

Entropy stable high order discontinuous Galerkin methods for nonlinear conservation laws

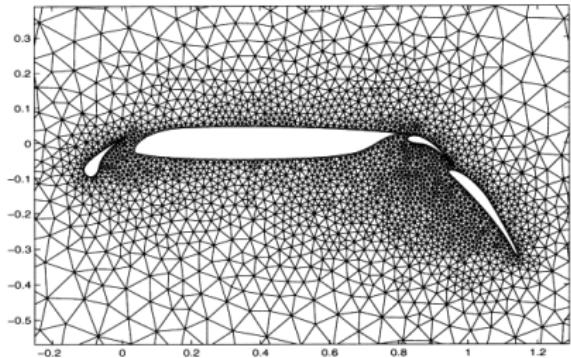
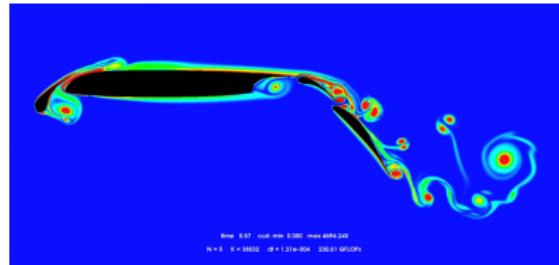
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October 22, 2018

High order finite element methods for hyperbolic PDEs

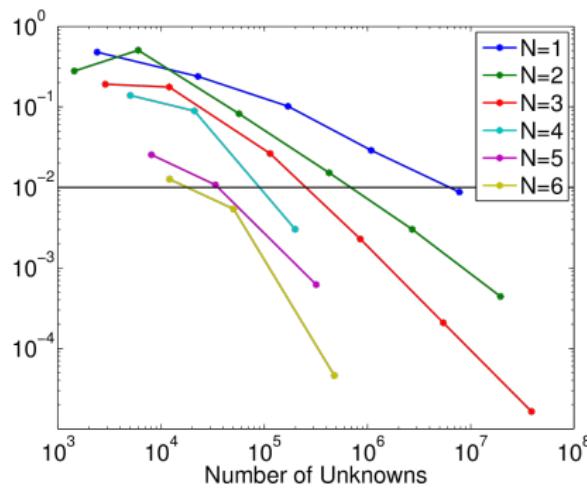
- Focus: **high accuracy** computational mechanics on **complex geometries**.
- Applications in fluid dynamics (waves, vorticular flows, turbulence, shocks).
- High order approximations are more accurate per unknown.
- High performance computing on many-core architectures (efficient explicit time-stepping).



Mesh from Slawig 2001.

High order finite element methods for hyperbolic PDEs

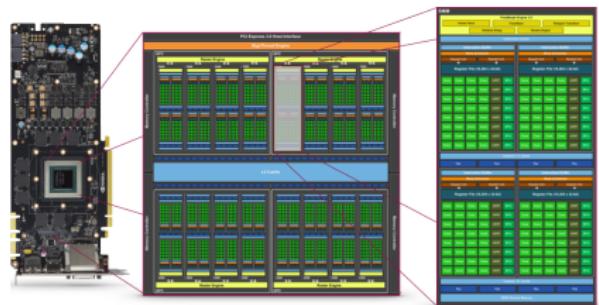
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For smooth solutions, high order methods deliver a lower error per degree of freedom.

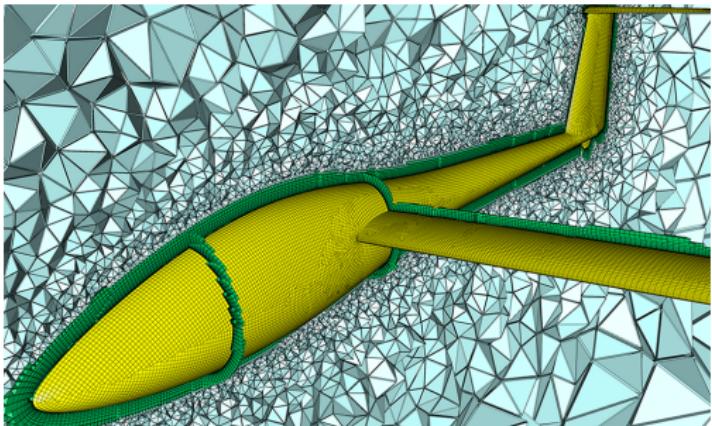
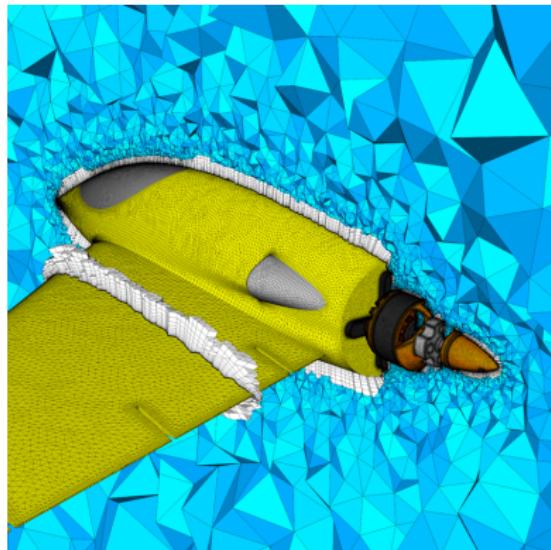
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Schematic of an NVIDIA graphics processing unit (GPU).

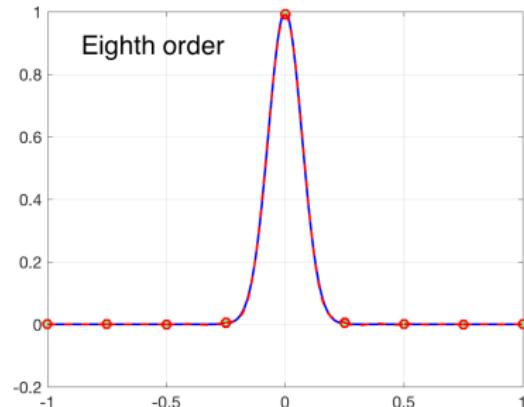
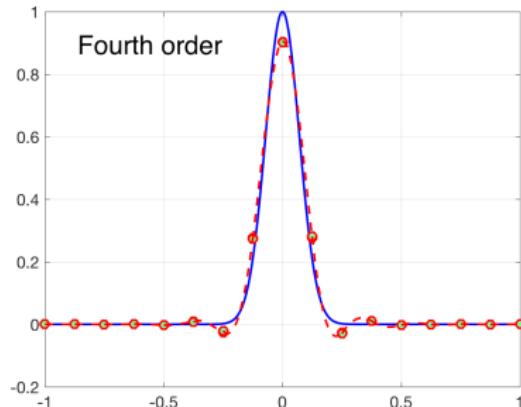
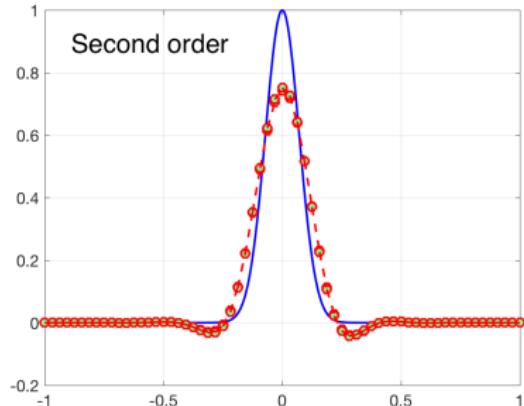
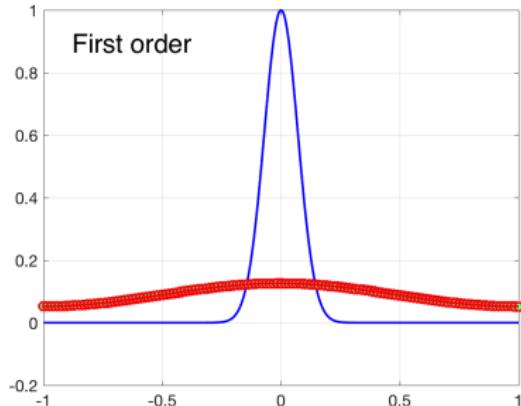
Why finite elements? General unstructured meshes



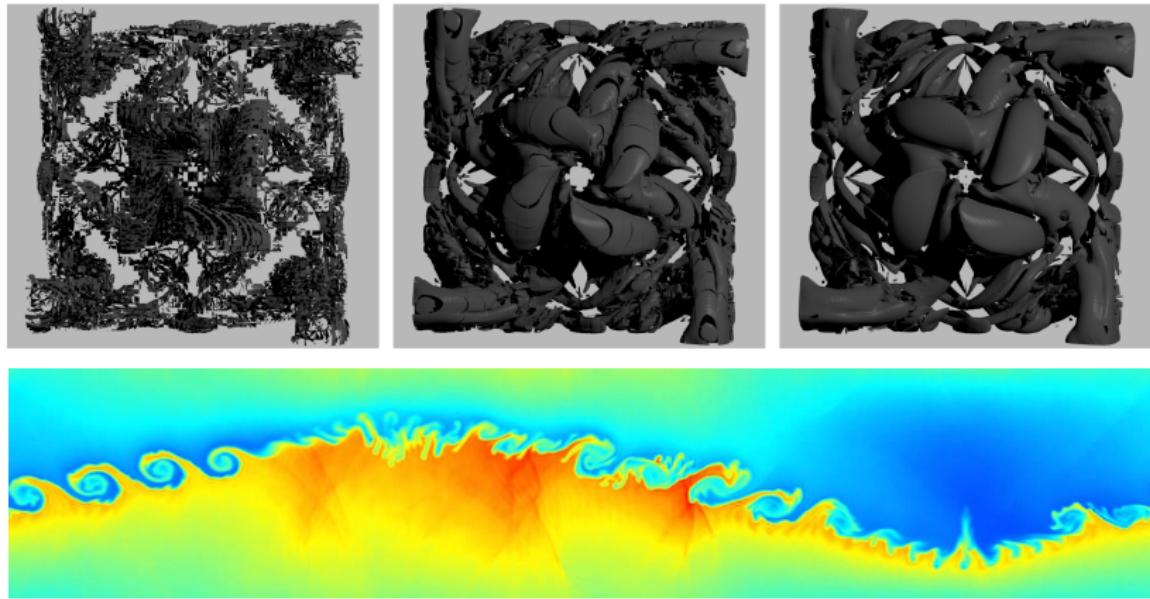
DG methods are compatible with unstructured meshes containing different types of elements (tetrahedra, hexahedra most common, but also prisms and pyramids).

Figures courtesy of Pointwise Inc (<https://www.pointwise.com>).

Why high order? Low numerical dissipation



Why high order? Low numerical dissipation



2nd, 4th, and 16th order Taylor-Green (top), 8th order Kelvin-Helmholtz (bottom).

Beck, Gassner (2012). *Numerical Simulation of the Taylor-Green Vortex at $Re=1600$ with the Discontinuous Galerkin Spectral Element Method for well-resolved and underresolved scenarios*

Peraire, Persson (2010). *High-Order Discontinuous Galerkin Methods for CFD*

Talk outline

- 1 Stability of high order DG: linear vs nonlinear PDEs
- 2 Summation by parts finite differences and high order DG
- 3 Entropy stable formulations and flux differencing
- 4 Numerical experiments
 - 1D experiments
 - Triangular and tetrahedral meshes
 - Quadrilateral and hexahedral meshes

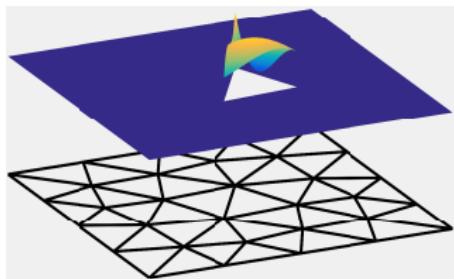
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Basics of discontinuous Galerkin methods

Discontinuous Galerkin (DG) methods:

- High order accuracy, geometric flexibility.
- Weak continuity across faces.
- Continuous PDE (example: advection)



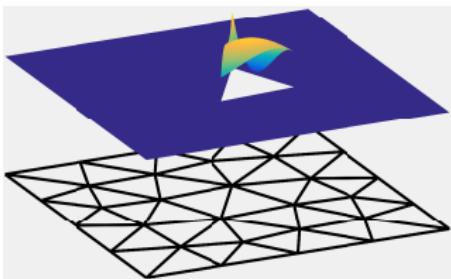
- Local DG form with numerical flux \mathbf{f}^* : find $u \in P^N(D^k)$ such that

$$\int_{D_k} \frac{\partial u}{\partial t} \phi = \int_{D_k} \frac{\partial f(u)}{\partial x} \phi + \int_{\partial D_k} \mathbf{n} \cdot (\mathbf{f}^* - \mathbf{f}(u)) \phi, \quad \forall \phi \in P^N(D^k).$$

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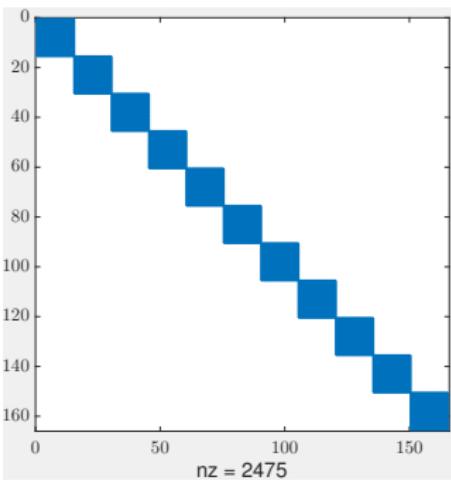
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DG in space yields system of ODEs

$$\mathbf{M}_\Omega \frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u}.$$

DG mass matrix decouples across elements,
inter-element coupling only through \mathbf{A} .



DG is semi-discretely energy stable for linear advection

- Linear periodic advection on $[-1, 1]$

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad u(-1) = u(1), \quad \Rightarrow \frac{\partial}{\partial t} \|u\|_{L^2([-1,1])}^2 = 0.$$

- DG numerical “penalty” flux, where $\llbracket u \rrbracket = u^+ - u^-$ and $\tau \geq 0$.

$$\sum_k \int_{D^k} \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} \right) v \, dx + \frac{1}{2} \int_{\partial D^k} (\llbracket u \rrbracket n_x + \tau \llbracket u \rrbracket) v \, dx = 0.$$

- Energy estimate: take $v = u$, chain rule in time, **integrate by parts**.

$$\sum_k \frac{\partial}{\partial t} \|u\|_{D^k}^2 \leq - \sum_k \frac{\tau}{2} \int_{\partial D^k} \llbracket u \rrbracket^2 \, dx.$$

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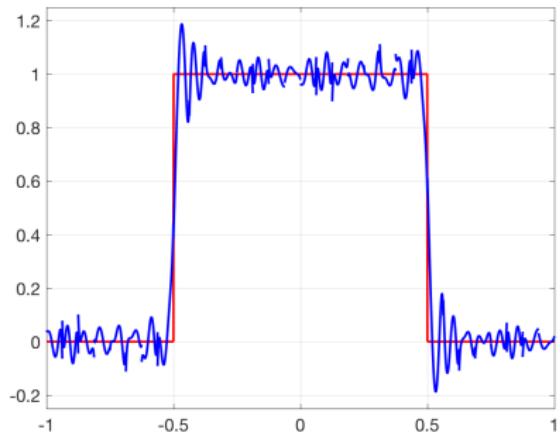
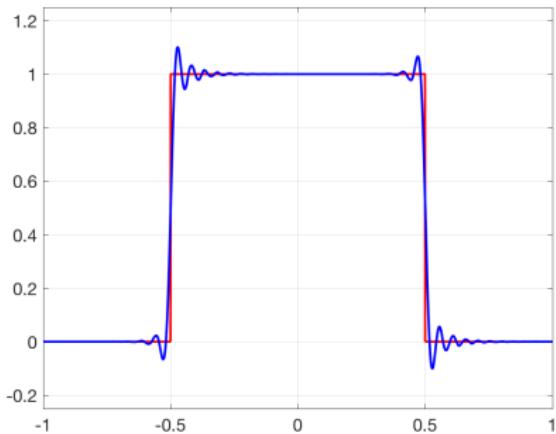
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Energy conservative vs. energy stable DG methods

- Energy estimate: implies $\|u\|$ is non-increasing if $\tau \geq 0$.
- Energy conservative (non-dissipative) “central” flux when $\tau = 0$.
- Energy stable (dissipative) “Lax-Friedrichs” flux when $\tau = 1$.

(a) Energy conservative ($\tau = 0$)(b) Energy stable ($\tau = 1$)

Generalization to nonlinear problems: entropy stability

- Generalizes energy stability to **nonlinear** systems of conservation laws (Burgers', shallow water, compressible Euler, MHD).

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0.$$

- Continuous entropy inequality: given a convex **entropy** function $S(\mathbf{u})$ and “entropy potential” $\psi(\mathbf{u})$,

$$\begin{aligned} \int_{\Omega} \mathbf{v}^T \left(\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} \right) = 0, \quad \mathbf{v} = \frac{\partial S}{\partial \mathbf{u}} \\ \implies \int_{\Omega} \frac{\partial S(\mathbf{u})}{\partial t} + \left(\mathbf{v}^T \mathbf{f}(\mathbf{u}) - \psi(\mathbf{u}) \right) \Big|_{-1}^1 \leq 0. \end{aligned}$$

- Proof of entropy inequality relies on **chain rule**, integration by parts.

Example: compressible flow and mathematical entropy

- Conservative variables: density, momentum, energy

$$\mathbf{u} = (\rho, \mathbf{m}, E), \quad \rho > 0, \quad E > \frac{1}{2}|\mathbf{m}|^2/\rho.$$

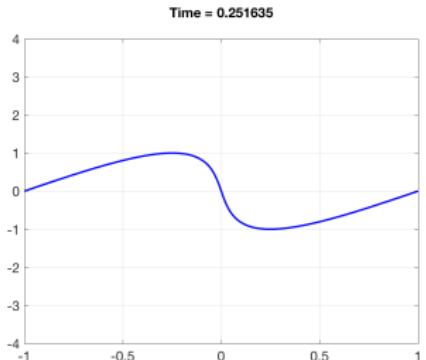
- Physical entropy $s(\mathbf{u})$ always increasing; mathematical entropy $S(\mathbf{u})$ always decreasing (analogous to energy).

$$s(\mathbf{u}) = \log \left(\frac{(\gamma - 1)\rho e}{\rho^\gamma} \right), \quad S(\mathbf{u}) = -\rho s(\mathbf{u}).$$

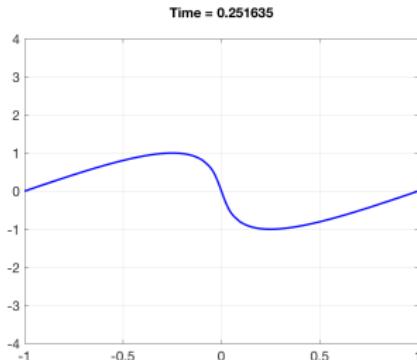
- Entropy variables $\mathbf{v}(\mathbf{u})$: invertible function of \mathbf{u}

$$\mathbf{v}(\mathbf{u}) = \frac{\partial S}{\partial \mathbf{u}} = \frac{1}{\rho e} \begin{pmatrix} \rho e(\gamma + 1 - s(\mathbf{u})) - E \\ \mathbf{m} \\ -\rho \end{pmatrix}$$

Why are discretizations of nonlinear PDEs unstable?



(a) Exact solution



(b) 8th order DG

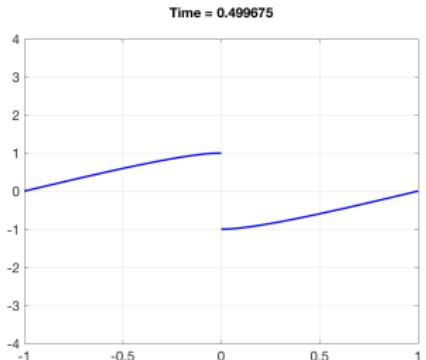
- Burgers' equation: $f(u) = u^2/2$. How to compute $\frac{\partial}{\partial x} f(u)$?

$$\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = 0, \quad u \in P^N(D^k), \quad u^2 \notin P^N(D^k).$$

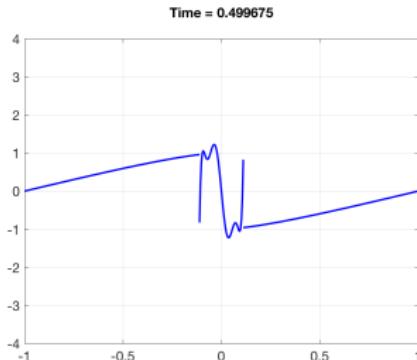
- Differentiating L^2 projection P_N + inexact quadrature: **no chain rule**.

$$\int_{D^k} \left(\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial}{\partial x} P_N u^2 \right) v \, dx = 0, \quad \frac{1}{2} \frac{\partial P_N u^2}{\partial x} \neq P_N \left(u \frac{\partial u}{\partial x} \right)$$

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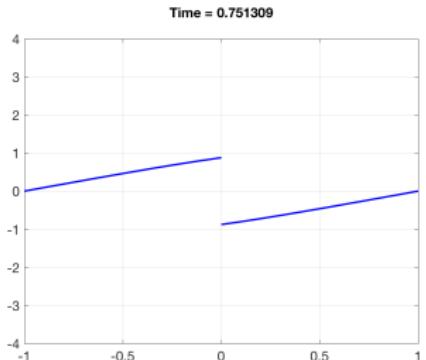
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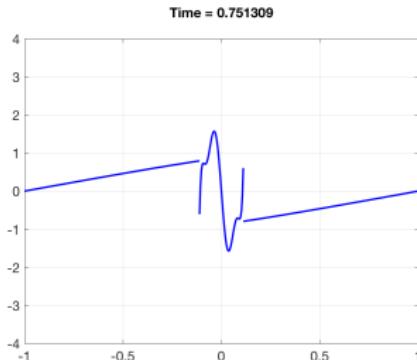
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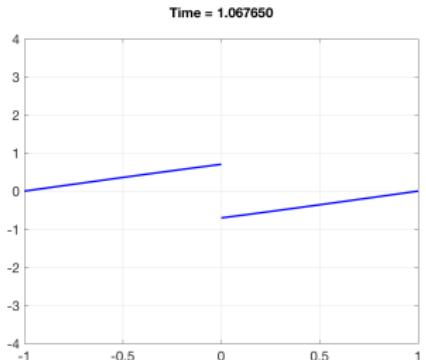
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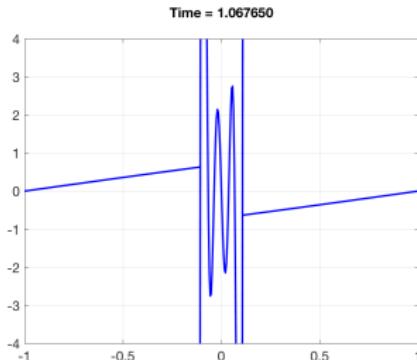
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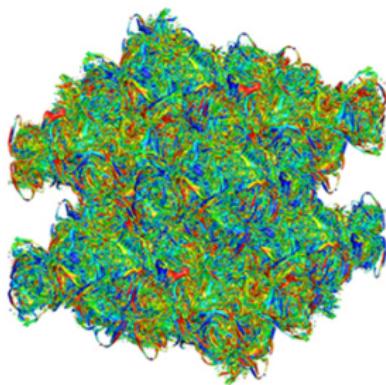
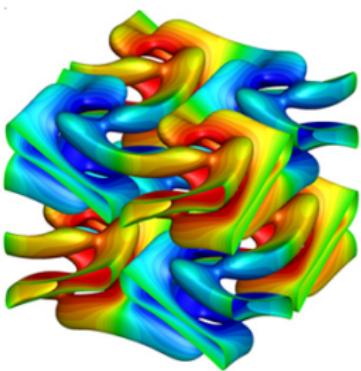
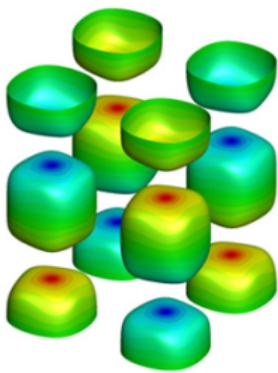
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Tradeoff: high order accuracy vs stability

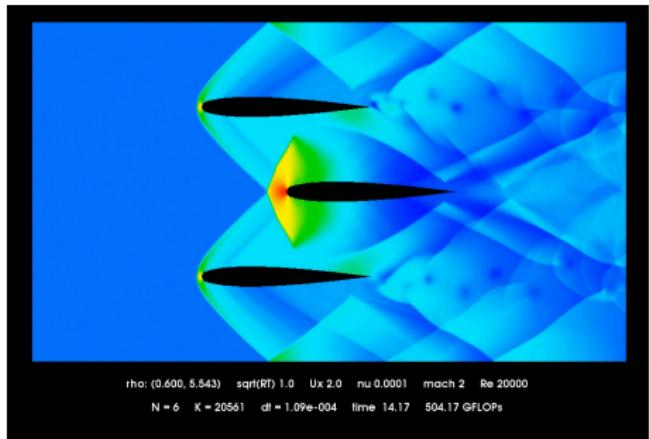
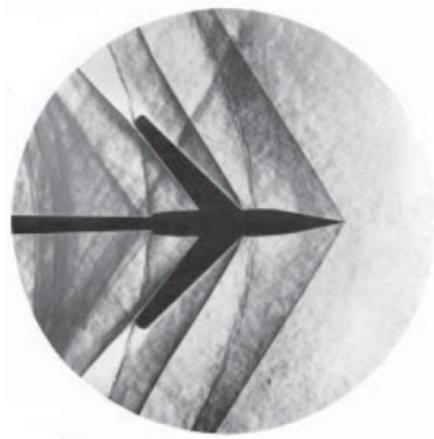
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- Common fix: stabilize by regularizing (limiters, filters, art. viscosity).



Under-resolved solutions: turbulence (inviscid Taylor-Green vortex).

Tradeoff: high order accuracy vs stability

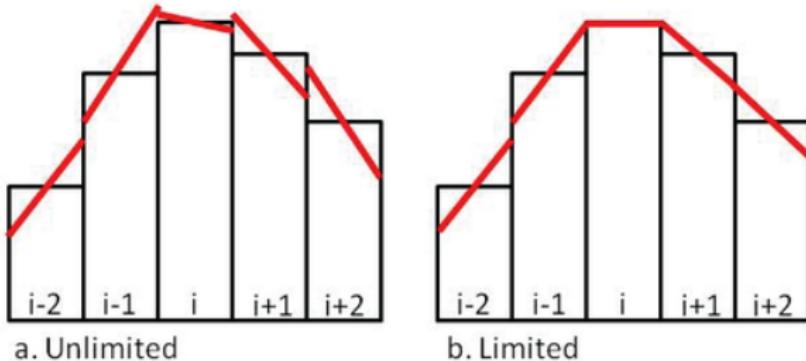
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Under-resolved solutions: shock waves.

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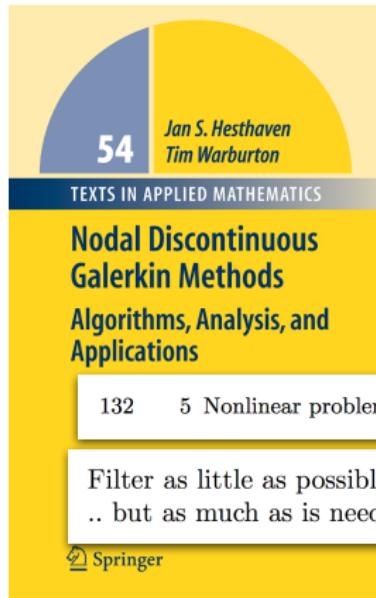
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Slope limiting for a finite volume method.

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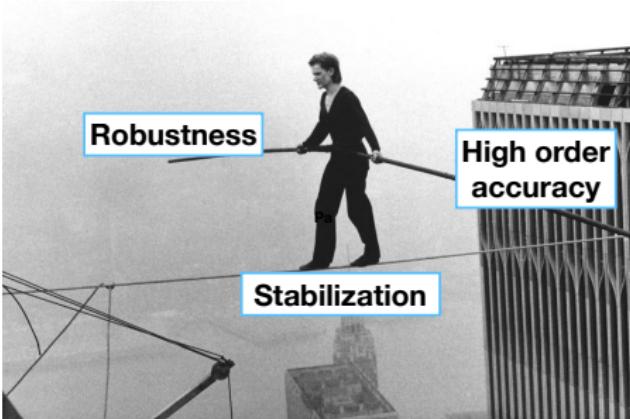
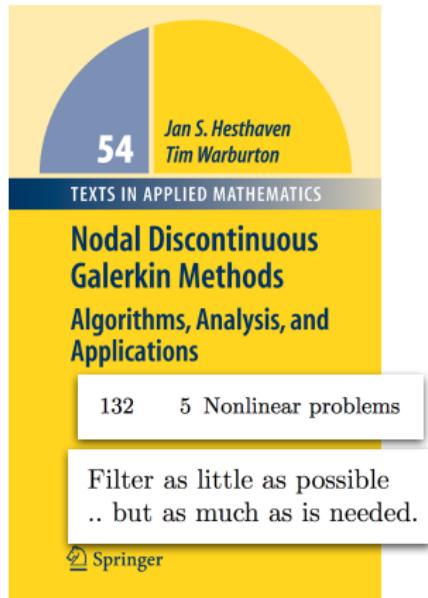
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Figures courtesy of Gregor Gassner, T. Warburton, Coastal Inlets Research Program (CIRP), "Man on Wire" (2008).

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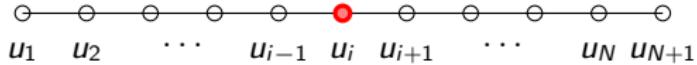


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Summation-by-parts (SBP) finite differences

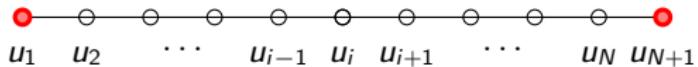


Simplest SBP finite difference matrix: combine 2nd order finite difference formulas at interior points with 1st order finite differences at boundary points .

$$\left. \frac{\partial u}{\partial x} \right|_{x=x_i} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad (\text{at interior points } x_i),$$

$$D = \frac{1}{2\Delta x} \begin{bmatrix} ? & ? & & \\ -1 & 0 & 1 & \\ & -1 & 0 & \ddots \\ & & \ddots & \ddots \end{bmatrix}, \quad M = \Delta x \begin{bmatrix} ? & & & \\ & 1 & & \\ & & 1 & \\ & & & \ddots \end{bmatrix}.$$

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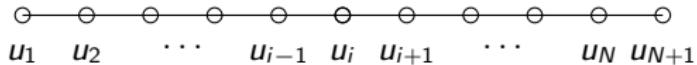


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$$\left. \frac{\partial u}{\partial x} \right|_{x=x_i} \approx \frac{u_2 - u_1}{\Delta x}, \quad \frac{u_{N+1} - u_N}{\Delta x} \quad (\text{at boundary pts } x_i)$$

$$\mathbf{D} = \frac{1}{2\Delta x} \begin{bmatrix} -2 & 2 & & & \\ -1 & 0 & 1 & & \\ & -1 & 0 & \ddots & \\ & & \ddots & \ddots & \end{bmatrix}, \quad \mathbf{M} = \Delta x \begin{bmatrix} 1/2 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & \ddots \end{bmatrix}.$$

Summation-by-parts (SBP) finite differences



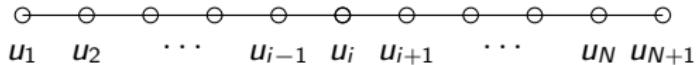
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$$\boldsymbol{MD} = \frac{1}{2} \begin{bmatrix} -1 & 1 & & & \\ -1 & 0 & 1 & & \\ & -1 & 0 & \ddots & \\ & & \ddots & \ddots & \end{bmatrix}, \quad \boldsymbol{MD} + \boldsymbol{D}^T \boldsymbol{M} = \underbrace{\begin{bmatrix} -1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}}_B.$$

Mimic integration by parts: difference matrix \boldsymbol{D} , SPD “norm” matrix \boldsymbol{M}

$$\boldsymbol{Q} = \boldsymbol{B} - \boldsymbol{Q}^T, \quad \boldsymbol{Q} = \boldsymbol{MD}, \quad \boldsymbol{M} \text{ diagonal.}$$

Summation-by-parts (SBP) finite differences



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Revisiting Burgers' equation: stable split formulations

- Rewrite Burgers' equation in **split form**

$$\frac{\partial u}{\partial t} + \frac{1}{3} \left(\frac{\partial u^2}{\partial x} + u \frac{\partial u}{\partial x} \right) = 0.$$

- SBP discretization of split formulation

$$\frac{d\mathbf{u}}{dt} + \frac{1}{3} (\mathbf{D}(\mathbf{u}^2) + \text{diag}(\mathbf{u}) \mathbf{D}\mathbf{u}) + \mathbf{M}^{-1} \mathbf{B} \mathbf{f}^* = 0, \quad \mathbf{f}^* = \begin{bmatrix} \mathbf{f}_0^* \\ \vdots \\ \mathbf{f}_N^* \end{bmatrix}.$$

- Semi-discrete stability: multiply by $\mathbf{u}^T \mathbf{M}$, use $\mathbf{Q} = \mathbf{M}\mathbf{D} + \text{diagonal}$ matrices commute + SBP to eliminate volume terms

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Revisiting Burgers' equation: stable split formulations

- Rewrite Burgers' equation in **split form**

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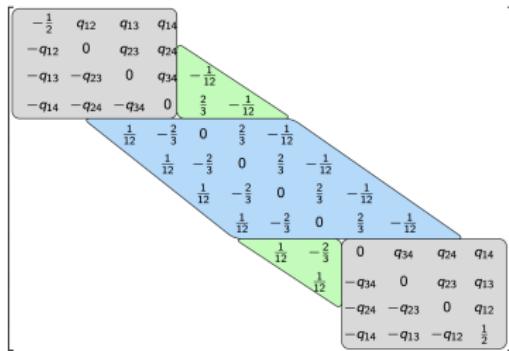
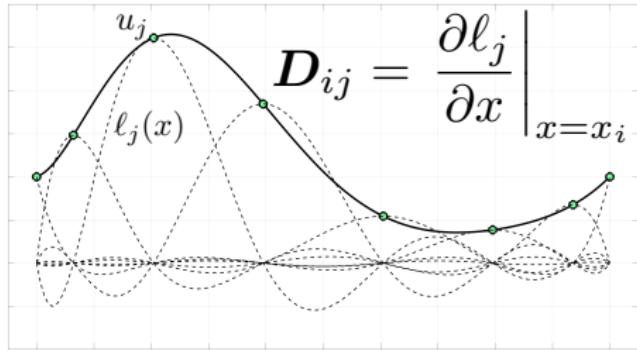
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$$\frac{1}{2} \frac{d}{dt} (\mathbf{u}^T \mathbf{M} \mathbf{u}) = 0, \quad (\text{for appropriate } \mathbf{f}^*).$$

Higher order SBP approximations

(a) 1D matrix ($N = 2$, equispaced)(b) 1D SBP ($N = 7$, GLL nodes)

- Solve for high order “diagonal-norm” SBP finite difference matrices.
- Nodal DG construction of diagonal-norm SBP matrices:
Gauss-Legendre-Lobatto **quadrature** + **nodal basis** + **mass lumping**.

Figure courtesy of David C. Del Rey Fernandez.

Fisher and Carpenter (2013). *High-order ES finite difference schemes for nonlinear conservation laws: Finite domains*.

Gassner, Winters, and Kopriva (2016). *Split form nodal DG schemes with SBP property for the comp. Euler equations*.

Key idea behind entropy stable schemes

- Traditional (unstable) scheme, ignoring boundary conditions:

$$\frac{d\mathbf{u}}{dt} + \mathbf{D}\mathbf{f}(\mathbf{u}) = 0 \implies \frac{d\mathbf{u}_i}{dt} + \sum_j \mathbf{D}_{ij}\mathbf{f}(\mathbf{u}_j) = 0.$$

- Flux differencing: $\mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_j) = \frac{\mathbf{u}_i + \mathbf{u}_j}{2}$ recovers traditional scheme

$$\frac{d\mathbf{u}_i}{dt} + \sum_j \mathbf{D}_{ij}2\mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_j) = 0 \implies \frac{d\mathbf{u}}{dt} + 2(\mathbf{D} \circ \mathbf{F}_S)\mathbf{1} = 0.$$

- Use “entropy conservative” finite volume numerical flux $\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R)$.
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$$\mathbf{1}^T \mathbf{M} \frac{dS(\mathbf{u})}{dt} + \mathbf{1}^T \mathbf{B} \left(\mathbf{v}^T \mathbf{f}(\mathbf{u}) - \psi(\mathbf{u}) \right) = 0.$$

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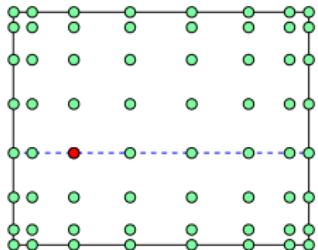
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Entropy stable SBP discretizations: current/challenges



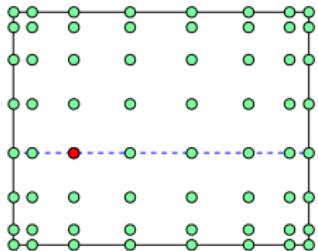
(a) GLL collocation

- (Current) **Discrete entropy inequality** using high order GLL hexes.
 - Gauss quadrature: more accurate but **expensive coupling conditions**.
 - Tetrahedra, wedges, pyramids? Over-integration?

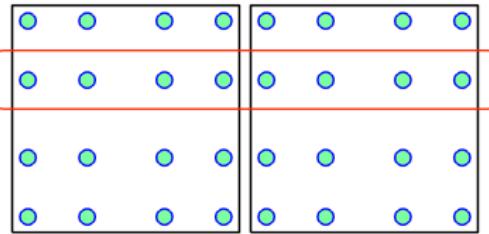
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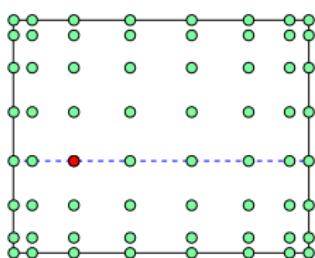
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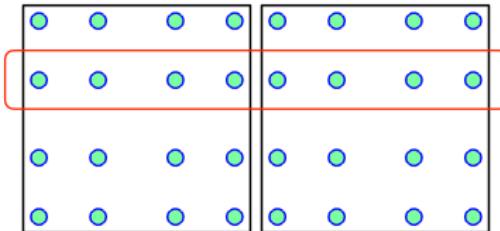
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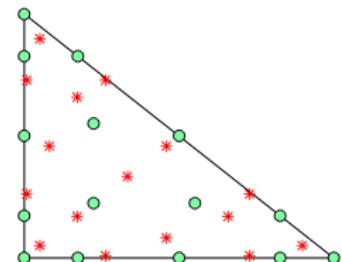
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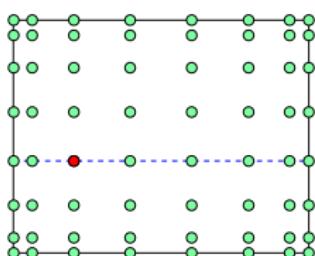
(c) Nodes vs quadrature

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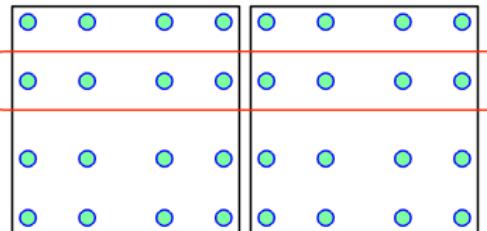
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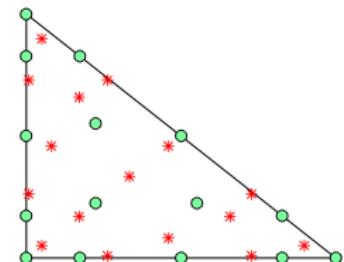
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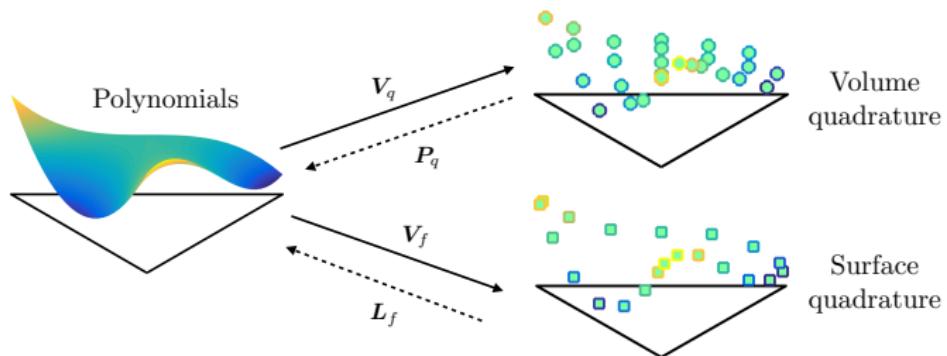
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Goal: **entropy stable** high order DG with **compact stencils** using arbitrary basis functions and volume/surface quadrature points.

Gassner, Winters, and Kopriva (2016). *Split form nodal DG schemes with SBP property for the comp. Euler equations*.

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Quadrature-based matrices for polynomial bases



- Assume degree $2N$ volume, surface quadratures $(\mathbf{x}_i^q, \mathbf{w}_i^q)$, $(\mathbf{x}_i^f, \mathbf{w}_i^f)$, and basis $\phi_1, \dots, \phi_{N_p}$. Define interpolation matrices \mathbf{V}_q , \mathbf{V}_f

$$(\mathbf{V}_q)_{ij} = \phi_j(\mathbf{x}_i^q), \quad (\mathbf{V}_f)_{ij} = \phi_j(\mathbf{x}_i^f).$$

- Introduce quadrature-based L^2 **projection** and **lifting** matrices

$$\mathbf{P}_q = \mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W}, \quad \mathbf{L}_f = \mathbf{M}^{-1} \mathbf{V}_f^T \mathbf{W}_f,$$

$$\mathbf{W} = \text{diag}(\mathbf{w}^q), \quad \mathbf{W}_f = \text{diag}(\mathbf{w}^f).$$

Quadrature-based differentiation matrices

- Matrix \mathbf{D}_q^i : evaluates derivative of L^2 projection at points \mathbf{x}^q .

$$\mathbf{D}_q^i = \mathbf{V}_q \mathbf{D}^i \mathbf{P}_q, \quad \mathbf{D}^i \text{ exactly differentiates polynomials.}$$

- Summation-by-parts involving L^2 projection:

$$\mathbf{W} \mathbf{D}_q^i + (\mathbf{W} \mathbf{D}_q^i)^T = (\mathbf{V}_f \mathbf{P}_q)^T \mathbf{W}_f \text{diag}(\mathbf{n}_i) \mathbf{V}_f \mathbf{P}_q.$$

- Equivalent to integration-by-parts + quadrature: for $u, v \in L^2(\widehat{D})$

$$\int_{\widehat{D}} \frac{\partial P_N u}{\partial x_i} v + \int_{\widehat{D}} u \frac{\partial P_N v}{\partial x_i} = \int_{\partial \widehat{D}} (P_N u)(P_N v) \widehat{n}_i$$

- Quadrature may not contain boundary points: complicated **interface terms** for coupling between neighboring elements or imposing BCs.

A “decoupled” block SBP operator

- Approx. derivatives also using **boundary traces** (compact coupling).
- On an element D^k with unit normal vector \mathbf{n} : approximate derivative with respect to the i th coordinate.

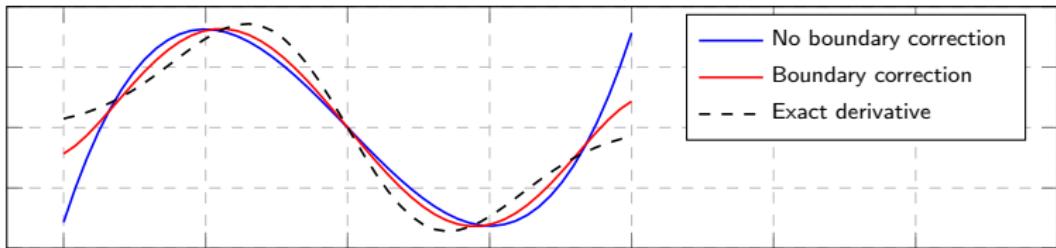
$$\mathbf{D}_N^i = \begin{bmatrix} \mathbf{D}_q^i - \frac{1}{2}\mathbf{V}_q \mathbf{L}_f \text{diag}(\mathbf{n}_i) \mathbf{V}_f \mathbf{P}_q & \frac{1}{2}\mathbf{V}_q \mathbf{L}_f \text{diag}(\mathbf{n}_i) \\ -\frac{1}{2}\text{diag}(\mathbf{n}_i) \mathbf{V}_f \mathbf{P}_q & \frac{1}{2}\text{diag}(\mathbf{n}_i) \end{bmatrix},$$

- \mathbf{D}_N^i satisfies a summation-by-parts (SBP) property

$$\mathbf{Q}_N^i = \begin{bmatrix} \mathbf{W} & \\ & \mathbf{W}_f \end{bmatrix} \mathbf{D}_N^i, \quad \mathbf{B}_N = \begin{bmatrix} 0 \\ \mathbf{W}_f \mathbf{n}_i \end{bmatrix},$$

$$\boxed{\mathbf{Q}_N^i + (\mathbf{Q}_N^i)^T = \mathbf{B}_N} \sim \boxed{\int_{D^k} \frac{\partial f}{\partial x_i} g + f \frac{\partial g}{\partial x_i} = \int_{\partial D^k} f g \mathbf{n}_i}.$$

Decoupled SBP operators: adding boundary corrections



- D_N^i produces a high order approximation of $f \frac{\partial g}{\partial x}$ at $\mathbf{x} = [\mathbf{x}^q, \mathbf{x}^f]$.

$$f \frac{\partial g}{\partial x} \approx [\begin{matrix} \mathbf{P}_q & \mathbf{L}_f \end{matrix}] \text{diag}(\mathbf{f}) D_N g, \quad \mathbf{f}_i, \mathbf{g}_i = f(\mathbf{x}_i), g(\mathbf{x}_i).$$

- Equivalent to a **skew-symmetric** variational problem for $u(\mathbf{x}) \approx f \frac{\partial g}{\partial x}$ (P_N is the degree N polynomial L^2 projection).

$$\int_{D^k} u(\mathbf{x}) v(\mathbf{x}) = \int_{D^k} f \frac{\partial P_N g}{\partial x} v + \int_{\partial D^k} (g - P_N g) \frac{(fv + P_N(fv))}{2}.$$

Talk outline

- 1 Stability of high order DG: linear vs nonlinear PDEs
- 2 Summation by parts finite differences and high order DG
- 3 Entropy stable formulations and flux differencing
- 4 Numerical experiments
 - 1D experiments
 - Triangular and tetrahedral meshes
 - Quadrilateral and hexahedral meshes

Burgers' equation: energy stable formulations

- Revisit split form of Burgers' equation:

$$\frac{\partial u}{\partial t} + \frac{1}{3} \left(\frac{\partial u^2}{\partial x} + u \frac{\partial u}{\partial x} \right) = 0$$

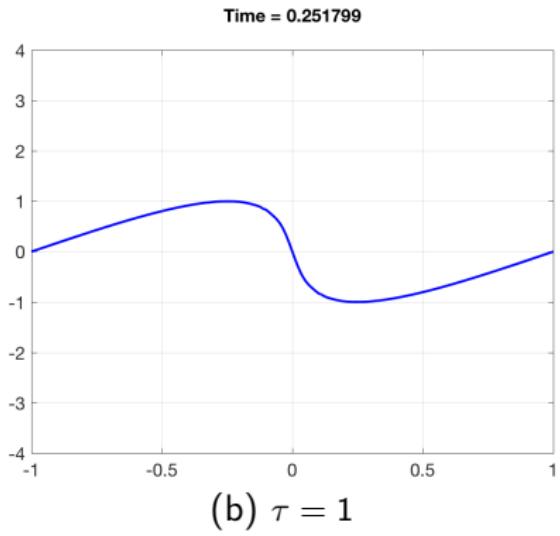
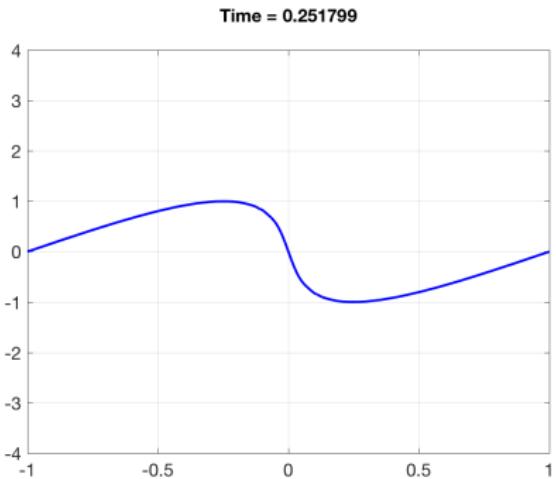
- Stable DG method: let $u(x) = \sum_j \hat{\mathbf{u}}_j \phi_j(x)$. Find $\hat{\mathbf{u}}$ such that

$$\begin{aligned} \mathbf{u} &= \begin{bmatrix} \mathbf{V}_q \\ \mathbf{V}_f \end{bmatrix} \hat{\mathbf{u}}, \quad \mathbf{f}^* = \mathbf{f}^*(u^+, u) = \text{numerical flux} \\ \frac{d\hat{\mathbf{u}}}{dt} + \frac{1}{3} [\mathbf{P}_q \quad \mathbf{L}_f] (\mathbf{D}_N (\mathbf{u}^2) + \text{diag}(\mathbf{u}) \mathbf{D}_N \mathbf{u}) + \mathbf{L}_f(\mathbf{f}^*) &= 0. \end{aligned}$$

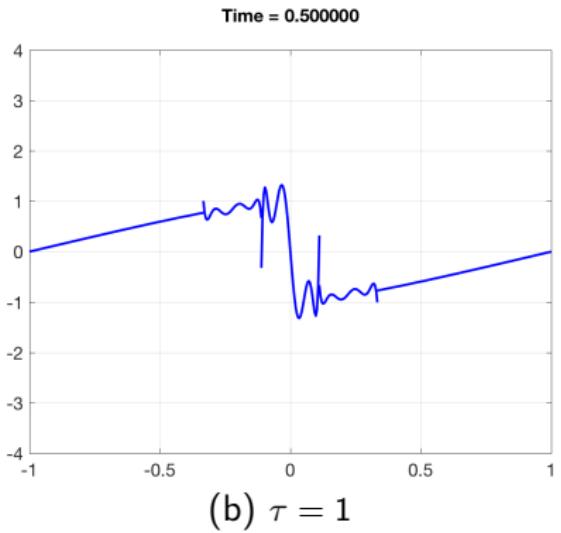
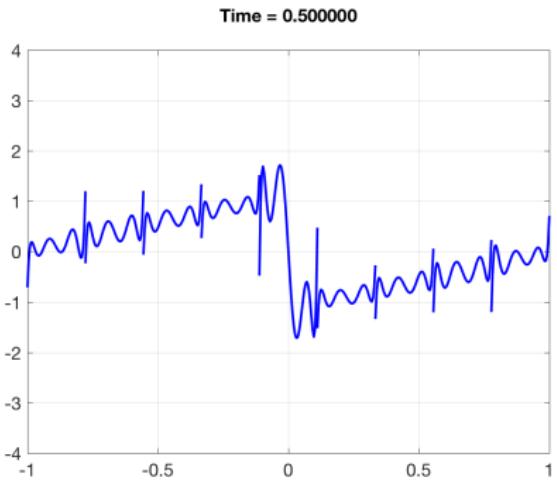
- Energy stability: multiply by $\hat{\mathbf{u}}^T \mathbf{M}$, use SBP, sum over D^k

$$\sum_k \frac{1}{2} \frac{d}{dt} \hat{\mathbf{u}}^T \mathbf{M} \hat{\mathbf{u}} = \sum_k \frac{1}{2} \frac{\partial}{\partial t} \|u\|_{L^2(D^k)}^2 \leq 0.$$

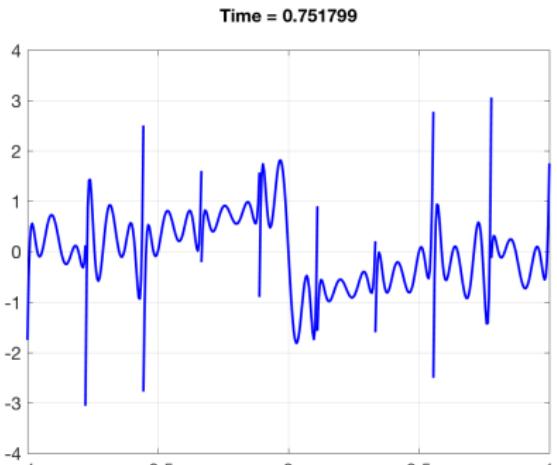
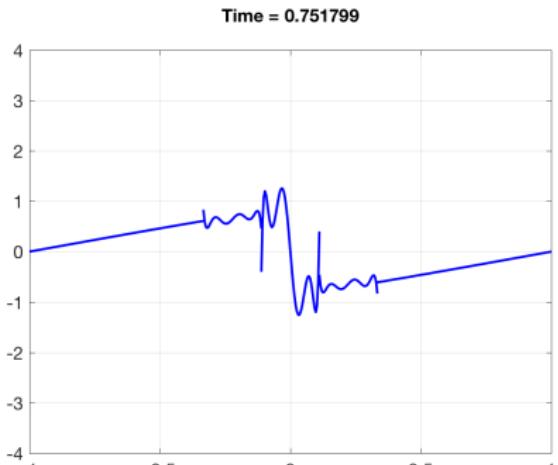
Burgers' equation: energy stable shock solution



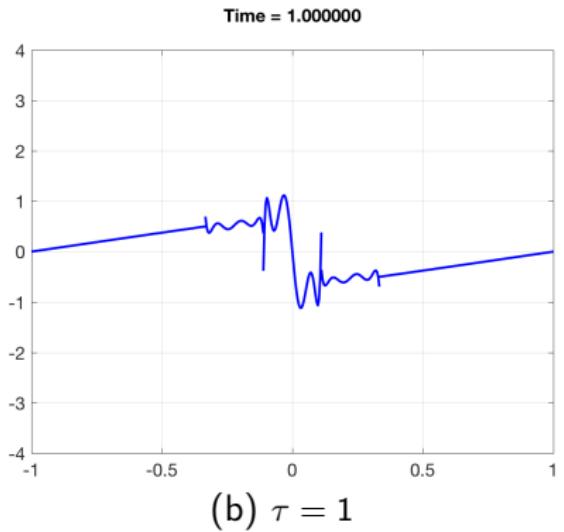
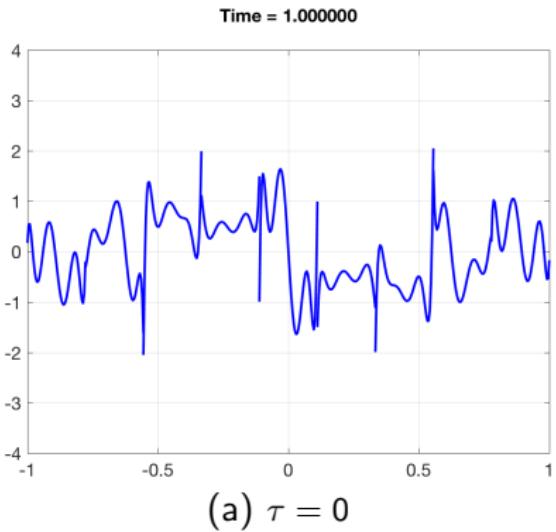
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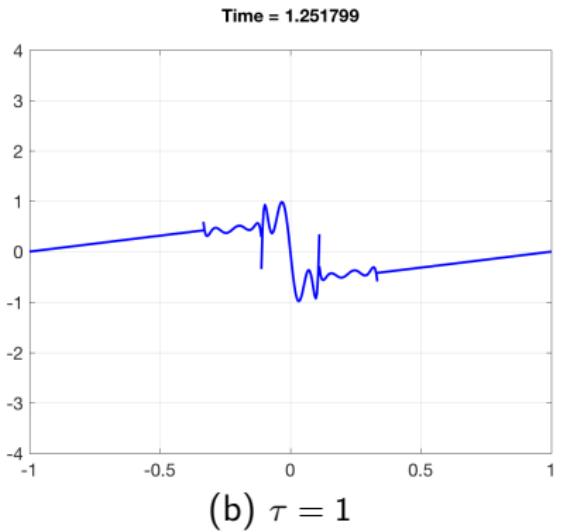
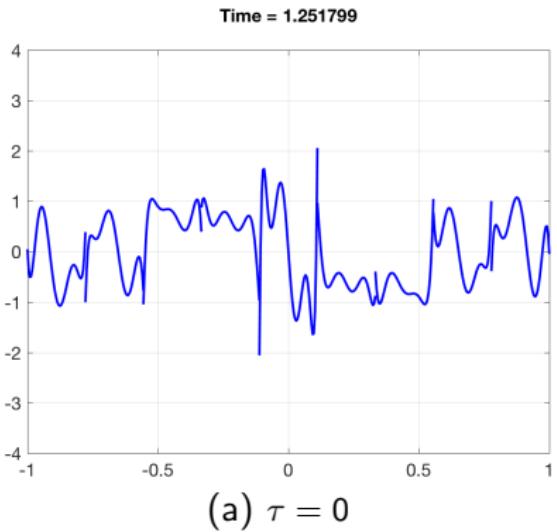
Burgers' equation: energy stable shock solution

(a) $\tau = 0$ (b) $\tau = 1$

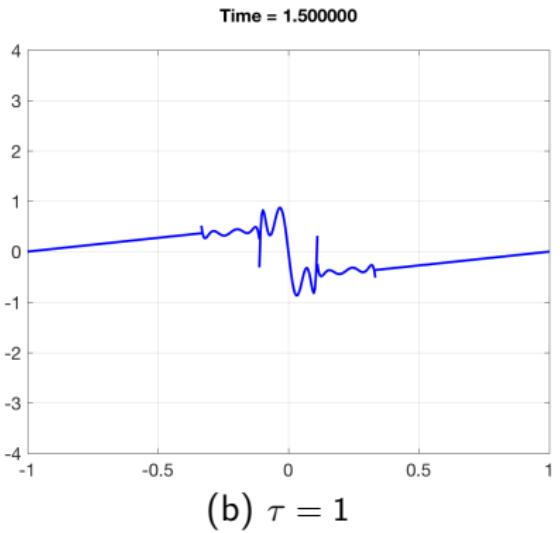
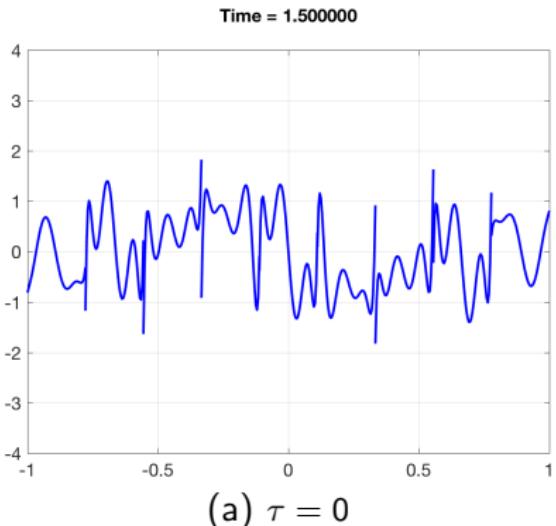
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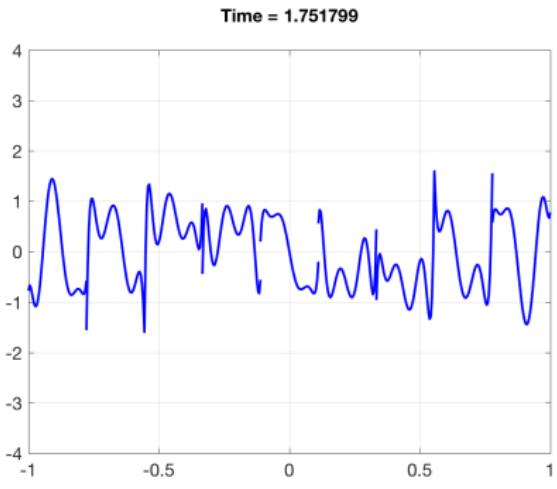
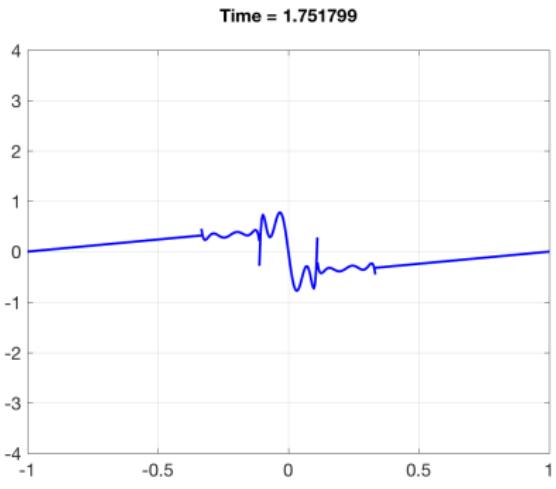
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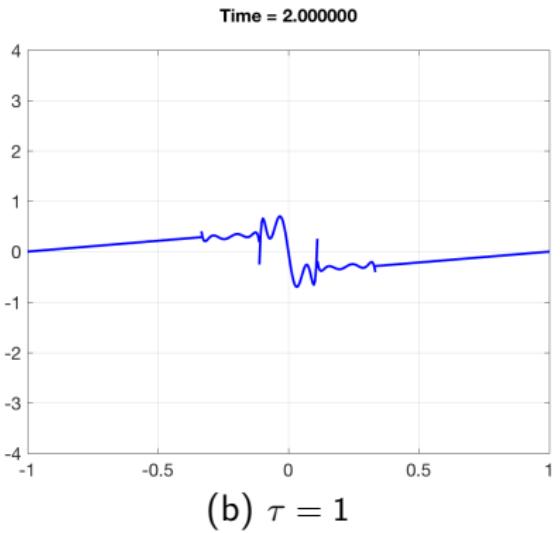
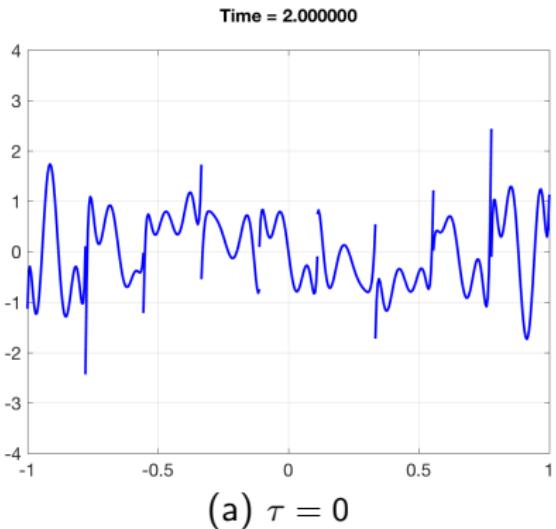
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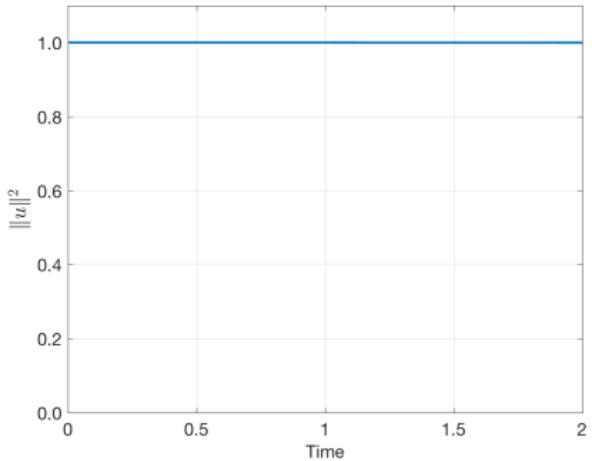
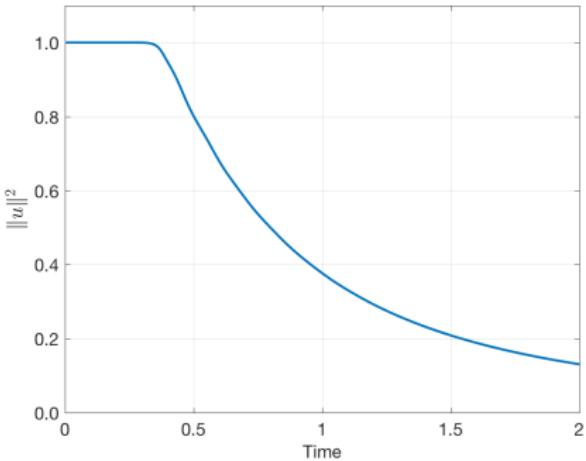
Burgers' equation: energy stable shock solution

(a) $\tau = 0$ (b) $\tau = 1$

Burgers' equation: energy stable shock solution



Burgers' equation: energy stable shock solution

(a) Energy conservative ($\tau = 0$)(b) Energy stable ($\tau = 1$)

Flux differencing: entropy conservative finite volume fluxes

- Tadmor's entropy conservative (mean value) numerical flux

$$\mathbf{f}_S(\mathbf{u}, \mathbf{u}) = \mathbf{f}(\mathbf{u}), \quad (\text{consistency})$$

$$\mathbf{f}_S(\mathbf{u}, \mathbf{v}) = \mathbf{f}_S(\mathbf{v}, \mathbf{u}), \quad (\text{symmetry})$$

$$(\mathbf{v}_L - \mathbf{v}_R)^T \mathbf{f}(\mathbf{u}_L, \mathbf{u}_R) = \psi_L - \psi_R, \quad (\text{conservation}).$$

- Example: entropy conservative flux for Burgers' equation

$$f_S(u_L, u_R) = \frac{1}{6} (u_L^2 + u_L u_R + u_R^2).$$

- Flux differencing: using finite volume numerical fluxes to evaluate high order derivatives in DG methods.

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Flux differencing: recovering split formulations

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$$\frac{\partial f(u)}{\partial x} \implies 2 \frac{\partial f_S(u(x), u(y))}{\partial x} \Big|_{y=x}$$

- Recovering the Burgers' split formulation

$$f_S(u(x), u(y)) = \frac{1}{6} (u(x)^2 + u(x)u(y) + u(y)^2)$$

$$2 \frac{\partial f_S(u(x), u(y))}{\partial x} \Big|_{y=x} = \frac{1}{3} \frac{\partial u^2}{\partial x} + \frac{1}{3} u \frac{\partial u}{\partial x} + \frac{1}{3} u^2 \cancel{\frac{\partial u}{\partial x}}.$$

Flux differencing: recovering split formulations

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Flux differencing: beyond split formulations

- Fluxes do not necessarily correspond to split formulations!
- Example: entropy conservative flux for 1D compressible Euler

$$f_S^1(\mathbf{u}_L, \mathbf{u}_R) = \{\{\rho\}\}^{\log} \{\{u\}\}$$

$$f_S^2(\mathbf{u}_L, \mathbf{u}_R) = \frac{\{\{\rho\}\}}{2 \{\{\beta\}\}} + \{\{u\}\} f_S^1$$

$$f_S^3(\mathbf{u}_L, \mathbf{u}_R) = f_S^1 \left(\frac{1}{2(\gamma - 1) \{\{\beta\}\}^{\log}} - \frac{1}{2} \{\{u^2\}\} \right) + \{\{u\}\} f_S^2,$$

- Rational functions: logarithmic mean and “inverse temperature” β

$$\{\{u\}\}^{\log} = \frac{u_L - u_R}{\log u_L - \log u_R}, \quad \beta = \frac{\rho}{2p}.$$

Flux differencing: implementational details

- Define \mathbf{F}_S by evaluating \mathbf{f}_S at all combinations of quadrature points

$$(\mathbf{F}_S)_{ij} = \mathbf{f}_S(u(\mathbf{x}_i), u(\mathbf{x}_j)), \quad \mathbf{x} = [\mathbf{x}^q, \mathbf{x}^f]^T.$$

- Replace $\frac{\partial}{\partial x}$ with \mathbf{D}_N + projection and lifting matrices.

$$2 \frac{\partial f_S(u(x), u(y))}{\partial x} \Big|_{y=x} \implies [\mathbf{P}_q \quad \mathbf{L}_f] \operatorname{diag}(2\mathbf{D}_N \mathbf{F}_S).$$

- Efficient **Hadamard product** reformulation of flux differencing
(efficient on-the-fly evaluation of \mathbf{F}_S)

$$\operatorname{diag}(2\mathbf{D}_N \mathbf{F}_S) = (2\mathbf{D}_N \circ \mathbf{F}_S) \mathbf{1}.$$

Flux differencing: avoiding the chain rule

- Test with entropy variables $\tilde{\mathbf{v}}$, integrate, and use SBP property:

$$\tilde{\mathbf{v}}^T (2\mathbf{Q}_N \circ \mathbf{F}_S) \mathbf{1} = \tilde{\mathbf{v}}^T \left(\left(\begin{bmatrix} 0 \\ \mathbf{W}_f \mathbf{n} \end{bmatrix} + \mathbf{Q}_N - \mathbf{Q}_N^T \right) \circ \mathbf{F}_S \right) \mathbf{1}.$$

- Only boundary terms appear in final estimate; volume terms become boundary terms using properties of $(\mathbf{F}_S)_{ij} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j)$

$$\begin{aligned} \tilde{\mathbf{v}}^T ((\mathbf{Q}_N - \mathbf{Q}_N^T) \circ \mathbf{F}_S) \mathbf{1} &= \tilde{\mathbf{v}}^T (\mathbf{Q}_N \circ \mathbf{F}_S) \mathbf{1} - \mathbf{1}^T (\mathbf{Q}_N \circ \mathbf{F}_S) \tilde{\mathbf{v}} \\ &= \sum_{i,j} (\mathbf{Q}_N)_{ij} (\tilde{\mathbf{v}}_i - \tilde{\mathbf{v}}_j)^T \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j). \end{aligned}$$

- Proof requires $\tilde{\mathbf{v}} = \mathbf{v}(\tilde{\mathbf{u}})$; the entropy variables $\tilde{\mathbf{v}}$ must be a function of the conservative variables $\tilde{\mathbf{u}}$.

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Modifying the conservative variables

- Conservative variables \mathbf{u}_h and test functions are polynomial, but the entropy variables $\mathbf{v}(\mathbf{u}_h) \notin P^N!$
- Evaluate flux \mathbf{f}_S using **modified** conservative variables $\tilde{\mathbf{u}}$

$$\tilde{\mathbf{u}} = \mathbf{u}(P_N \mathbf{v}(\mathbf{u}_h)).$$

- If $\mathbf{v}(\mathbf{u})$ is an invertible mapping, this choice of $\tilde{\mathbf{u}}$ ensures that

$$\tilde{\mathbf{v}} = \mathbf{v}(\tilde{\mathbf{u}}) = P_N \mathbf{v}(\mathbf{u}_h) \in P^N.$$

- Local conservation w.r.t. a generalized Lax-Wendroff theorem.

A discretely entropy conservative DG method

Theorem (Chan 2018)

Let $\mathbf{u}_h(\mathbf{x}) = \sum_j \hat{\mathbf{u}}_j \phi_j(\mathbf{x})$ and $\tilde{\mathbf{u}} = \mathbf{u}(P_N \mathbf{v})$. Let $\hat{\mathbf{u}}$ locally solve

$$\frac{d\hat{\mathbf{u}}}{dt} + \sum_{i=1}^d \begin{bmatrix} \mathbf{P}_q & \mathbf{L}_f \end{bmatrix} (2\mathbf{D}_N^i \circ \mathbf{F}_S^i) \mathbf{1} + \mathbf{L}_f \left(\mathbf{f}_S^i(\tilde{\mathbf{u}}^+, \tilde{\mathbf{u}}) - \mathbf{f}^i(\tilde{\mathbf{u}}) \right) \mathbf{n}_i = 0.$$

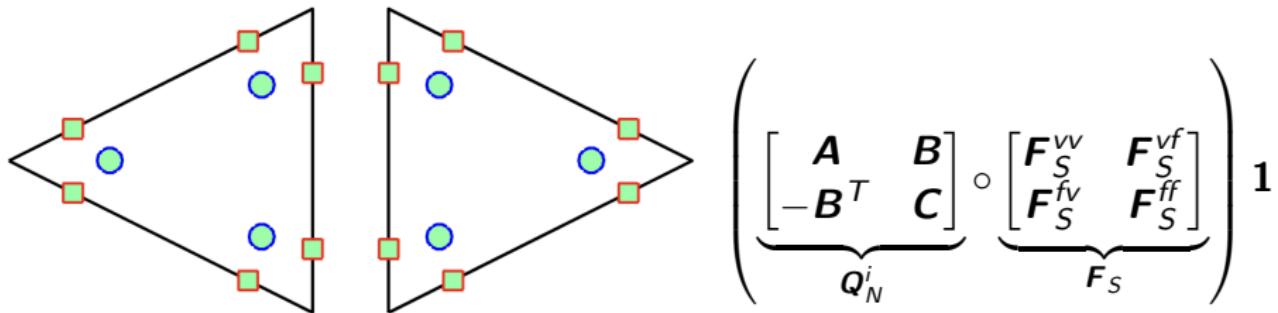
Assuming continuity in time, $\mathbf{u}_h(\mathbf{x})$ satisfies the quadrature form of

$$\int_{\Omega} \frac{\partial S(\mathbf{u}_h)}{\partial t} + \sum_{i=1}^d \int_{\partial\Omega} \left((P_N \mathbf{v})^T \mathbf{f}^i(\tilde{\mathbf{u}}) - \psi_i(\tilde{\mathbf{u}}) \right) \mathbf{n}_i = 0.$$

- Can modify interface flux (e.g. Lax-Friedrichs or matrix dissipation) to change the entropy equality to an entropy **inequality**.

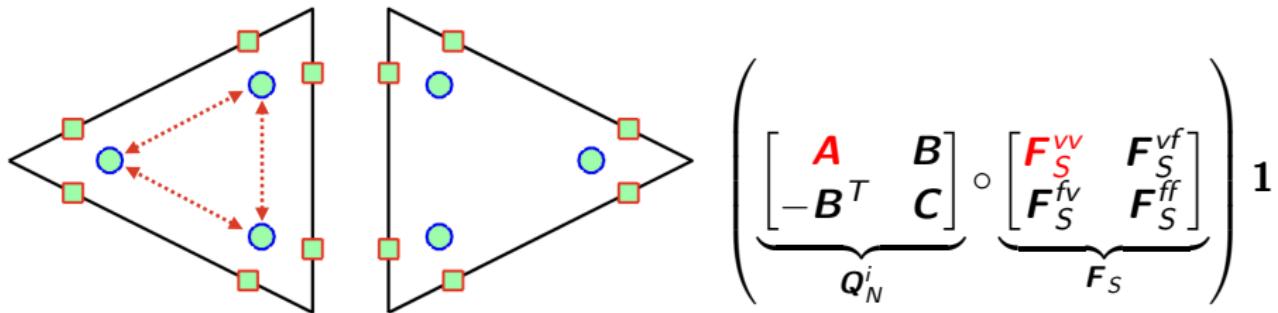
Winters, Derigs, Gassner, and Walch (2017). A uniquely defined entropy stable matrix dissipation operator for high Mach number ideal MHD and compressible Euler simulations.

Illustration of main steps of ESDG



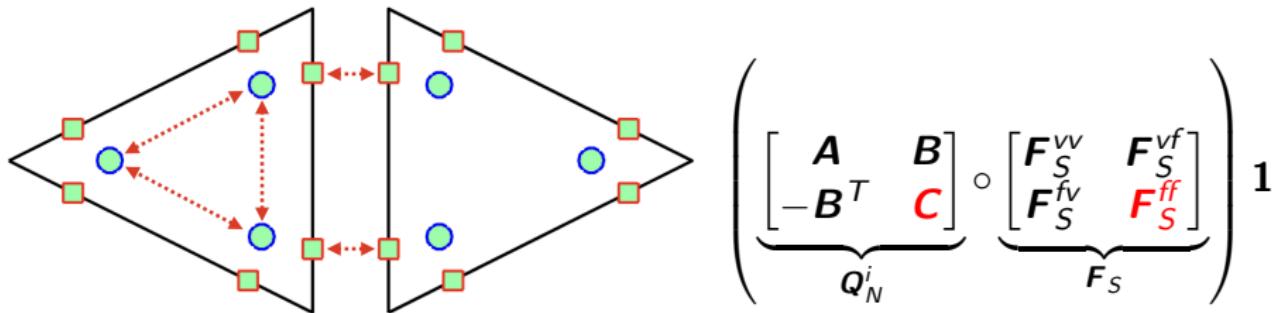
- Interpolate projected entropy variables $P_N \mathbf{v}(\mathbf{u})$ to all nodes.
- Compute interactions $f_S(\mathbf{u}_L, \mathbf{u}_R)$ between volume quadrature nodes.
- Compute interactions between surface nodes of neighboring elements
- Compute interactions between volume/surface nodes.

Illustration of main steps of ESDG



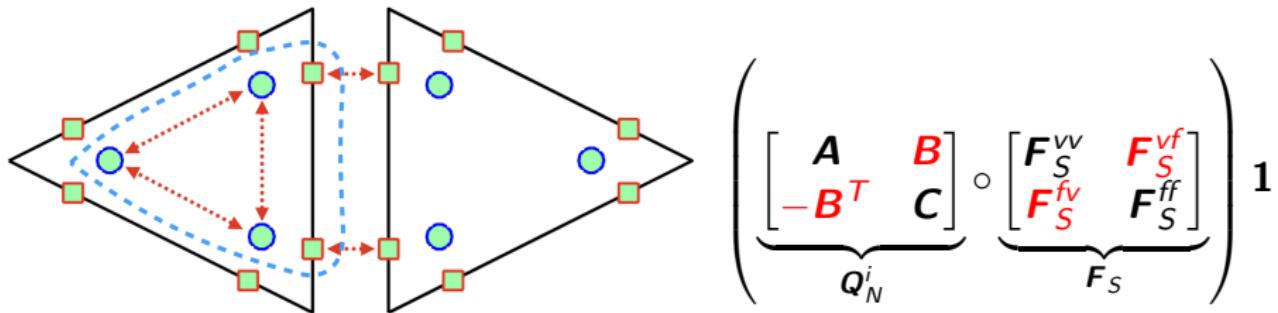
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Talk outline

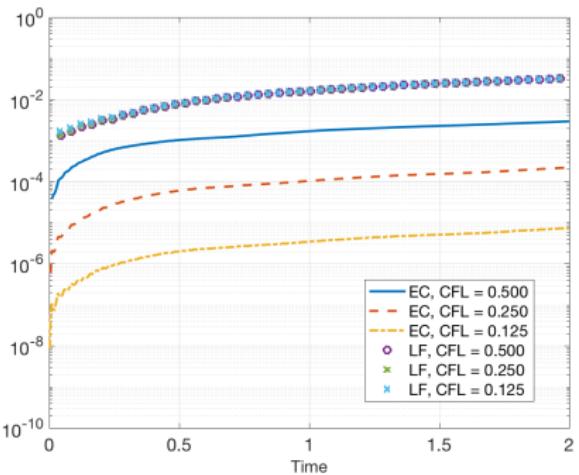
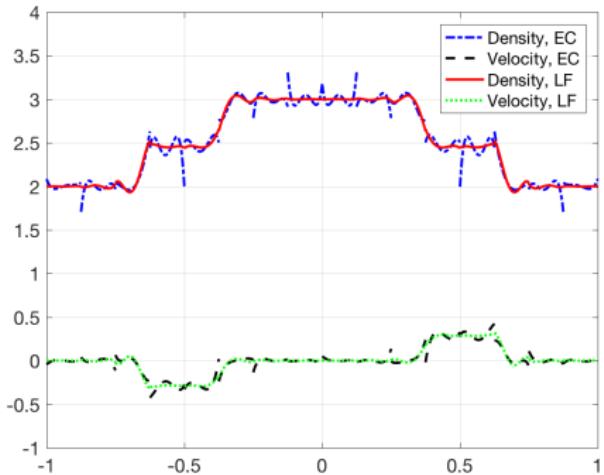
- 1 Stability of high order DG: linear vs nonlinear PDEs
- 2 Summation by parts finite differences and high order DG
- 3 Entropy stable formulations and flux differencing
- 4 Numerical experiments
 - 1D experiments
 - Triangular and tetrahedral meshes
 - Quadrilateral and hexahedral meshes

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Conservation of entropy: semi-discrete vs. fully discrete

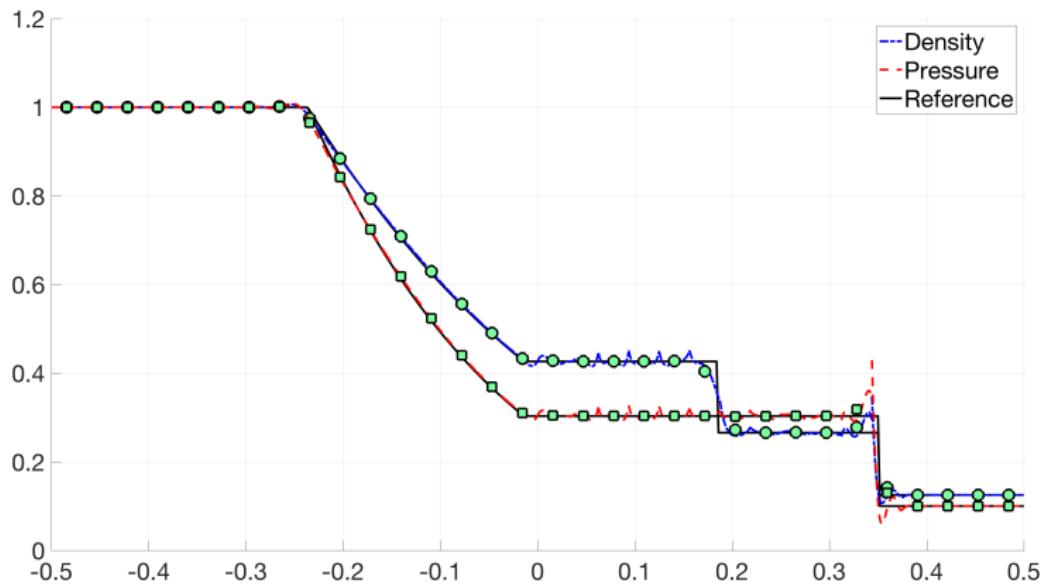
$$\Delta S(\mathbf{u}) = |S(\mathbf{u}(x, t)) - S(\mathbf{u}(x, 0))| \rightarrow 0 \text{ as } \Delta t \rightarrow 0.$$

(a) $\Delta S(\mathbf{u})$ for various Δt (b) $\rho(x), u(x)$ ($N = 4, K = 16$)

Solution and change in entropy $\Delta S(\mathbf{u})$ for entropy conservative (EC) and Lax-Friedrichs (LF) fluxes (using GQ- $(N+2)$ quadrature).

1D Sod shock tube

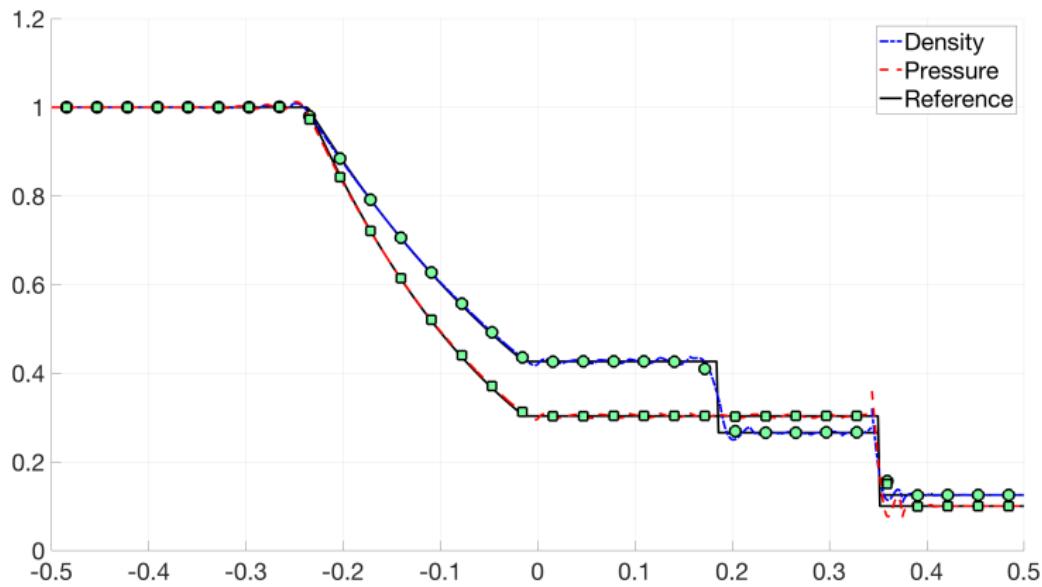
- Circles are cell averages.
- CFL of .125 used for both GLL- $(N + 1)$ and GQ- $(N + 2)$.



$N = 4, K = 32, (N + 1)$ point Gauss-Lobatto-Legendre quadrature.

1D Sod shock tube

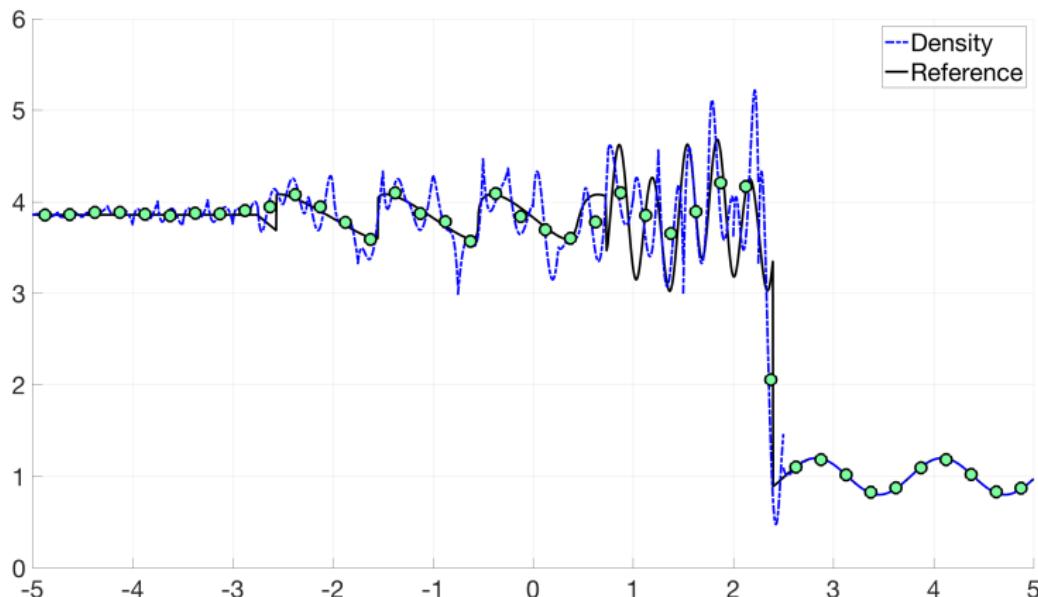
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1D sine-shock interaction

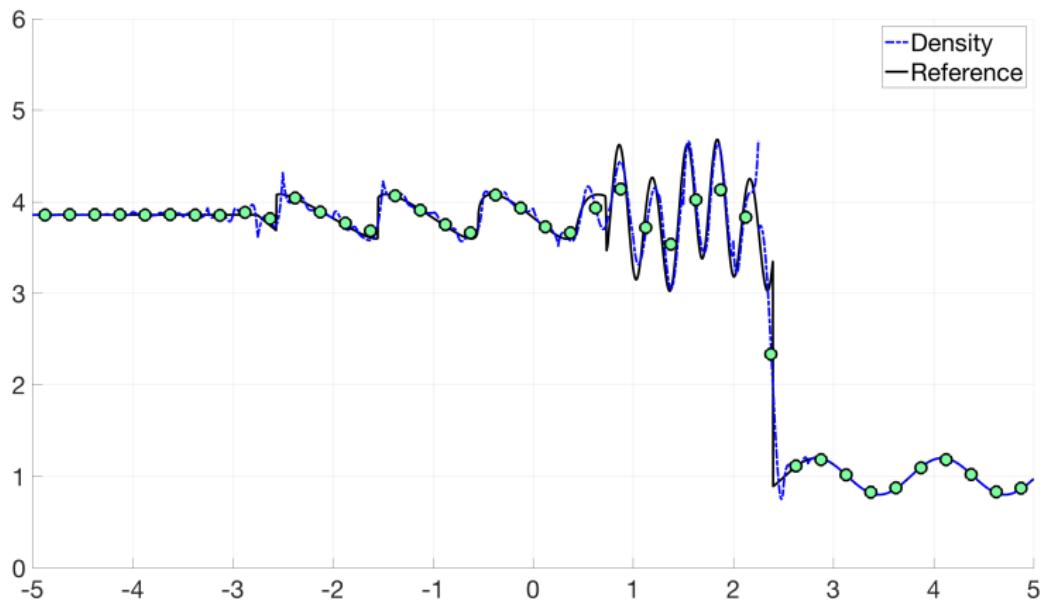
- GQ- $(N + 2)$ needs smaller CFL (.05 vs .125) for stability.



$N = 4, K = 40, \text{CFL} = .05, (N + 1)$ point Gauss-Lobatto-Legendre quadrature.

1D sine-shock interaction

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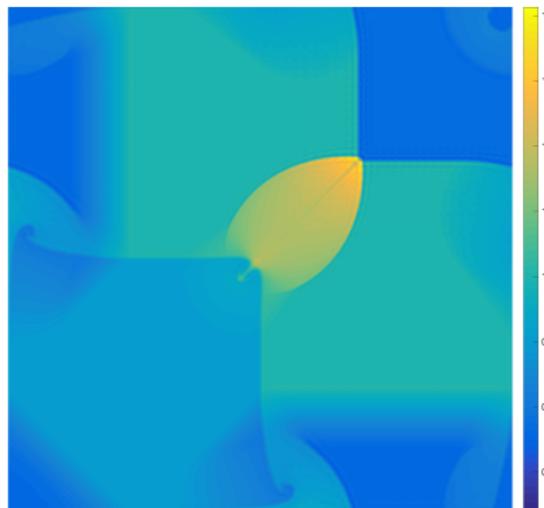
$N = 4, K = 40, \text{CFL} = .05, (N + 2)$ point Gauss quadrature.

Talk outline

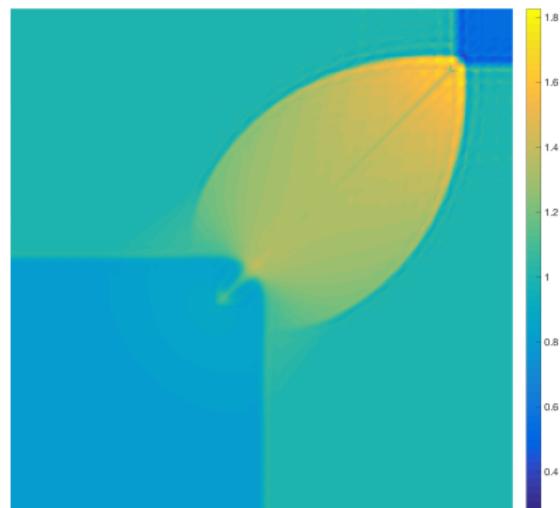
- 1 Stability of high order DG: linear vs nonlinear PDEs
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- 4 Numerical experiments
 - 1D experiments
 - **Triangular and tetrahedral meshes**
 - Quadrilateral and hexahedral meshes

2D Riemann problem

- Uniform 64×64 mesh: $N = 3$, CFL .125, Lax-Friedrichs stabilization.
- No limiting or artificial viscosity required to maintain stability!
- Periodic on larger domain (“natural” boundary conditions unstable).

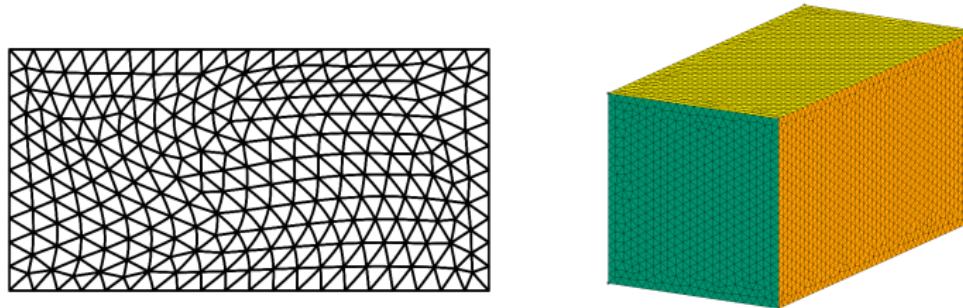


(a) $\Omega = [-1, 1]^2$



(b) $\Omega = [-0.5, 0.5]^2$, 32×32 elements

Smooth isentropic vortex and curved meshes in 2D/3D



(a) 2D triangular mesh

(b) 3D tetrahedral mesh

Figure: Example of 2D and 3D meshes used for convergence experiments.

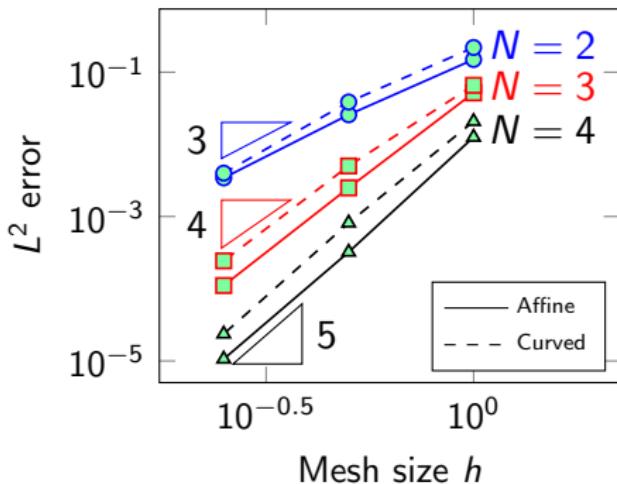
- Entropy stability: needs discrete geometric conservation law (GCL).
- Generalized mass lumping: weight-adjusted mass matrices.
- Modify $\tilde{\mathbf{u}} = \mathbf{u}(\tilde{\mathbf{v}})$, $\tilde{\mathbf{v}} = \tilde{P}_N^k \mathbf{v}(\mathbf{u}_h)$ using weight-adjusted projection \tilde{P}_N^k .

Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.

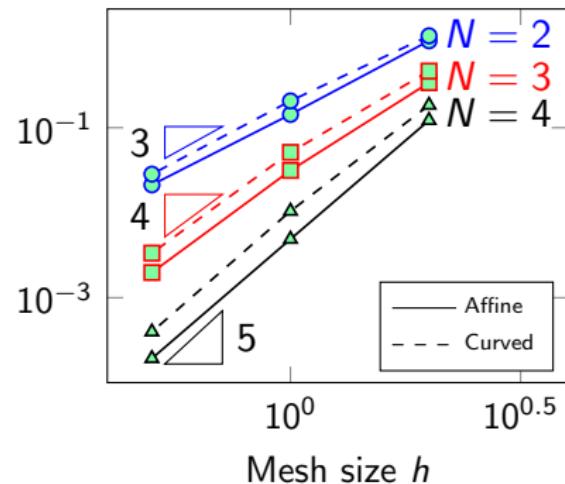
Kopriva (2006). Metric identities and the discontinuous spectral element method on curvilinear meshes.

Chan, Hewett, and Warburton (2016). *Weight-adjusted discontinuous Galerkin methods: curvilinear meshes*.

Smooth isentropic vortex and curved meshes in 2D/3D



(a) 2D results



(b) 3D results

L^2 errors for 2D/3D isentropic vortex at $T = 5$ on affine, curved meshes.

Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.

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Taylor-Green vortex

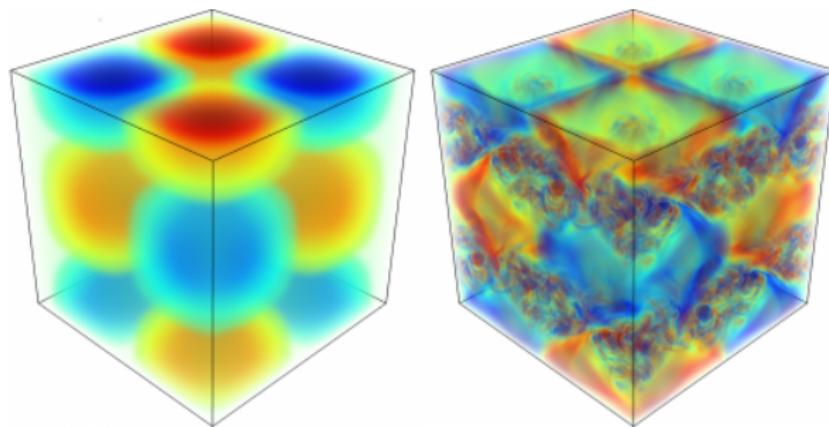
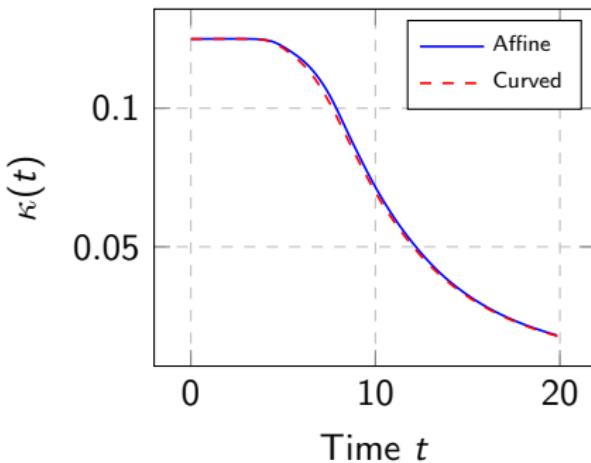


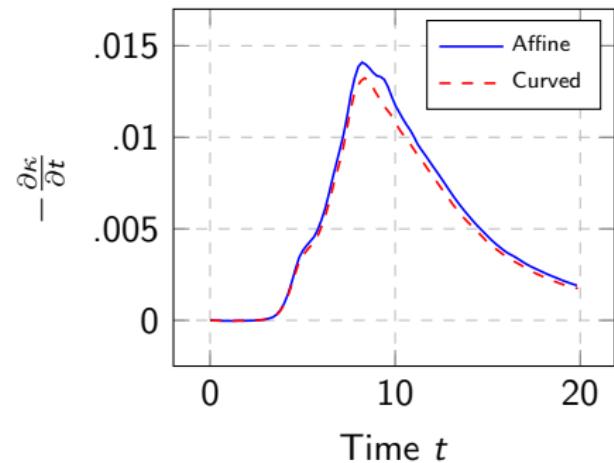
Figure: Isocontours of z -vorticity for Taylor-Green at $t = 0, 10$ seconds.

- Simple turbulence-like behavior (generation of small scales).
- Inviscid Taylor-Green: tests robustness w.r.t. under-resolved solutions.

Taylor-Green vortex: kinetic energy dissipation rate



(a) Kinetic energy



(b) KE dissipation rate

Figure: Evolution of kinetic energy $\kappa(t)$ and kinetic energy dissipation rate $-\frac{\partial \kappa}{\partial t}$ for $N = 3$, $h = \pi/8$, CFL = .25 on affine and curved meshes.

Taylor-Green vortex: kinetic energy dissipation rate

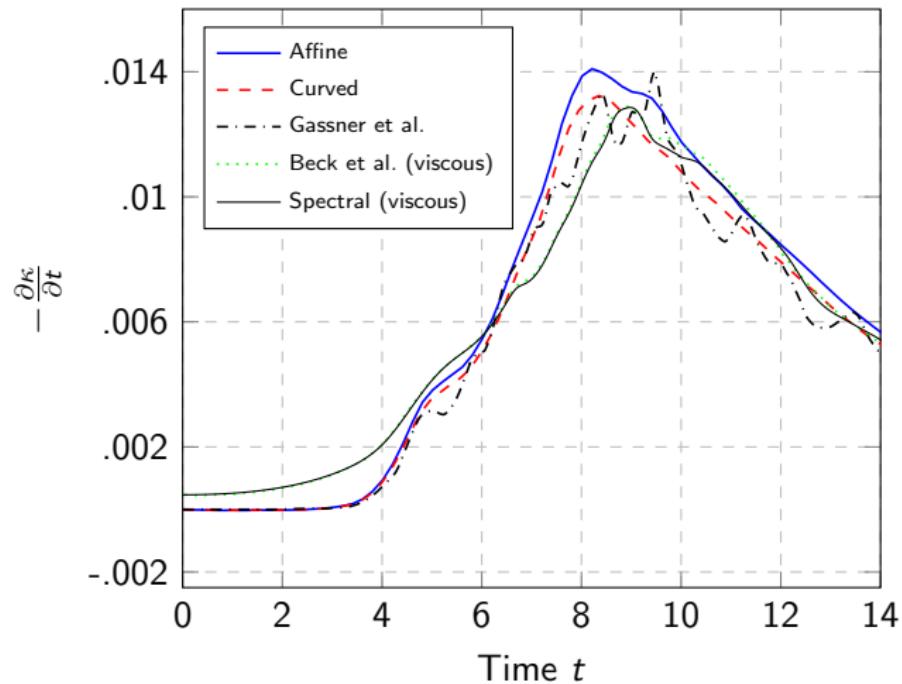
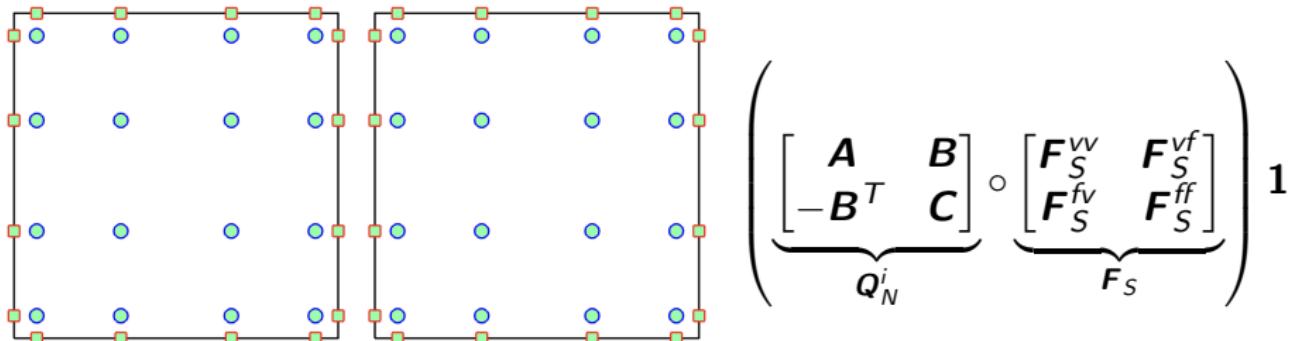


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Talk outline

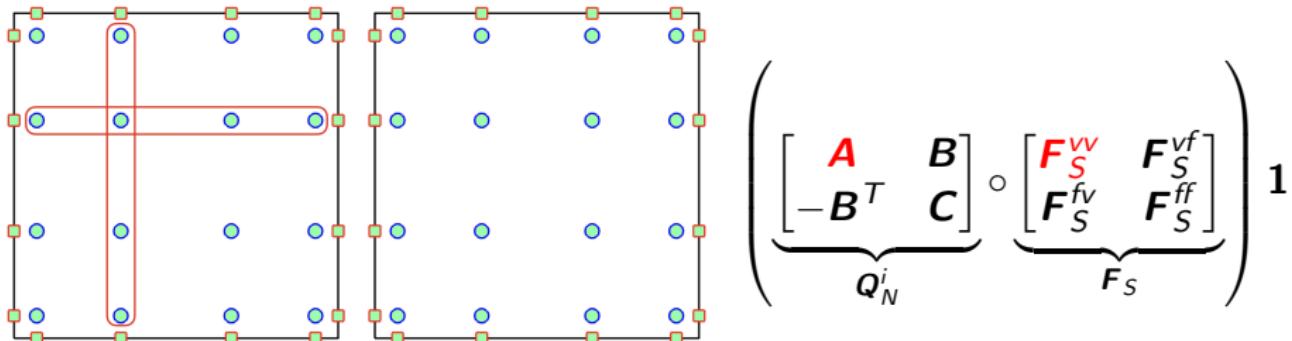
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Entropy stable Gauss collocation: main steps



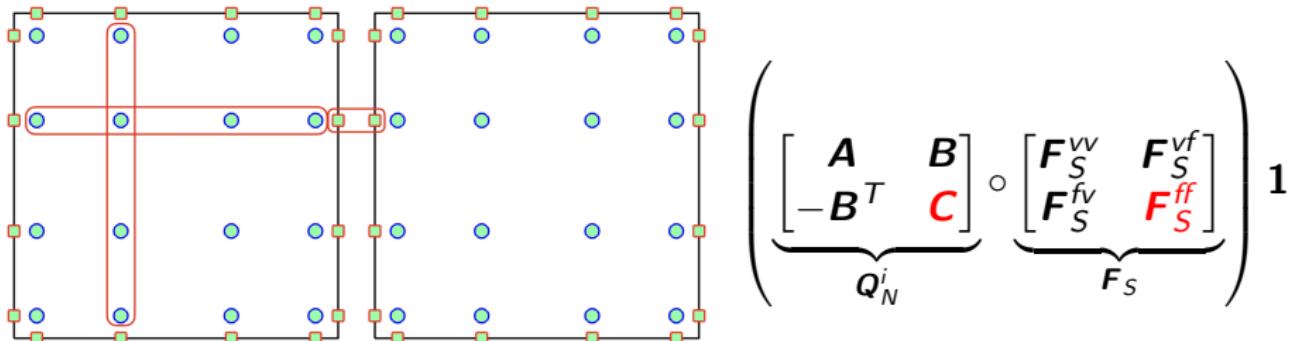
- Advantage over tetrahedral elements: tensor product structure.
- Reduces computational costs from $O(N^6)$ to $O(N^4)$ in 3D.
- New approach: collocate at Gauss nodes instead of GLL nodes.

Entropy stable Gauss collocation: main steps



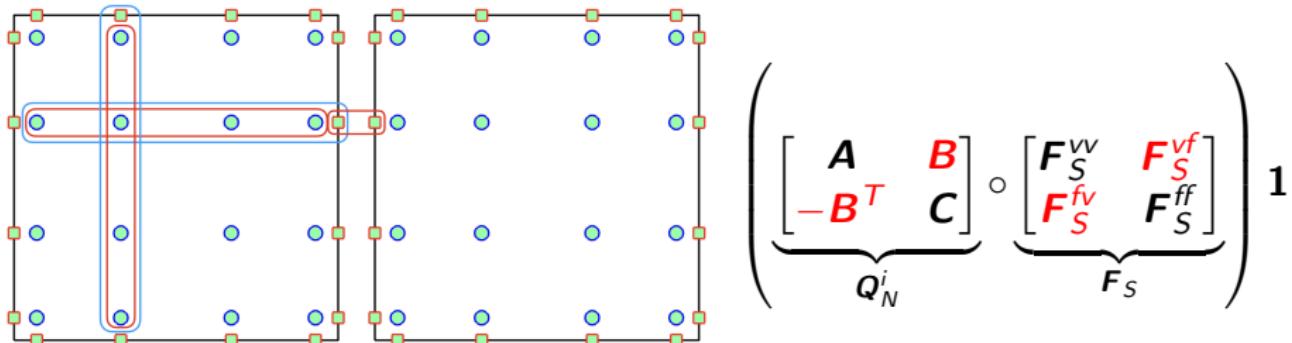
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Improved errors on curved meshes

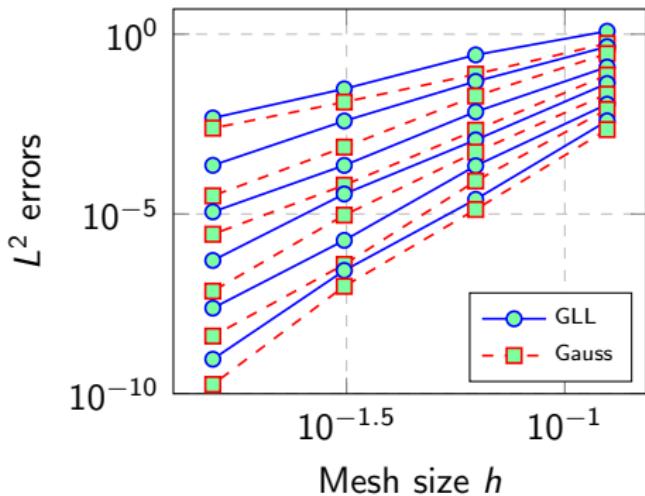
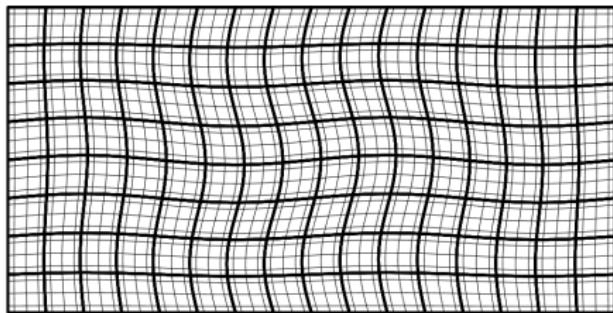


Figure: L^2 errors for the 2D isentropic vortex at time $T = 5$ for degree $N = 2, \dots, 7$ GLL and Gauss collocation schemes (similar behavior in 3D).

Improved errors on curved meshes

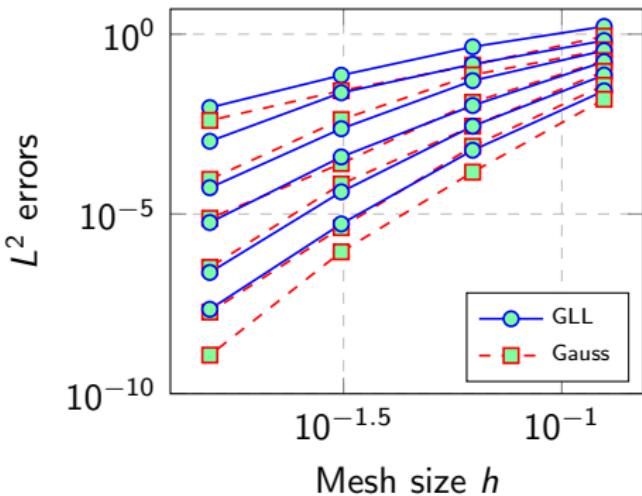
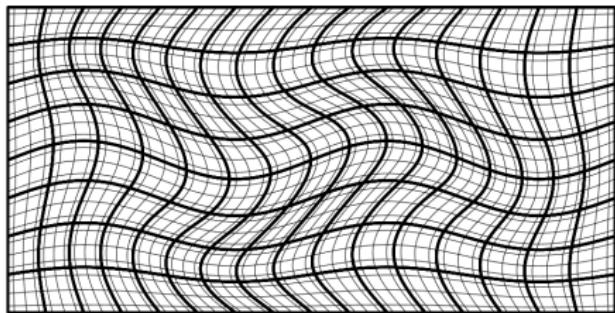


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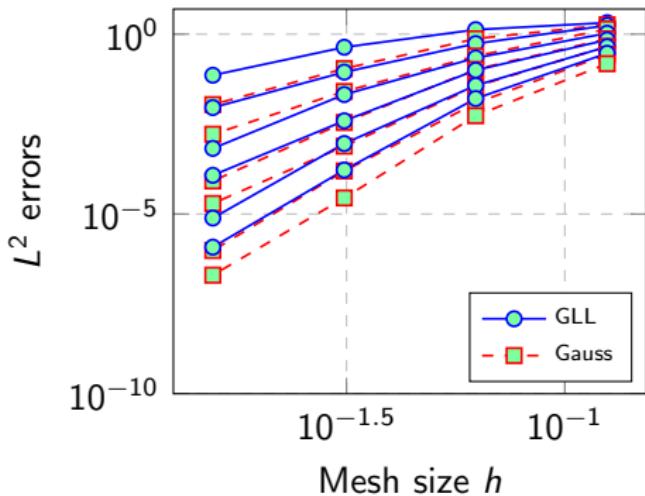
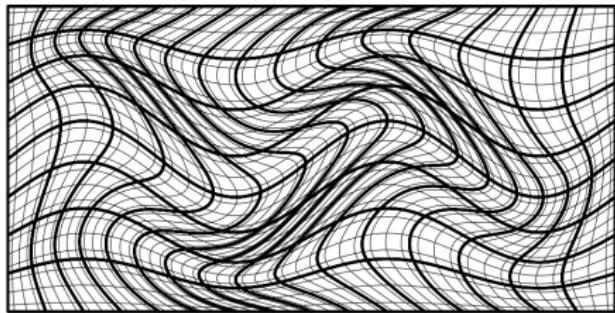
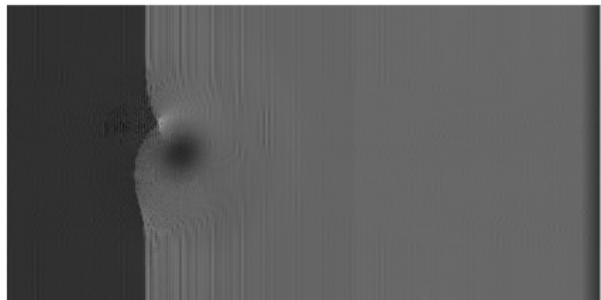
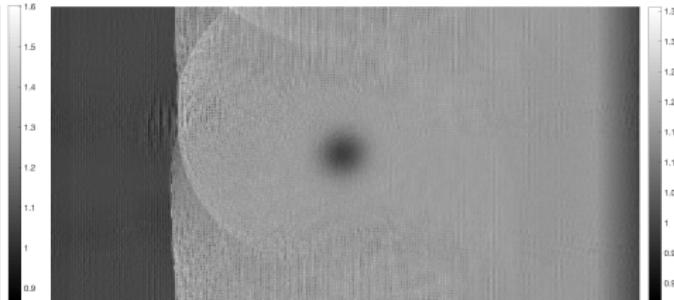


Figure: L^2 errors for the 2D isentropic vortex at time $T = 5$ for degree $N = 2, \dots, 7$ GLL and Gauss collocation schemes (similar behavior in 3D).

Shock vortex interaction



(a) Entropy conservative flux, $T = .3$



(b) Entropy conservative flux, $T = .7$

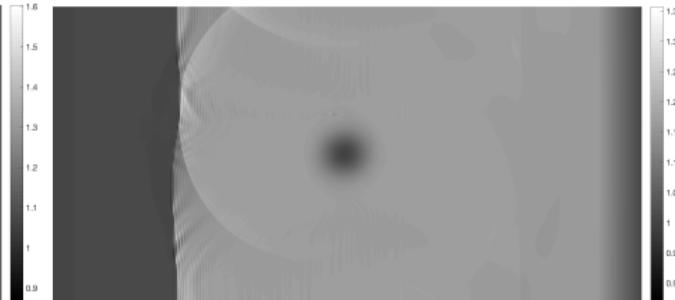
Figure: Shock vortex interaction problem using high order entropy stable Gauss collocation schemes with $N = 4, h = 1/100$.

Winters, Derigs, Gassner, and Walch (2017). *A uniquely defined entropy stable matrix dissipation operator for high Mach number ideal MHD and compressible Euler simulations.*

Shock vortex interaction



(a) Lax-Friedrichs flux, $T = .3$



(b) Lax-Friedrichs flux, $T = .7$

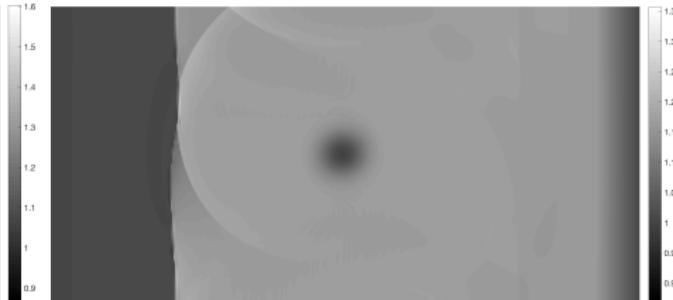
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Shock vortex interaction



(a) Matrix dissipation flux, $T = .3$

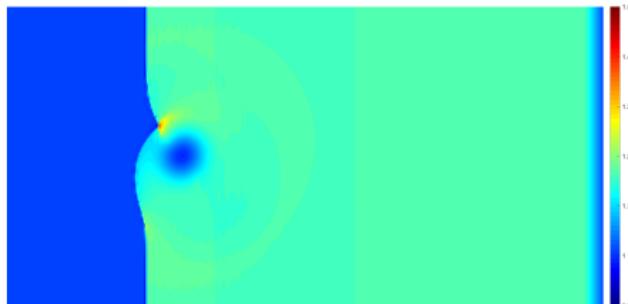


(b) Matrix dissipation flux, $T = .7$

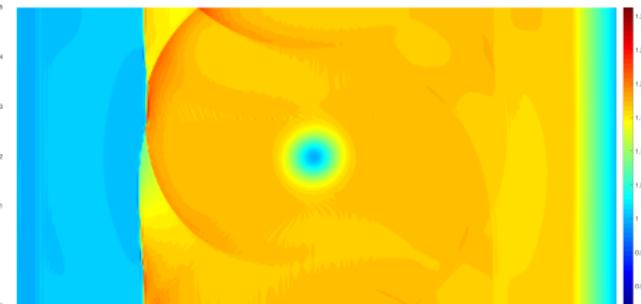
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(a) Matrix dissipation flux, $T = .3$



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Summary and future work

- Entropy stable high order discontinuous Galerkin methods:
semi-discrete stability, improved robustness.
- Additional work required for strong shocks, positivity preservation.
- Currently: hybrid + non-conforming meshes, multi-GPU.
- This work is supported by DMS-1719818 and DMS-1712639.

Thank you! Questions?



Chan, Del Rey Fernandez, Carpenter (2018). *Efficient entropy stable Gauss collocation methods*.

Chan, Wilcox (2018). *On discretely entropy stable weight-adjusted DG methods: curvilinear meshes*.

Chan, Hewett, and Warburton (2016). *Weight-adjusted discontinuous Galerkin methods: curvilinear meshes*.

Chan (2017). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods*.

Additional slides

Over-integration is ineffective without L^2 projection

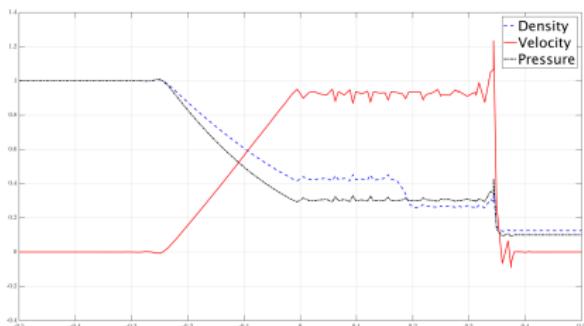
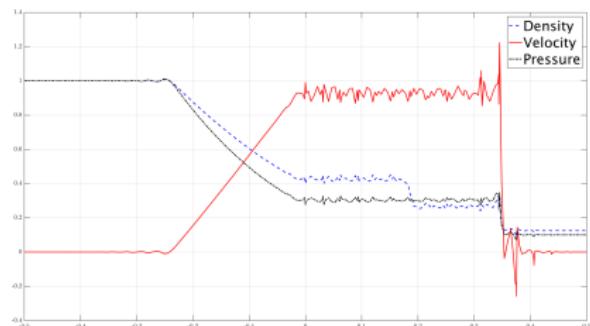
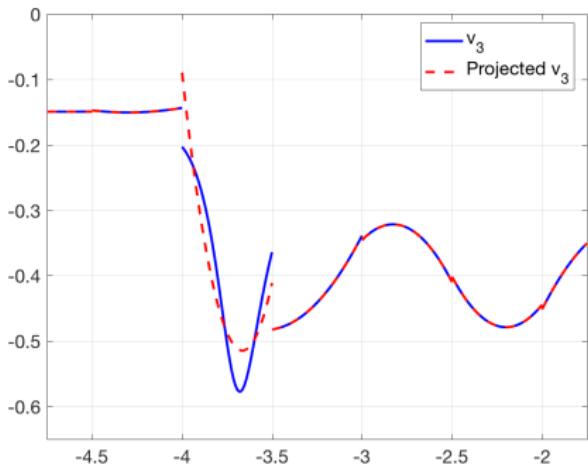
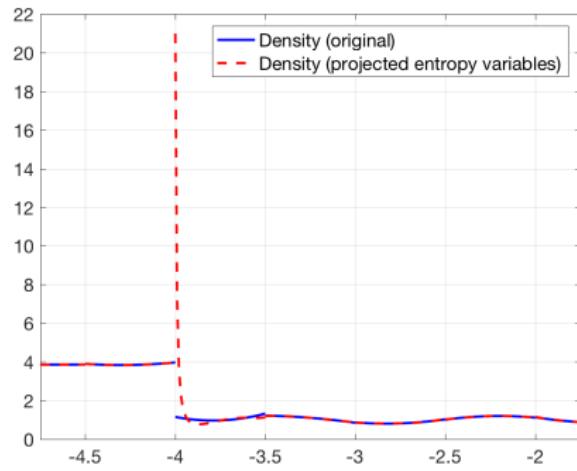
(a) $(N + 1)$ points(b) $(N + 4)$ points

Figure: Numerical results for the Sod shock tube for $N = 4$ and $K = 32$ elements. Over-integrating by increasing the number of quadrature points does not improve solution quality.

On CFL restrictions

- For GLL- $(N + 1)$ quadrature, $\tilde{\mathbf{u}} = \mathbf{u} (P_N \mathbf{v}) = \mathbf{u}$ at GLL points.
- For GQ- $(N + 2)$, discrepancy between L^2 projection and interpolation.
- Still need **positivity** of thermodynamic quantities for stability!

(a) $v_3(x), (P_N v_3)(x)$ (b) $\rho(x), \rho((P_N \mathbf{v})(x))$

High order DG on many-core (GPU) architectures

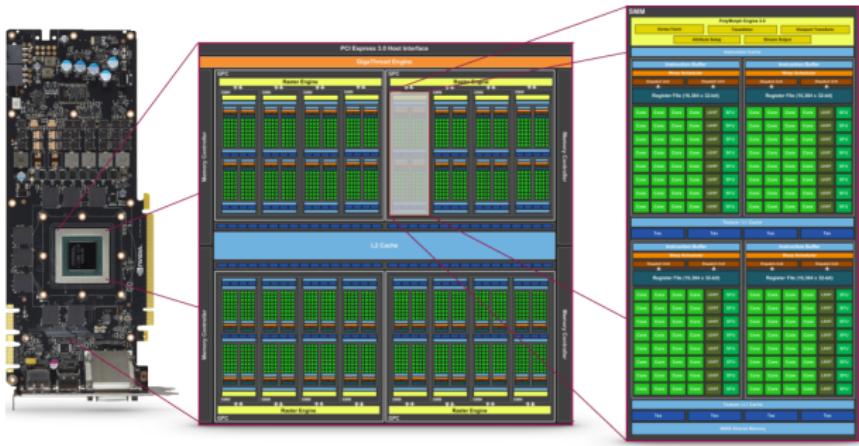


Figure: NVIDIA Maxwell GM204 GPU: 16 cores, 4 SIMD clusters of 32 units.

- Thousands of processing units organized in synchronized groups.
- No free lunch: **memory costs** (accesses, transfer, latency, storage).

High order DG on many-core (GPU) architectures

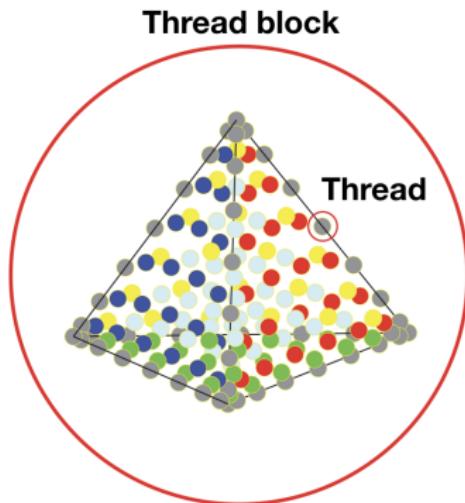


Figure: Thread blocks process elements, threads process degrees of freedom.

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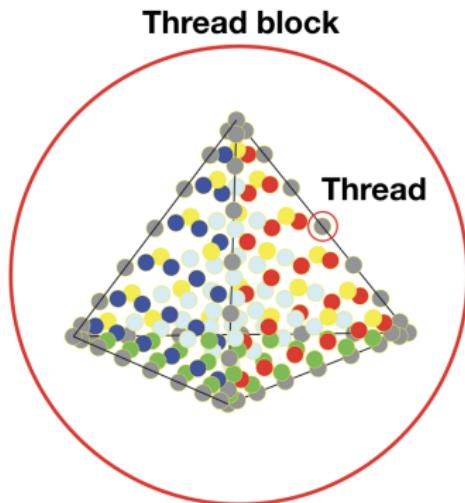


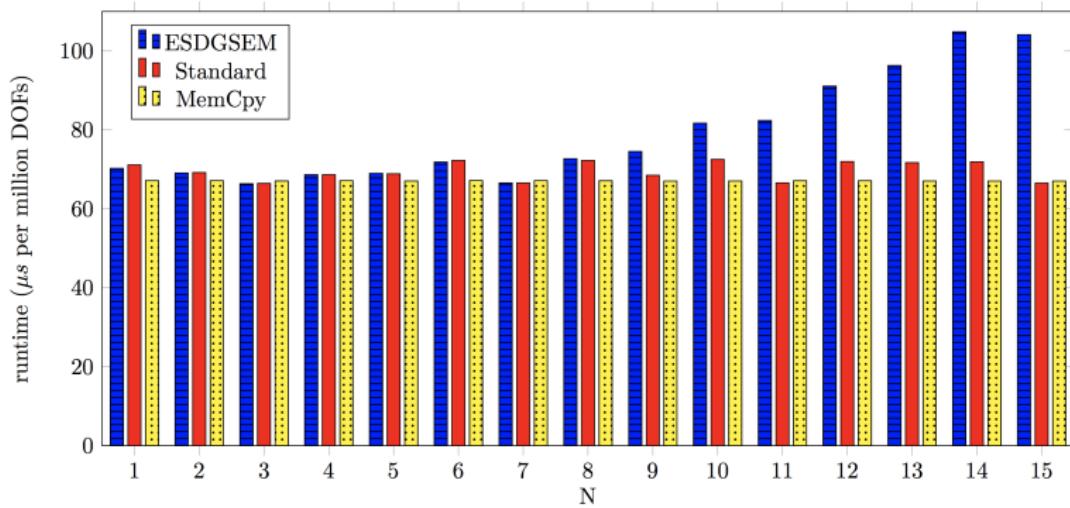
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Implementing high order entropy stable DG on GPUs

- “FLOPS are free, **but** . . . ”
(bytes are expensive) / (memory is dear) / (**postage is extra**)
- Standard considerations: minimize CPU-GPU transfers, structured data layouts, reduce global memory accesses, maximize data reuse.
- Arithmetic vs memory latency: need roughly **$O(10)$ operations per byte** of memory accessed (high arithmetic intensity).
- Standard mat-vec: **only $1/10 - 1/2$ FLOPS per byte!**

GPUs and flux differencing: when FLOPS are free



- High arithmetic intensity: compute while waiting for global memory.
- On GPUs, extra operations don't increase runtime until $N \geq 9$!

Wintermeyer, Winters, Gassner, Warburton (2018). *An entropy stable discontinuous Galerkin method for the shallow water equations on curvilinear meshes with wet/dry fronts accelerated by GPUs*.