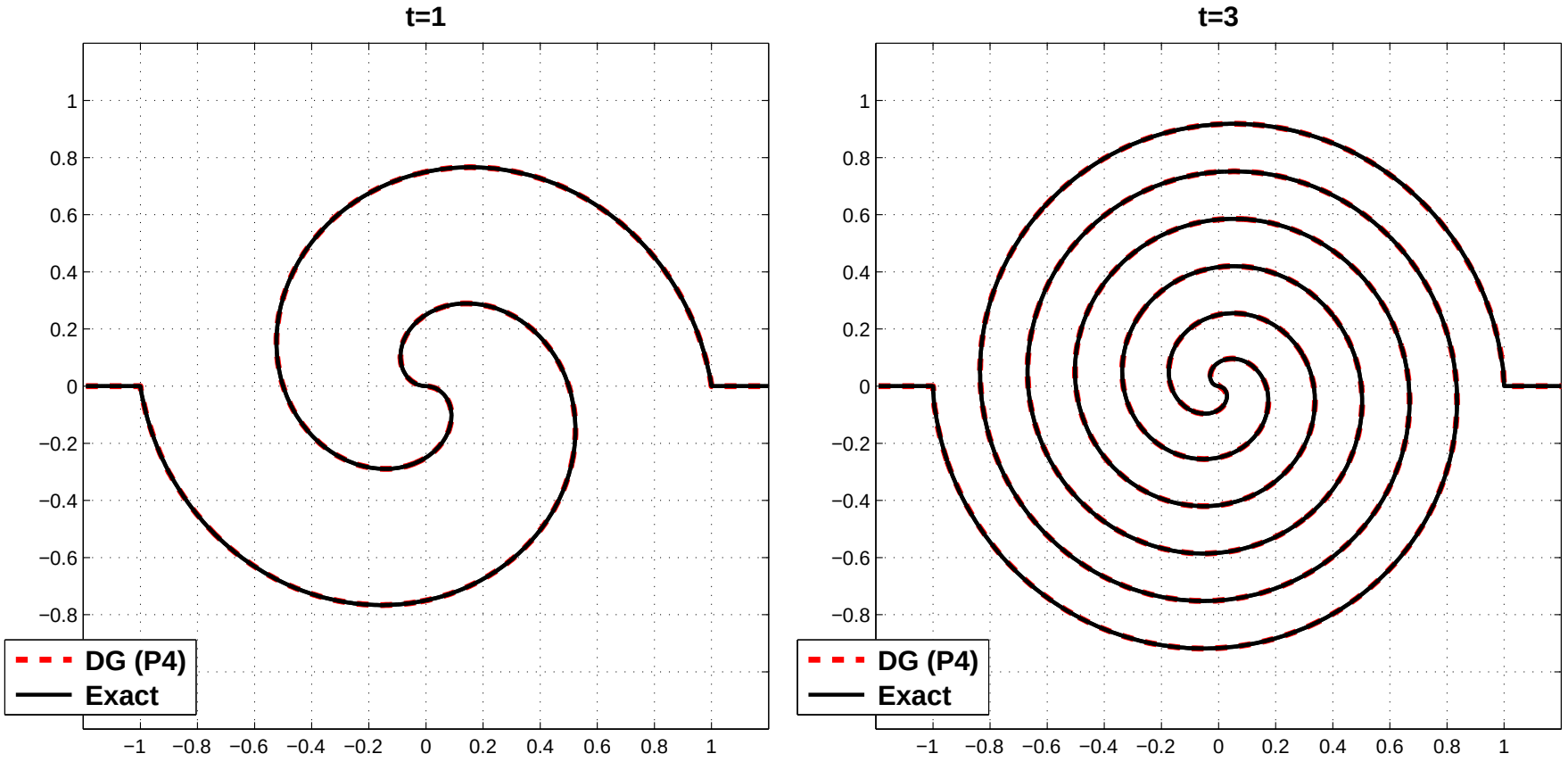


Figure 1: Plots at times $t = 1$ and $t = 3$ with P^4 and 24×24 mesh cells.

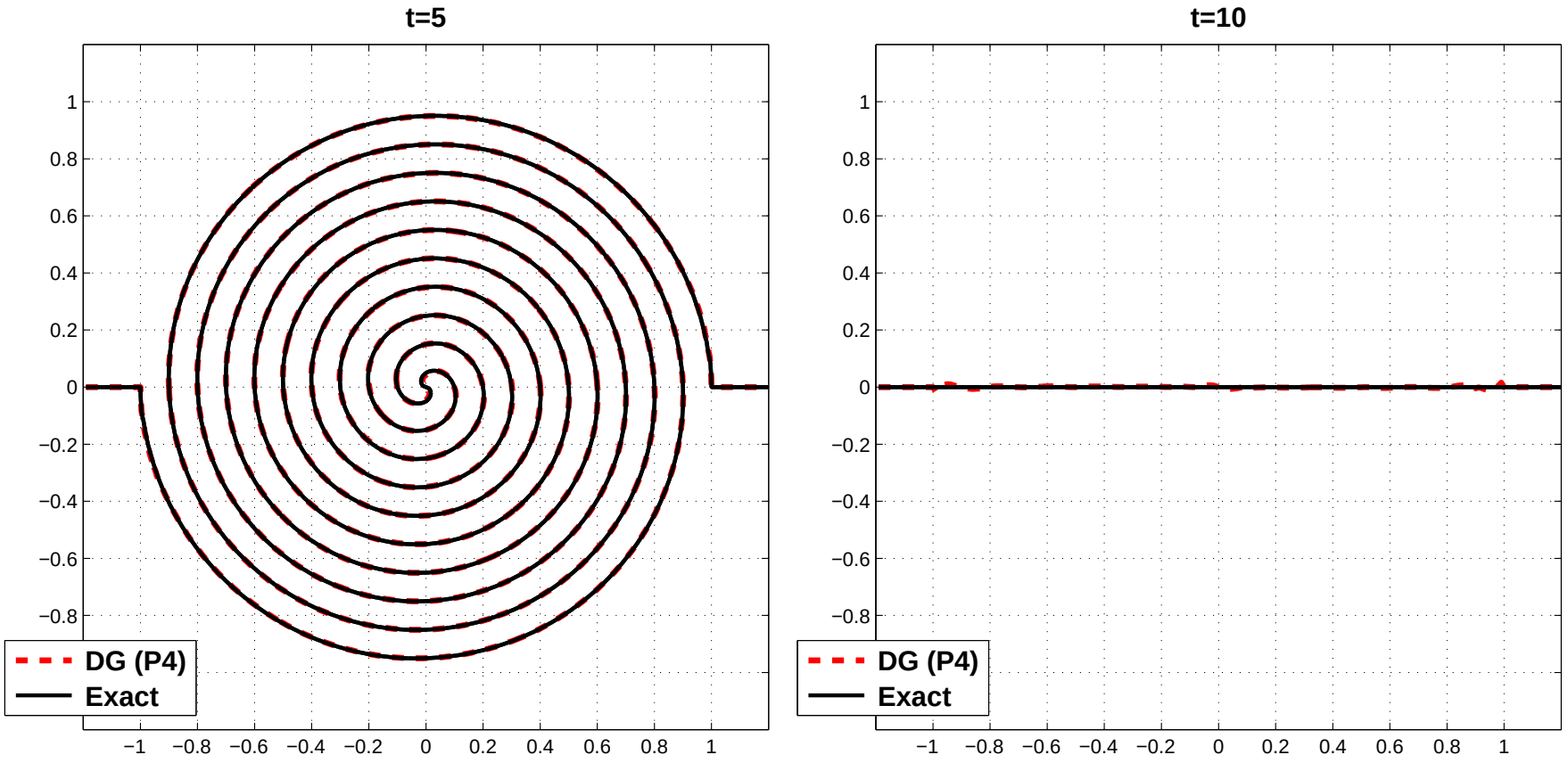


Figure 2: Plots at times $t = 5$ and $t = 10$ (return to initial data), with P^4 and 24×24 mesh cells.

The second example is the pressureless Euler equations. For such equations density can evolve into δ-functions from smooth or bounded initial conditions. Our DG algorithm in Yang, Wei and Shu, JCP 13) is high-order, positivity-preserving for density, and L^1 stable.

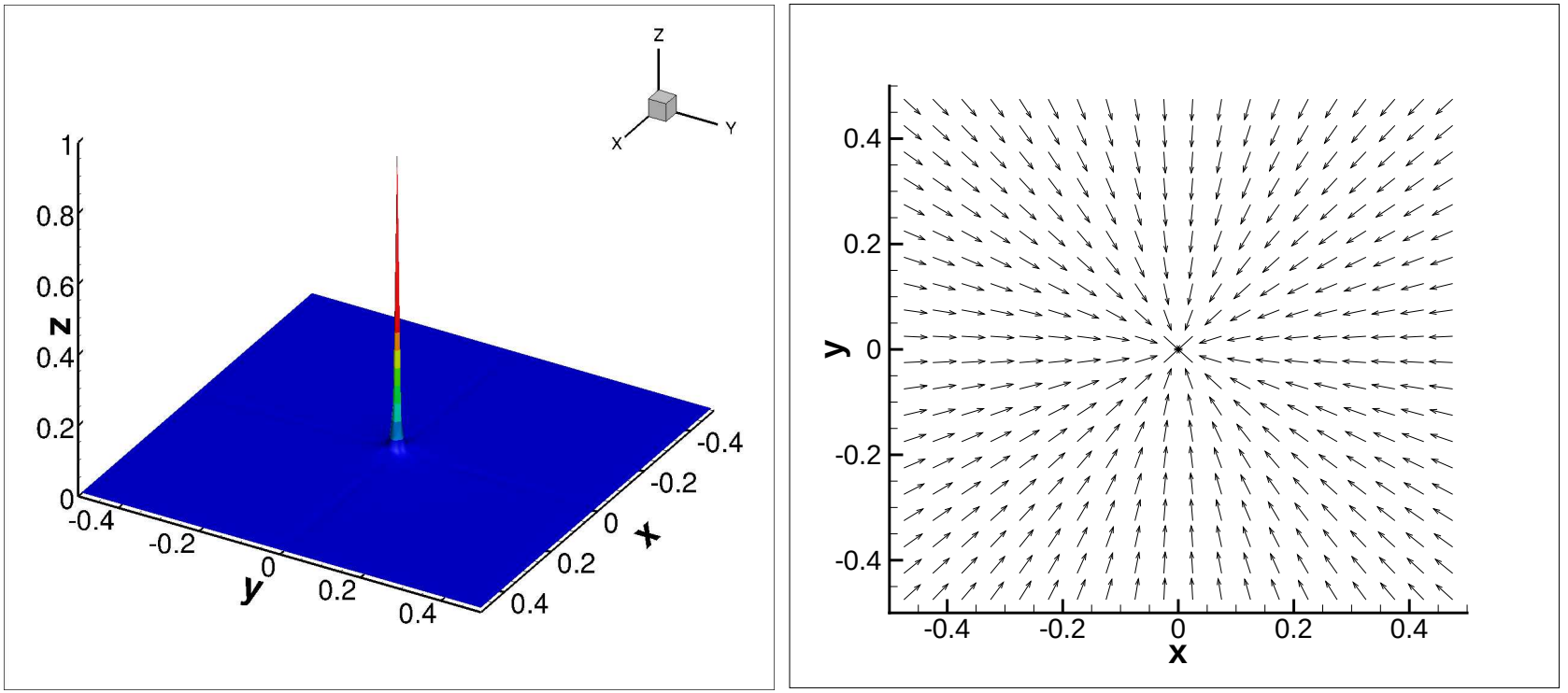


Figure 3: Numerical density (left) and velocity field (right) at $t = 0.5$ for the example of a single δ at origin.

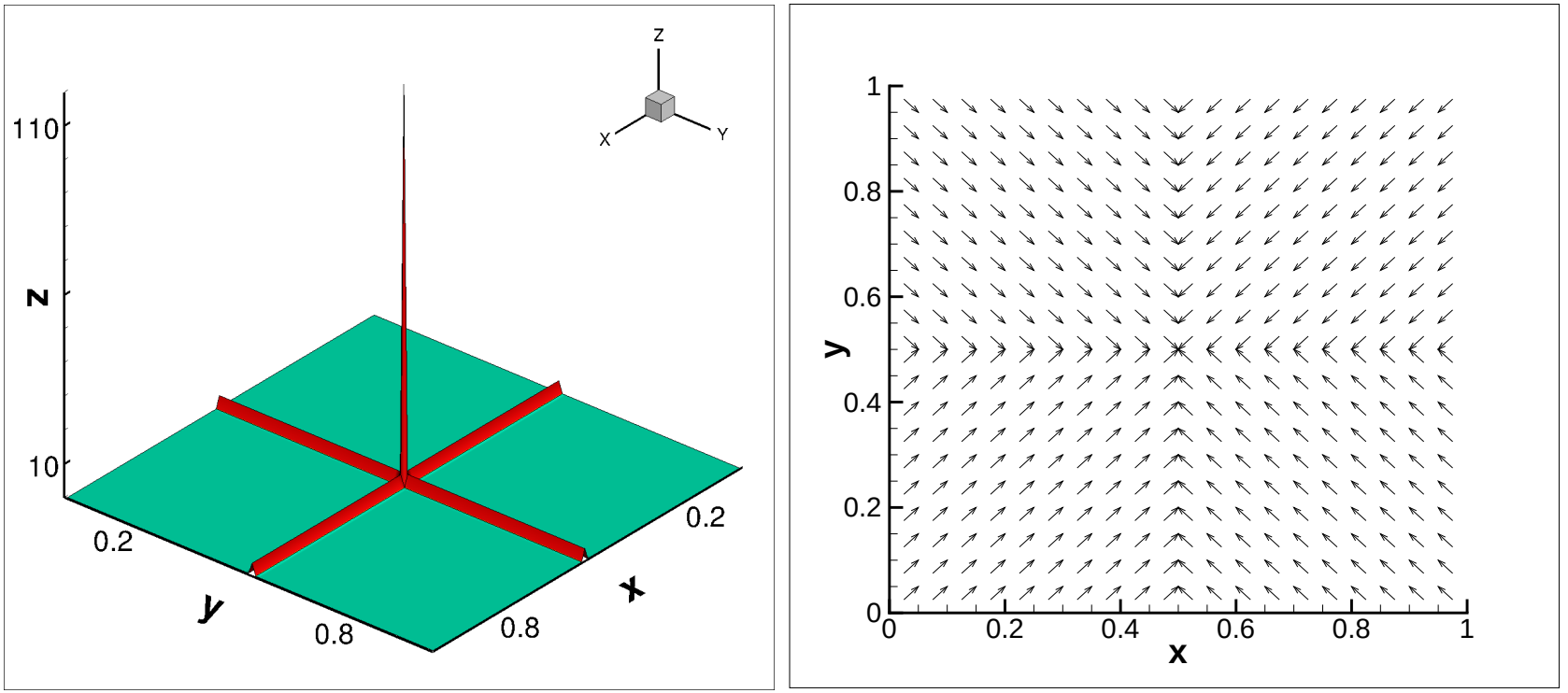


Figure 4: Numerical density (left) and velocity field (right) at $t = 0.5$ for the example of δ-singularities located at the origin and the two axes.

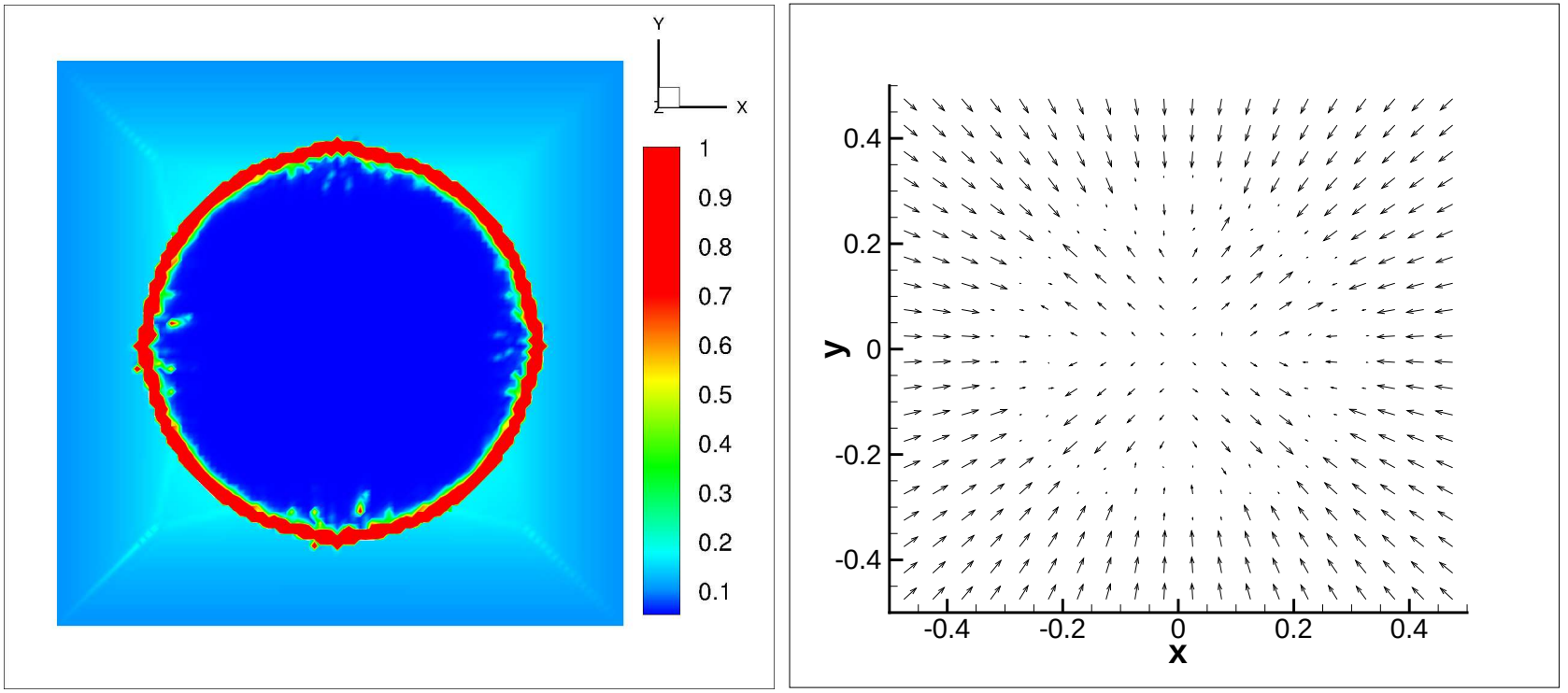


Figure 5: Numerical density (left) and velocity field (right) at $t = 0.5$ for the example with δ-shocks located on a circle and vacuum inside.

Positivity-preserving high order DG methods

We assume the exact solution of the PDE has a convex invariant region G:

- If $u(\cdot, 0) \in G$, then $u(\cdot, t) \in G$ for all $t > 0$.

For a convex region G, if $u_1, \cdots, u_m \in G$, $\alpha_i \geq 0$, $\sum_{i=1}^{m} \alpha_i = 1$, then $u = \sum_{i=1}^{m} \alpha_i u_i \in G$. We will heavily use this property when building our high order bound-preserving schemes.

Several examples:

- For a scalar conservation law, an important property of the entropy solution (which may be discontinuous) is that it satisfies a strict maximum principle: If

$$M = \max_{\mathbf{x}} u_0(\mathbf{x}), \quad m = \min_{\mathbf{x}} u_0(\mathbf{x}), \tag{3}$$

  then $u(\mathbf{x}, t) \in [m, M]$ for any $\mathbf{x}$ and t.

  Therefore, $G = [m, M]$ is an invariant region. It is clearly convex.

- For the compressible Euler equations:

$$u_t + f(u)_x = 0$$

with

$$u = \begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix}, \qquad f(u) = \begin{pmatrix} \rho v \\ \rho v^2 + p \\ v(E+p) \end{pmatrix},$$

where $E = e + \frac{1}{2}\rho v^2$. The internal energy e is related to density and pressure through the equation of states (EOS). For the ideal gas, we have $e = \frac{p}{\gamma - 1}$ with $\gamma = 1.4$ for air.

In this case, we can verify that the set

$$G = \{u : \rho \geq 0, e \geq 0\} \tag{4}$$

is invariant. It is also easy to check that G is convex (for this we need to check that the internal energy e is a concave function of the conservative variable u, then Jensen's inequality implies the convexity of G).

For many EOS, e.g. that for the ideal gas, the region G defined in (4) is equivalent to

$$G = \{u : \rho \geq 0, p \geq 0\}.$$

Framework for explicit time stepping

It is of course desirable to have the invariant region G also to be an invariant region for the numerical solution. That is, we wish that, if the initial condition $u(\cdot, 0) \in G$ then $u(\cdot, t) \in G$ for later time $t > 0$. This time u stands for the numerical solution.

We first review a framework to achieve this under explicit time stepping. The framework consists of the following ingredients:

- We start with a first order scheme which can be proved to be bound preserving under a certain CFL condition

$$\lambda = \frac{\Delta t}{\Delta x} \leq \lambda_0.$$

For example, for the scalar conservation laws

$$u_t + f(u)_x + g(u)_y = 0,$$

the first order monotone schemes satisfy maximum principles; for Euler equations of compressible gas dynamics, many first order schemes, including Godunov, Lax-Friedrichs, kinetic and HLLC schemes are proved to be positivity-preserving for density and internal energy.

We emphasize that sometimes it is already non-trivial to find first order schemes which are bound-preserving, e.g. for MHD equations. Since our high order bound-preserving schemes discussed later are built upon first order bound-preserving schemes, the very first task when one would like to solve a new PDE is to find a first order bound-preserving scheme.

- We will call a high order finite volume or DG scheme bound-preserving, if we have

$$m \leq u^{n+1}(x) \leq M, \qquad \forall x$$

provided

$$m \leq u^{n}(x) \leq M, \qquad \forall x.$$

Here $u^n(x)$ refers to the piecewise polynomial numerical solution, either reconstructed in a finite volume scheme or evolved for a DG scheme.

A suitable modification to evaluate the bounds only at certain quadrature points will be given later to facilitate easy implementation.

The flowchart for designing a high order finite volume or DG bound-preserving scheme (we use maximum principle in scalar case below as an example) is as follows:

1. Start with $u^n(x)$ which is high order accurate

$$|u(x,t^n) - u^n(x)| \leq C\Delta x^p$$

and satisfies

$$m \leq u^n(x) \leq M, \qquad \forall x$$

therefore of course we also have

$$m \leq \bar{u}_j^n \leq M, \qquad \forall j.$$

2. Evolve for one time step to get

$$m \leq \bar{u}_j^{n+1} \leq M, \qquad \forall j. \tag{5}$$

   This is usually the most difficult step, since it must be proved for the unmodulated scheme.

3. Given (5) above, use a simple scaling limiter to obtain $u^{n+1}(x)$ (reconstruction or evolution) which
   - satisfies the maximum principle

$$m \leq u^{n+1}(x) \leq M, \qquad \forall x;$$

   - is high order accurate

$$|u(x, t^{n+1}) - u^{n+1}(x)| \leq C\Delta x^p.$$

In Zhang and Shu, JCP 2010a, a procedure is designed to obtain

$$m \leq \bar{u}_j^{n+1} \leq M, \qquad \forall j$$

with simple Euler forward or SSP Runge-Kutta or multi-step methods using the unmodulated finite volume or DG scheme.

Now, given

$$m \leq \bar{u}_j^{n+1} \leq M, \qquad \forall j$$

for the unmodulated finite volume or DG scheme, again in Zhang and Shu, JCP 2010a, a procedure is designed to obtain a bound-preserving $u^{n+1}(x)$ with a very simple scaling limiter, which only requires the evaluation of unmodulated $u^{n+1}(x)$ at certain pre-determined quadrature points and does not destroy accuracy:

We replace $p_j(x)$ by the limited polynomial $\tilde{p}_j(x)$ defined by

$$\tilde{p}_j(x) = \theta_j(p_j(x) - \bar{u}_j^n) + \bar{u}_j^n$$

where

$$\theta_j = \min\left\{ \left| \frac{M - \bar{u}_j^n}{M_j - \bar{u}_j^n} \right|, \left| \frac{m - \bar{u}_j^n}{m_j - \bar{u}_j^n} \right|, 1 \right\},$$

with

$$M_j = \max_{x \in S_j} p_j(x), \qquad m_j = \min_{x \in S_j} p_j(x)$$

where S_j is the set of Legendre Gauss-Lobatto quadrature points of cell I_j. Clearly, this limiter is just a simple scaling of the original polynomial around its average.

The following lemma, guaranteeing the maintenance of accuracy of this simple limiter, is proved in Zhang and Shu, JCP 2010a:

Lemma: Assume $\bar{u}_j^n \in [m, M]$ and $p_j(x)$ is an $O(\Delta x^p)$ approximation, then $\tilde{p}_j(x)$ is also an $O(\Delta x^p)$ approximation.

We have thus obtained a high order accurate scheme satisfying the following maximum principle: If

$$m \leq u^n(x) \leq M, \qquad \forall x \in S_j,$$

then

$$m \leq u^{n+1}(x) \leq M, \qquad \forall x \in S_j.$$

Recall that S_j is the set of Legendre Gauss-Lobatto quadrature points of cell I_j.

Clearly, the framework easily generalizes to 2D (or higher dimensions) in structured or unstructured meshes, and to high order time accuracy through explicit SSP (also called TVD) Runge-Kutta or multi-step time discretizations.

Implicit time stepping

Many first order implicit schemes (e.g. for scalar equations, first order monotone schemes with backward Euler time discretization) can be proved to be unconditionally bound-preserving. Unfortunately, this does not easily generalize to higher order schemes.

In (Qin and Shu, SISC to appear), we have developed a general framework to obtain high order bound-preserving finite volume or DG schemes with backward Euler time discretization, which consists of the following ingredients:

- We first establish the following property:

  Property: If the numerical solution $u^n(x)$ is within the desired bounds at the Gauss-Lobatto quadrature points, then the cell averages $\bar{u}_j^{n+1}$ of the numerical solution for the unmodulated high order finite volume or DG scheme is within the desired bounds under the following lower bound of the CFL condition

$$\lambda \geq \lambda_0. \tag{6}$$

  This property is rigorously proved for the linear equations and demonstrated numerically for nonlinear equations including Euler equations of compressible gas dynamics.

- Given that the cell averages $\bar{u}_j^{n+1}$ of the numerical solution for the unmodulated high order finite volume or DG scheme is within the desired bounds, we may use the same scaling limiter as described above to obtain a high order accurate solution $u^{n+1}(x)$ (without changing the cell averages) within the desired bounds at the Gauss-Lobatto quadrature points.

Unlike in the explicit case, here the lower bound in (6) actually improves (becomes smaller) with higher order of accuracy:

Table 1: Values of λ_0 for polynomial degrees $k = 1, \ldots, 5$ in the finite volume or DG scheme, and for Legendre-Gauss-Lobatto (LGL) and Legendre-Gauss quadrature rules respectively.

	LGL rule		LG rule	
k	N_q	λ_0	N_q	r^k
1	3	0.333	2	0.333
2	4	0.262	3	0.344
3	5	0.177	4	0.177
4	6	0.177	5	0.212
5	7	0.121	6	0.121

Example 1. Steady-state solution to Burgers' problems.

Table 2: Error table for the approximation of the steady state solution to the Burgers' equation without the positivity preserving limiter.

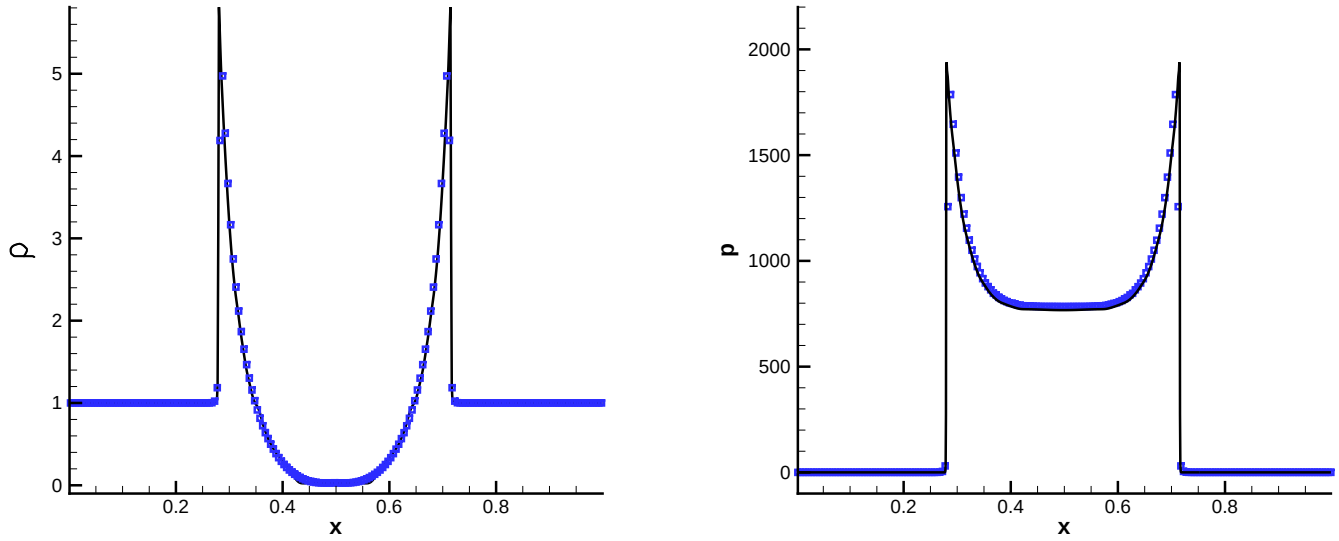
k	N	L^2 error	order	L^∞ error	order	$\min u_h$
2	20	2.915 E-6	–	5.085 E-6	–	-8.073 E-6
	40	3.508 E-7	3.05	6.358 E-7	3.00	-1.009 E-6
	80	4.293 E-8	3.03	7.948 E-8	3.00	-1.261 E-7
	160	5.304 E-9	3.02	9.934 E-9	3.00	-1.577 E-8
3	20	2.336 E-9	–	1.648 E-9	–	-3.855 E-10
	40	1.445 E-10	4.02	1.030 E-10	4.00	-1.204 E-11
	80	9.010 E-11	4.00	6.525 E-11	3.98	-3.763 E-13
	160	6.031 E-12	3.90	4.978 E-12	3.71	-1.175 E-14
4	20	3.403 E-10	–	6.312 E-10	–	-1.497 E-9
	40	1.010 E-11	5.07	1.970 E-11	5.00	-4.678 E-11
	80	3.116 E-13	5.02	5.398 E-13	5.19	-1.462 E-12

Table 3: Error table for the approximation of the steady state solution to the Burgers' equation with the positivity preserving limiter.

k	N	L^2 error	order	L^∞ error	order	$\min u_h$
2	20	3.207 E-6	–	4.408 E-6	–	1.000 E-13
	40	3.696 E-7	3.12	6.010 E-7	2.87	1.000 E-13
	80	4.435 E-8	3.06	8.171 E-8	2.88	1.000 E-13
	160	5.414 E-9	3.03	1.083 E-8	2.92	1.000 E-13
3	20	2.338 E-9	–	1.648 E-9	–	1.000 E-13
	40	1.445 E-10	4.02	1.030 E-10	4.00	1.000 E-13
	80	9.010 E-11	4.00	6.511 E-11	3.98	1.000 E-13
	160	6.031 E-12	3.90	4.987 E-12	3.71	1.051 E-14
4	20	4.792 E-10	–	9.061 E-10	–	1.000 E-13
	40	1.253 E-11	5.26	3.102 E-11	4.87	1.000 E-13
	80	3.653 E-13	5.10	1.086 E-12	4.84	1.000 E-13

Example 2. Sedov point-blast wave.

Initially the gas is steady with uniform density one in the whole domain. The pressure is set to be $p = 10^{-9}$, except in the central cell, where the pressure is as high as $p = 10^4$. Then a blast-wave starts to propagate from the central cell with a shock front. In Figure 6 we present the numerical approximation and the exact solution for the pressure and density respectively. The positivity-preserving limiter not only helps keep the low-density region positive, but also add robustness to the nonlinear solver. Without it, the code breaks down due to the failure of convergence of the nonlinear solver.



(a) density (b) Pressure

Figure 6: Sedov point-blast wave. $T = 0.003$, with $N = 200$ and $CFL = 2$. With the positivity-preserving limiter on. Solid line is the exact solution and blue squares are the numerical approximations.

Conclusions and future work

- Discontinuous Galerkin (DG) methods are very flexible to geometry, boundary condition and h-p adaptivity.
- Stable and accurate DG methods can be designed for a wide spectrum of PDEs including conservation laws and convection dominated convection-diffusion equations and dispersive wave equations.
- We have designed bound-preserving high order DG schemes for both explicit and implicit time discretizations.

- Future research is needed for the design of stable DG methods for more nonlinear PDEs in applications, for efficient time discretization (preconditioning, multigrid, exponential type time discretization, deferred correction, ...), for a posteriori error estimates to guide adaptivity, and for more general bound-preserving DG methods.

THANK YOU!