

Discretely entropy stable discontinuous Galerkin methods

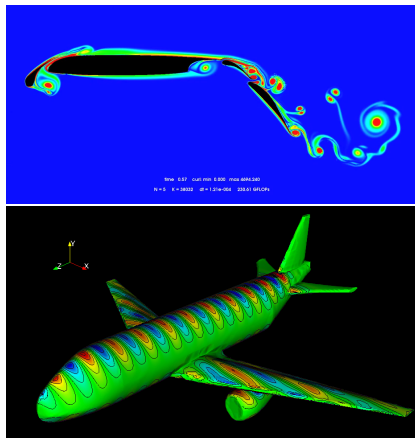
Jesse Chan

¹Department of Computational and Applied Math

TAMES 2017
September 22, 2017

High order methods for hyperbolic PDEs

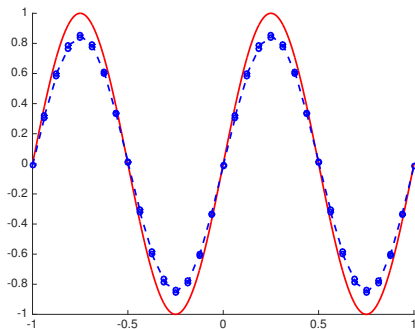
- Time-dependent solutions of wave and fluid PDEs.
- Low numerical dissipation and dispersion (waves and vortices).
- High order approximations: more accurate per unknown.
- Many-core architectures (matrix free explicit time-stepping).



Figures courtesy of T. Warburton.

High order methods for hyperbolic PDEs

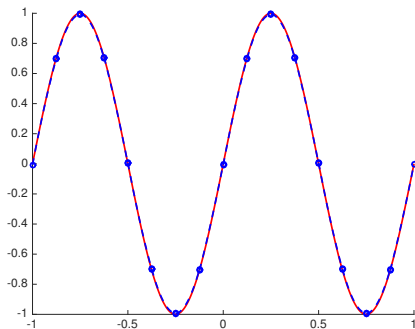
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Fine linear approximation.

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Coarse quadratic approximation.

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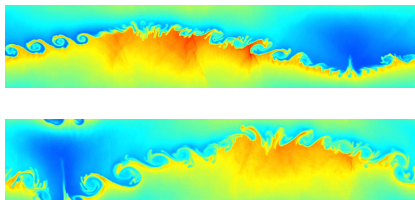


Figure courtesy of Per-Olof Persson.

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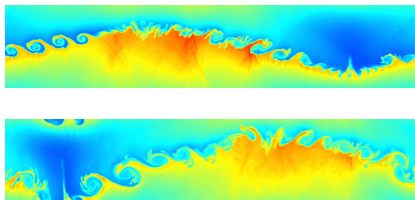
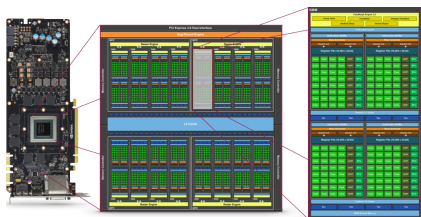


Figure courtesy of Per-Olof Persson.

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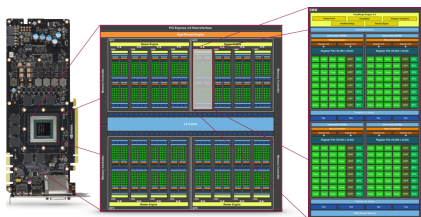
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A graphics processing unit (GPU).

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Goal: address inherent **instability** of high order methods!

Talk outline

- 1 High order DG methods
- 2 Nonlinear stability for conservation laws
- 3 Continuous entropy stable formulations
- 4 Numerical experiments, higher dimensions, curved meshes

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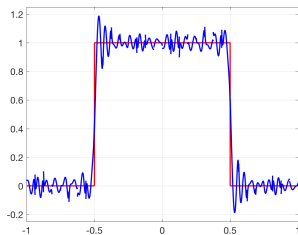
High order DG methods for linear problems

- Constant **linear** advection on $[-1, 1]$

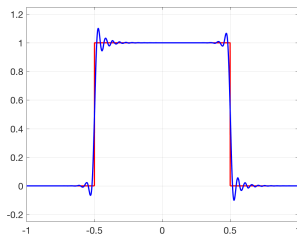
$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad u(-1) = u(1).$$

- Semi-discrete form: let $[[u]] = u^+ - u^-$ and $\tau \geq 0$

$$\sum_k \int_{D^k} \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} \right) v + \int_{\partial D^k} \frac{n_x - \tau |n_x|}{2} [[u]] v = 0, \quad \forall v \in V_h.$$



(a) Central flux ($\tau = 0$)



(b) Upwind flux ($\tau = 1$)

DG energy estimates for linear advection

- Let $V_h = \bigoplus_k P^N(D^k)$, define global DG derivative $D_h^x : V_h \rightarrow V_h$:

$$(D_h^x u, v)_\Omega = \sum_{D^k} \left(\frac{\partial u}{\partial x}, v \right)_{D^k} + \frac{1}{2} \langle \llbracket u \rrbracket, v \rangle_{\partial D^k}, \quad v \in V_h,$$

$$(D_h^x u, v)_\Omega = \langle u, v \rangle_{\partial \Omega} - (u, D_h^x v)_\Omega, \quad (\text{integration-by-parts}).$$

- Advection formulation: semi-definite penalization $s(u, v)$

$$\left(\frac{\partial u}{\partial t} + D_h^x u, v \right)_\Omega + \underbrace{\sum_k \left\langle -\tau \frac{|n_x|}{2} \llbracket u \rrbracket, v \right\rangle_{\partial D^k}}_{s(u, v), \text{ pos. semi-def.}}.$$

- Energy method (periodic domains): take $v = u$, integrate by parts

$$\frac{1}{2} \frac{\partial}{\partial t} \|u\|_{L^2(\Omega)}^2 = -s(u, u) \leq 0.$$

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Entropy stability for nonlinear conservation laws

- System of nonlinear conservation laws, convex **entropy** $S(\mathbf{u})$

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

- **Nonlinear** entropy inequality: chain rule + entropy potential ψ

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

- Periodic linear advection: square entropy, $\mathbf{v} = \mathbf{u}$

$$\int_{\Omega} \frac{\partial S(u)}{\partial t} \leq 0, \quad S(u) = \frac{u^2}{2}.$$

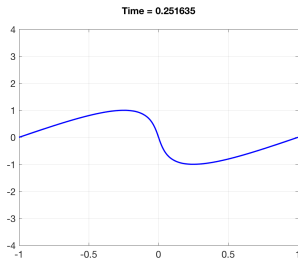
Discrete instability for nonlinear conservation laws

- How to differentiate $f(u)$? Burgers' equation: $f(u) = u^2/2$

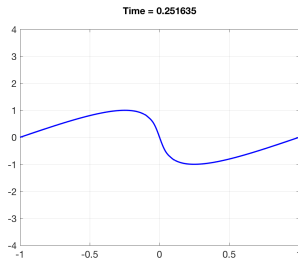
$$\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = 0, \quad u \in V_h, \quad u^2 \notin V_h.$$

- Loss of chain rule with L^2 projection P_N or inexact quadrature.

$$\left(\frac{\partial u}{\partial t} + \frac{1}{2} D_h^x P_N u^2, v \right)_\Omega = 0, \quad \frac{1}{2} \frac{\partial P_N u^2}{\partial x} \neq P_N \left(u \frac{\partial u}{\partial x} \right)$$



(a) $N = 7, K = 8$



(b) $N = 7, K = 9$

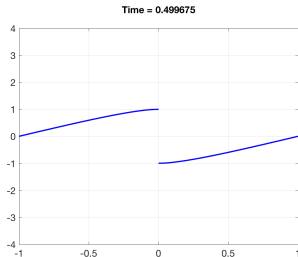
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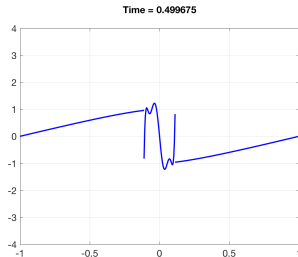
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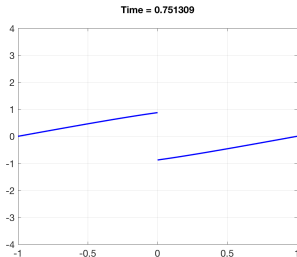
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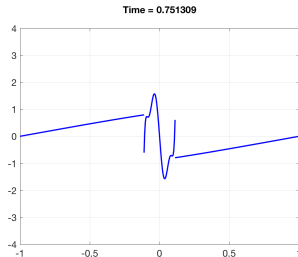
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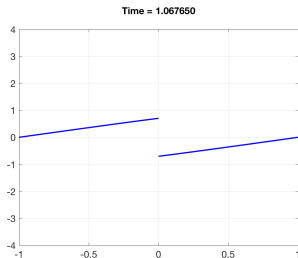
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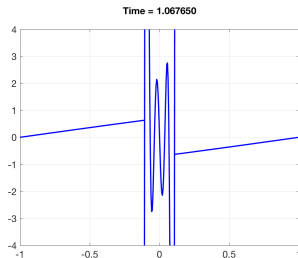
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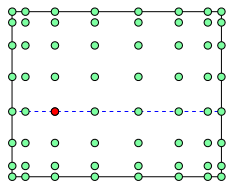
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Entropy stable (ES) summation-by-parts (SBP) methods

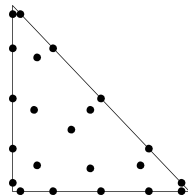
- Entropy conservation: needs **mass lumping, nodal collocation!**

$$(\mathbf{I}_n \otimes \mathbf{M}) \frac{\partial \mathbf{u}}{\partial t} + (2(\mathbf{I}_n \otimes \mathbf{S}) \circ \mathbf{F}_S) \mathbf{1} = 0, \quad (\text{Semi-discrete form})$$

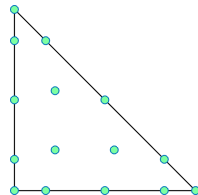
$$\implies \mathbf{1}^T \left(\mathbf{M} \frac{\partial S}{\partial t} + \mathbf{B} (\mathbf{v}^T \mathbf{f} - \psi) \right) = 0, \quad (\text{Entropy conservation})$$



(c) Tensor product SBP nodes (GLL quadrature)



(d) Diag-norm SBP nodes ($N = 4, 22$ pts)



(e) Non-SBP nodes ($N = 4, 15$ pts)

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.*

Chen and Shu (2017). *ES high order DG methods with suitable quadrature rules for hyperbolic conservation laws.*

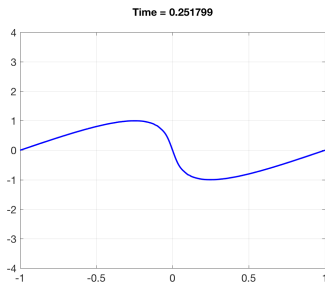
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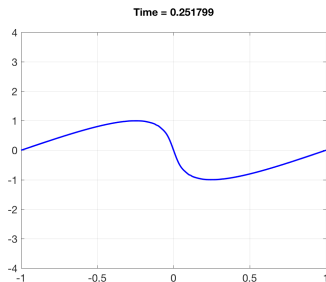
Burgers' equation: energy stable formulations

- Split formulation (replace $\frac{\partial}{\partial x}$ with some D_h^\times + stabilization for DG).

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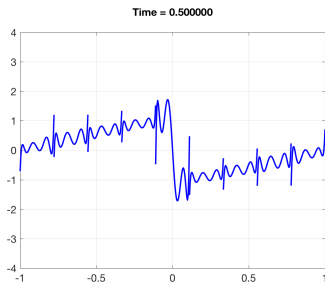
(b) $\tau = 1$

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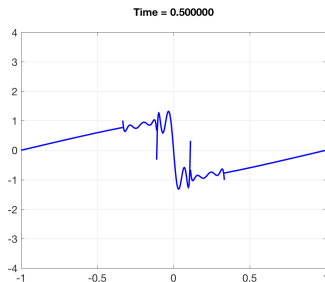
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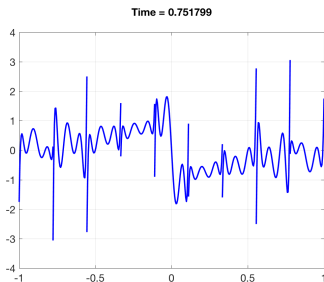


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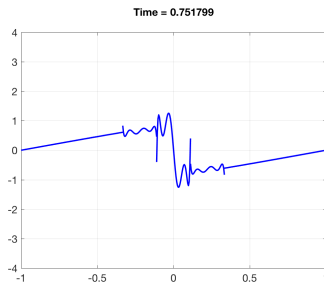
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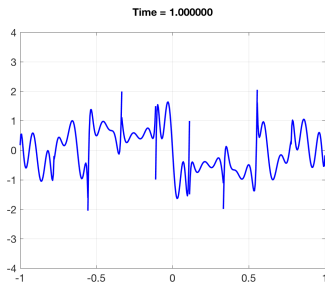


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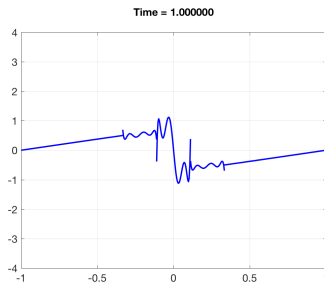
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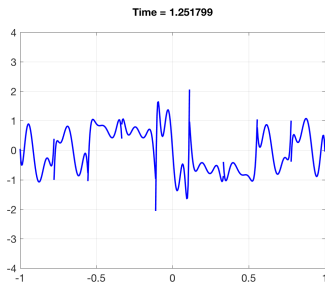


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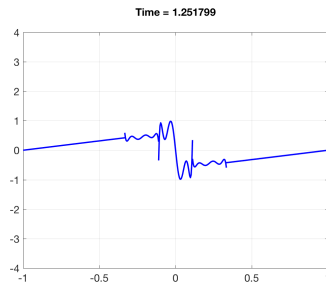
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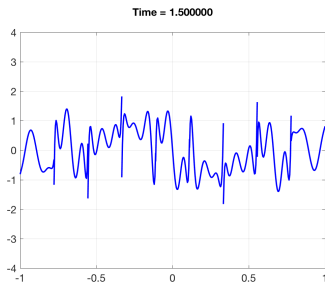
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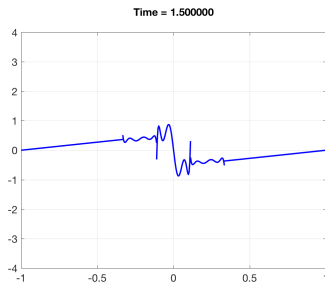
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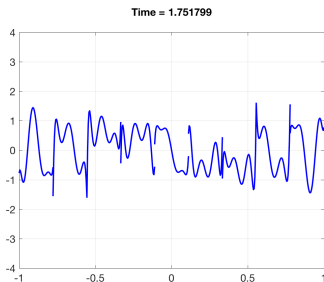
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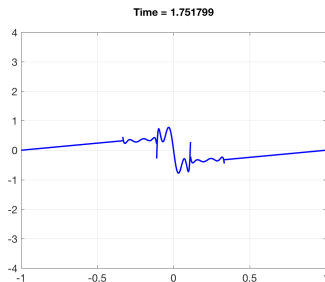
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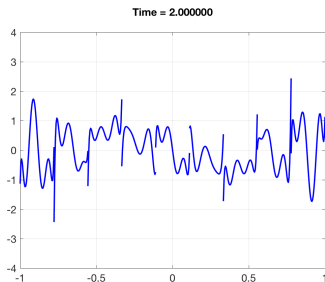
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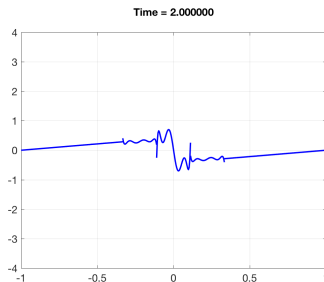
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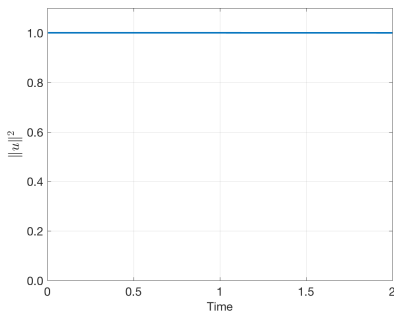
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Burgers' equation: energy stable formulations

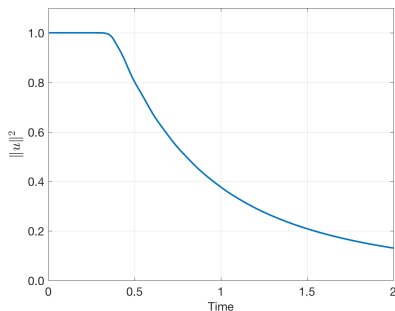
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(a) Energy conservative ($\tau = 0$)



(b) Energy stable ($\tau = 1$)

Flux differencing: split formulations and beyond

- Tadmor's entropy conservative finite volume flux

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

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

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

- Easy example: Burgers' equation, let $u_L = u(x)$, $u_R = u(y)$

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

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

- Harder example: compressible Euler (entropy conservative mass flux)

$$f_S^\rho(\mathbf{u}_L, \mathbf{u}_R) = \{\{\rho\}\}^{\log} \{\{u\}\}, \quad \{\{u\}\}^{\log} = \frac{u_L - u_R}{\log u_L - \log u_R}.$$

Flux differencing: split formulations and beyond

- Tadmor's entropy conservative finite volume flux

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

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

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

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Discrete entropy conservation: a continuous formulation

Theorem (Chan 2017)

Let $\mathbf{u}_x = \mathbf{u}((P_N \mathbf{v})(x))$, $\mathbf{u}_y = \mathbf{u}((P_N \mathbf{v})(y))$, and let \mathbf{u} solve

$$\left(\frac{\partial \mathbf{u}}{\partial t} + (2D_h^\times \mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y))|_{y=x}, \mathbf{w} \right)_\Omega = 0, \quad \forall \mathbf{w} \in V_h.$$

Then \mathbf{u} satisfies $\int_\Omega \frac{\partial S(\mathbf{u})}{\partial t} + \int_{\partial\Omega} P_N \mathbf{v}^T \mathbf{f}(\mathbf{u}_x) - \psi(\mathbf{u}_x) = 0$.

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Sketch of proof

Step 1 (time term): take $\mathbf{w} = P_N \mathbf{v}(\mathbf{u})$. For method of lines, $\frac{\partial \mathbf{u}}{\partial t} \in V_h$.

$$\left(\frac{\partial \mathbf{u}}{\partial t}, P_N \mathbf{v} \right)_{\Omega} = \left(\frac{\partial \mathbf{u}}{\partial t}, \mathbf{v} \right)_{\Omega} = \left(\frac{\partial S}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial t}, 1 \right)_{\Omega} = \left(\frac{\partial S(\mathbf{u})}{\partial t}, 1 \right)_{\Omega}.$$

Discrete entropy conservation: a continuous formulation

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Sketch of proof

Step 2 (spatial term): integrate by parts.

$$\begin{aligned} & \left((D_h^x \mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y))|_{y=x}, P_N \mathbf{v} \right)_{\Omega} \\ & + \langle \mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_x), (P_N \mathbf{v}) \mathbf{n}_x \rangle_{\partial \Omega} - \left(D_h^x (\mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y)(P_N \mathbf{v})(x))|_{y=x}, 1 \right)_{\Omega}. \end{aligned}$$

Discrete entropy conservation: a continuous formulation

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Let $\mathbf{u}_x = \mathbf{u}((P_N \mathbf{v})(x))$, $\mathbf{u}_y = \mathbf{u}((P_N \mathbf{v})(y))$, and let \mathbf{u} solve

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Then \mathbf{u} satisfies $\int_{\Omega} \frac{\partial S(\mathbf{u})}{\partial t} + \int_{\partial \Omega} P_N \mathbf{v}^T \mathbf{f}(\mathbf{u}_x) - \psi(\mathbf{u}_x) = 0$.

Sketch of proof

Step 2 (spatial term): gather volume terms, use conservation and IBP.

$$\begin{aligned} & \left(D_h^x (\mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y) ((P_N \mathbf{v})(x) - (P_N \mathbf{v})(y)))|_{y=x}, 1 \right)_{\Omega} \\ &= \left(D_h^x (\psi(\mathbf{u}_x) - \psi(\mathbf{u}_y))|_{y=x}, 1 \right)_{\Omega} = \langle \psi(\mathbf{u}_x), 1 \mathbf{n}_x \rangle_{\partial \Omega}. \end{aligned}$$

Discrete entropy conservation: a continuous formulation

Theorem (Chan 2017)

Let $\mathbf{u}_x = \mathbf{u}((P_N \mathbf{v})(x))$, $\mathbf{u}_y = \mathbf{u}((P_N \mathbf{v})(y))$, and let \mathbf{u} solve

$$\left(\frac{\partial \mathbf{u}}{\partial t} + (2D_h^x \mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y))|_{y=x}, \mathbf{w} \right)_{\Omega} = 0, \quad \forall \mathbf{w} \in V_h.$$

Then \mathbf{u} satisfies $\int_{\Omega} \frac{\partial S(\mathbf{u})}{\partial t} + \int_{\partial \Omega} P_N \mathbf{v}^T \mathbf{f}(\mathbf{u}_x) - \psi(\mathbf{u}_x) = 0$.

- Difficulty: $\mathbf{u} \in V_h$, but $\mathbf{v}(\mathbf{u}) \notin V_h$! Need $\mathbf{u} = \mathbf{u}(P_N \mathbf{v})$ for

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

- Proof requires only (inexact) quadrature-based L^2 projection + IBP.
- Jump stabilization $s(u, v)$ gives entropy **inequality**.

Entropy stable high order DG: implementation

- Efficient reformulation (Hadamard product: low-memory evaluation)

$$\begin{aligned}
 & P_N \left(\left. \frac{\partial P_N \mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y)}{\partial x} \right|_{y=x} \right) \\
 &= \mathbf{P}_q \text{diag}(\mathbf{V}_q \mathbf{D} \mathbf{P}_q \mathbf{F}_S) = \mathbf{P}_q ((\mathbf{V}_q \mathbf{D} \mathbf{P}_q \circ \mathbf{F}_S) \mathbf{1}).
 \end{aligned}$$

- Explicit time-stepping right hand side evaluation:

- 1 Compute $P_N(\mathbf{v}(\mathbf{u}))$.
- 2 Evaluate $\mathbf{u} = \mathbf{u}(P_N(\mathbf{v}(\mathbf{u})))$ at volume, face quadratures.
- 3 Compute $\mathbf{RHS}(\mathbf{u}) = 2(\mathbf{D}_h \circ \mathbf{F}_S(\mathbf{u}_x, \mathbf{u}_y)) \mathbf{1}$

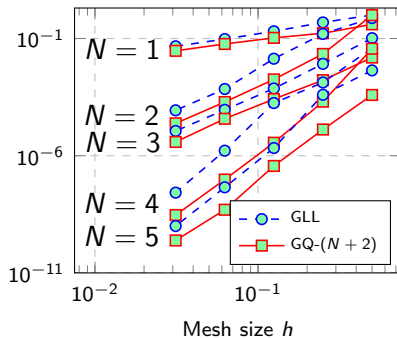
- Simplifications for diag-norm SBP (nodal collocation): avoid computing projections, combine volume + surface operations.

Talk outline

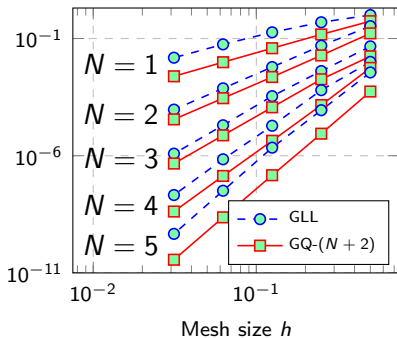
- 1 High order DG methods
- 2 Nonlinear stability for conservation laws
- 3 Continuous entropy stable formulations
- 4 Numerical experiments, higher dimensions, curved meshes

Numerical experiments: compressible Euler equations

- Entropy conservative (EC) and Lax-Friedrichs (LF) fluxes.
- No additional stabilization, filtering, or limiting.
- L^2 rates: odd/even decoupling for EC, $O(h^{N+1})$ for LF.



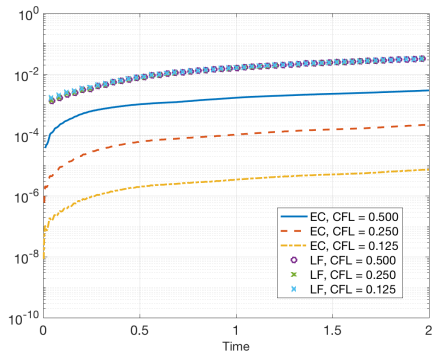
(c) Entropy conservative flux



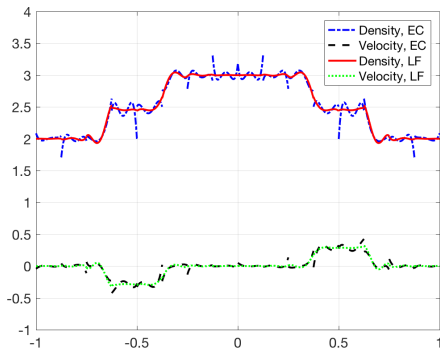
(d) With Lax-Friedrichs penalization

Numerical experiments: entropy conservation

- Entropy conservation: *semi-discrete*, not fully discrete.
- $\Delta S(\mathbf{u}) = |S(\mathbf{u}(x, t)) - S(\mathbf{u}(x, 0))| \rightarrow 0$ as $\Delta t \rightarrow 0$.



(e) $\Delta S(\mathbf{u})$ for various Δt

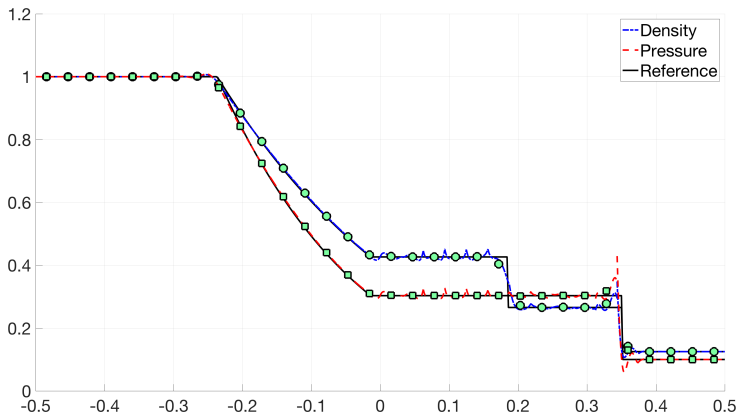


(f) $\rho(x), u(x)$ ($N = 4, K = 16$)

$\Delta S(\mathbf{u})$ and solution for entropy conservative (EC) and Lax-Friedrichs (LF) fluxes.

Numerical experiments: Sod shock tube

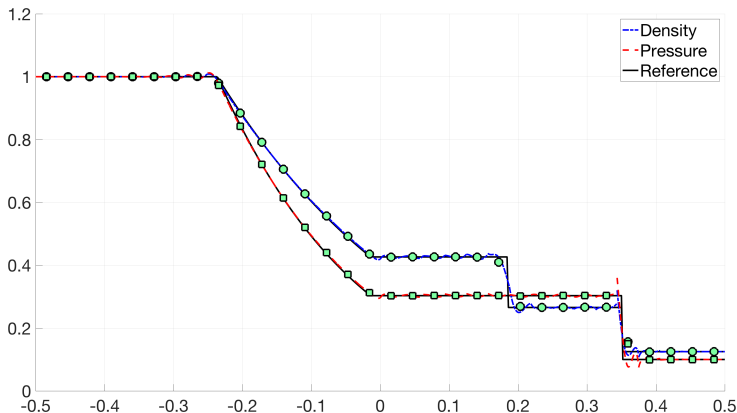
- Cell averages overlaid as circles.
- CFL of .125 used for both GLL- $(N + 1)$ and GQ- $(N + 2)$.



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

Numerical experiments: Sod shock tube

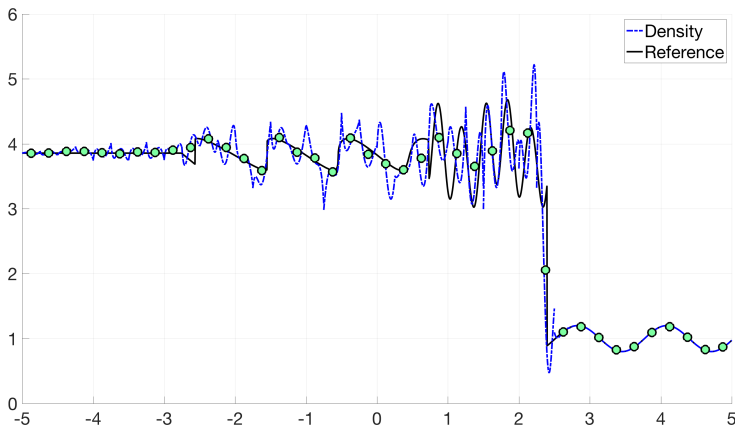
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$N = 4, K = 32, (N + 2)$ point Gaussian quadrature.

Numerical experiments: sine-shock interaction

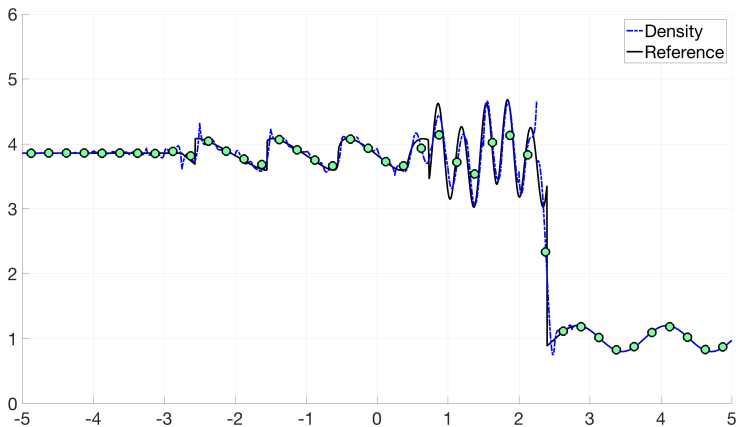
- Reference solution, smaller CFL (.05 vs .125) for GQ- $(N + 2)$.



$N = 4$, $K = 40$, $(N + 1)$ point Gauss-Lobatto-Legendre quadrature.

Numerical experiments: sine-shock interaction

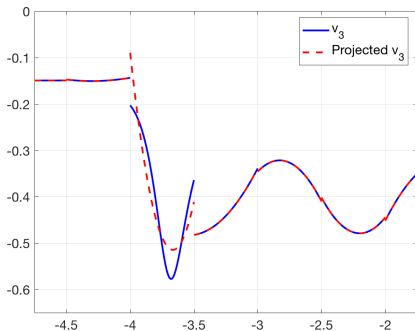
- Reference solution, smaller CFL (.05 vs .125) for GQ- $(N + 2)$.



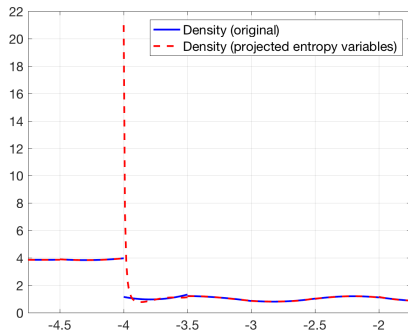
$N = 4, K = 40, (N + 2)$ point Gaussian quadrature.

Numerical experiments: CFL restrictions

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



(g) $v_3(x), (P_N v_3)(x)$



(h) $\rho(x), \rho((P_N \mathbf{v})(x))$

Extension to higher dimensions

- Define global gradient, divergence, e.g.

$$(\nabla_h \cdot \mathbf{u}, v)_\Omega = \sum_k (\nabla \cdot \mathbf{u}, v)_{D^k} + \left\langle \frac{1}{2} \llbracket \mathbf{u} \rrbracket \cdot \mathbf{n}, v \right\rangle_{\partial D^k}$$

$$(\nabla_h u, \mathbf{v})_\Omega = \sum_k (\nabla u, \mathbf{v})_{D^k} + \left\langle \frac{1}{2} \llbracket u \rrbracket \mathbf{n}, \mathbf{v} \right\rangle_{\partial D^k}$$

- Flux differencing: let $\mathbf{u}_x = \mathbf{u}(P_N \mathbf{v}(\mathbf{x}))$, $\mathbf{u}_y = \mathbf{u}(P_N \mathbf{v}(\mathbf{y}))$

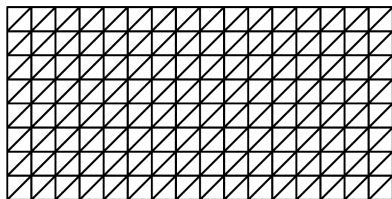
$$\left(\frac{\partial \mathbf{u}}{\partial t} + (2\nabla_h \cdot \mathbf{f}_S(\mathbf{u}_x, \mathbf{u}_y))|_{\mathbf{y}=\mathbf{x}}, \mathbf{w} \right)_\Omega = 0, \quad \forall \mathbf{w} \in V_h.$$

- Entropy stability on curved meshes: modify flux using $\mathbf{G}_{ij} = \frac{\partial \mathbf{x}_i}{\partial \hat{\mathbf{x}}_j}$

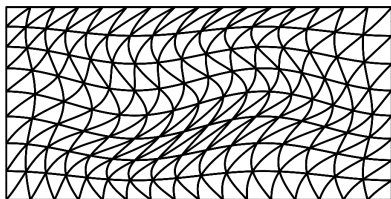
$$\tilde{\mathbf{f}}_S(\mathbf{u}_L, \mathbf{u}_R) = \{\{J\mathbf{G}\}\} \mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R).$$

Numerical results: two-dimensional curvilinear meshes

- Vortex problem at $T = 5$, $\Omega = [0, 20] \times [-5, 5]$, CFL = .25.
- Avoid weighted mass inverse using weight-adjusted approximation.



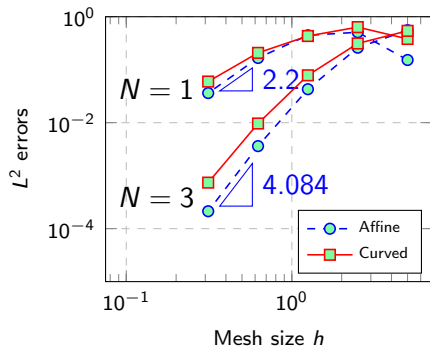
(a) Uniform mesh



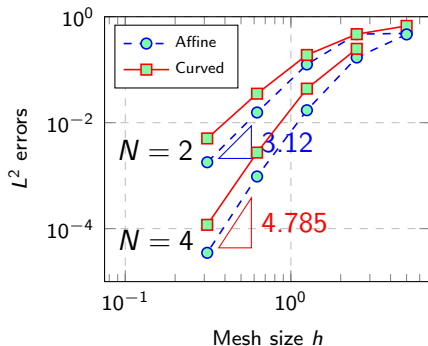
(b) Warped mesh

Numerical results: two-dimensional curvilinear meshes

L^2 error converges at $O(h^{N+1})$ up to time-stepper accuracy (LSERK-45).



(a) Degree $N = 1, N = 3$



(b) Degree $N = 2, N = 4$

Summary and acknowledgements

- Derived discretely entropy stable high order discontinuous Galerkin methods using a continuous formulation.
- Future work: regularization, multi-GPU (with Lucas Wilcox).
- This research is supported by the National Science Foundation under awards DMS-1712639 and DMS-1719818.

Thank you! Questions?



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

Global DG differentiation operator

- Let $v \in V_h$, $u, w \notin V_h$ with u, w bounded; modified D_h^x

$$\begin{aligned} (D_h^x u, vw)_\Omega &= \sum_k \left(\frac{\partial P_N u}{\partial x}, vw \right)_{D^k} \\ &\quad + \frac{1}{2} \langle u^+ - P_N u, vw \mathbf{n}_x \rangle_{\partial D^k} \\ &\quad + \frac{1}{2} \langle u - P_N u, P_N(vw) \mathbf{n}_x \rangle_{\partial D^k}. \end{aligned}$$

- Integration-by-parts property

$$(D_h^x u, vw)_\Omega = \langle u, vw \rangle_{\partial\Omega} - (u, D_h^x(vw))_\Omega.$$

- Coupling only through **surface** values (in contrast to D_h^x with $\llbracket P_N u \rrbracket$).