Discretely entropy stable high order methods for nonlinear conservation laws

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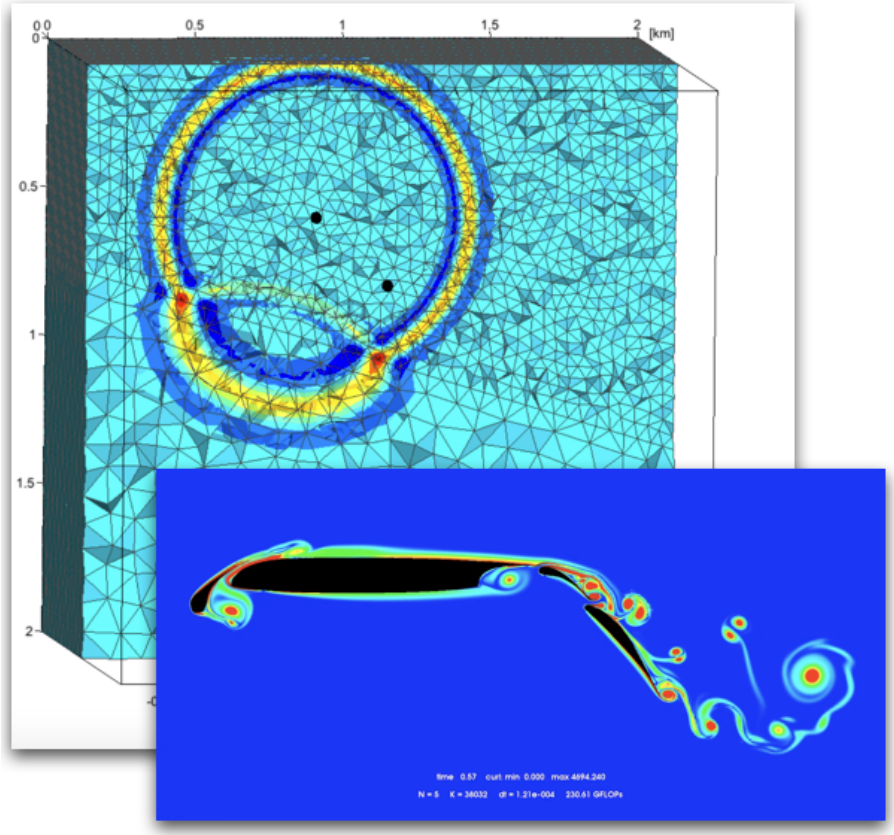
High order methods for time-dependent hyperbolic PDEs

- Accurate resolution of propagating waves and vortices.
- High order: low numerical dissipation and dispersion.
- High order approximations: more accurate per unknown.
- Many-core architectures (efficient explicit time-stepping).



Figures courtesy of T. Warburton, A. Modave.

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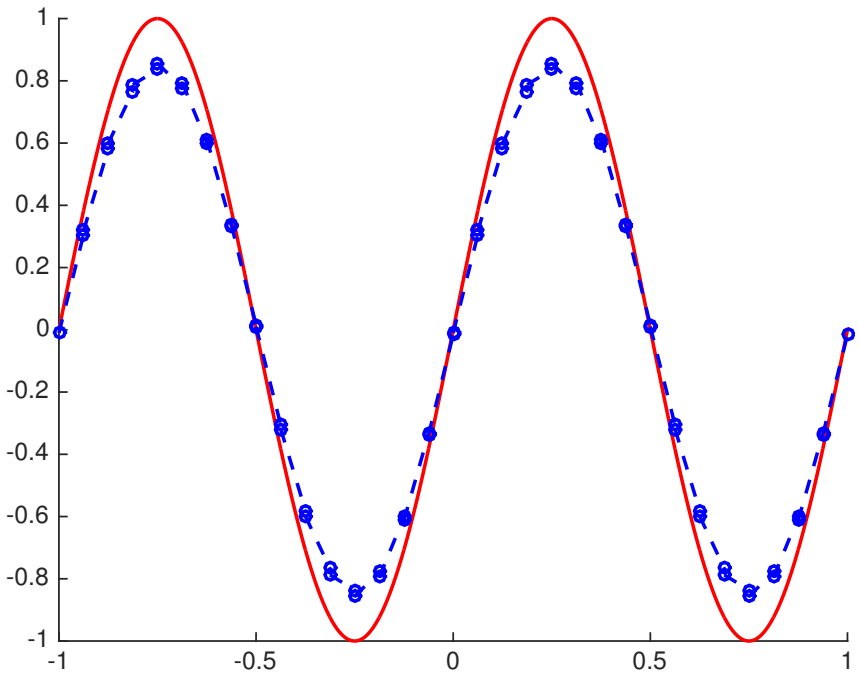

Fine linear approximation.

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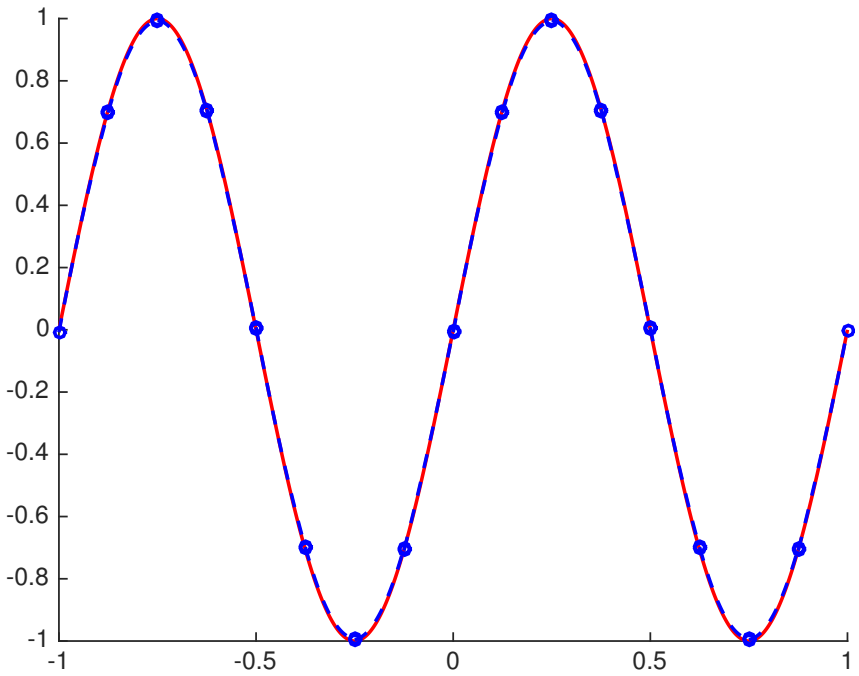

Coarse quadratic approximation.

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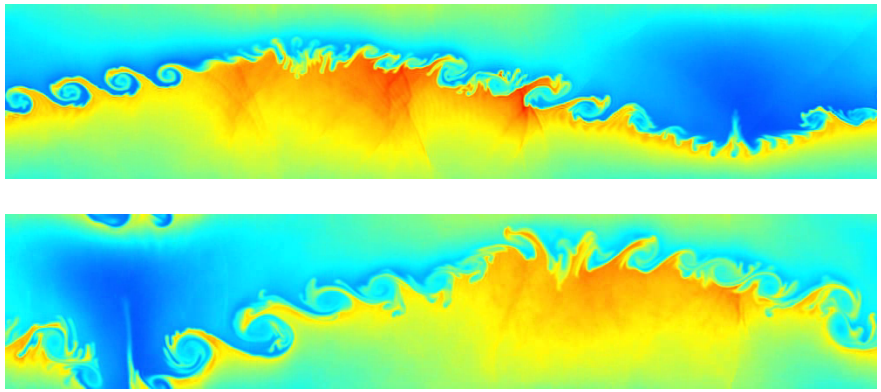

Figure from Per-Olof Persson.

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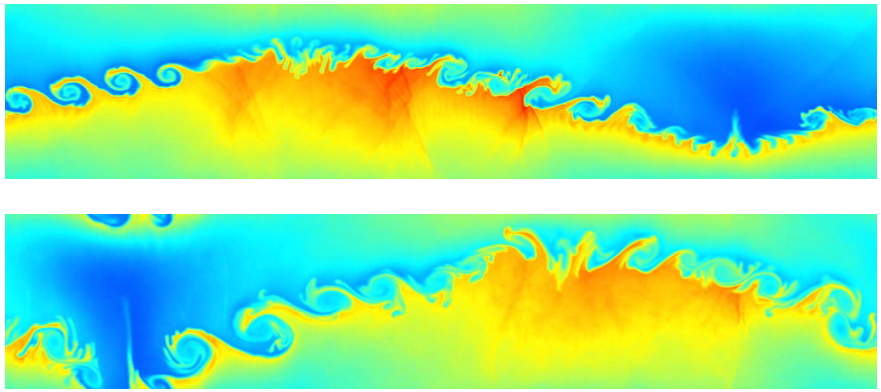

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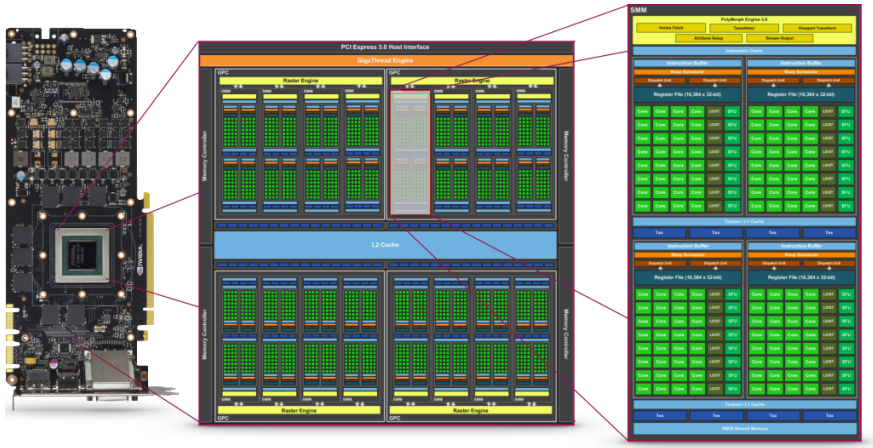
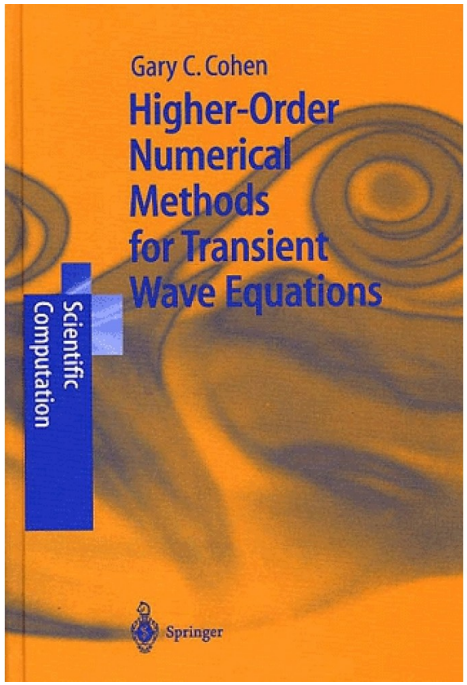


A graphics processing unit (GPU).

What is considered "high order"? Waves vs CFD



- Stability for time-dependent waves, incompressible flow: well established, independent of degree of approx. N.
- High order for waves: $N = 8, 9, 10$ not uncommon (up to $N \approx 20$).
- High order for CFD: $N > 1$ (considered much less robust than low order!)

Goal: address robustness of efficient high order methods for time-dependent systems of nonlinear conservation laws.

Wang, Fidkowski, Abgrall, Bassi, Caraeni, Cary, Deconinck, Hartmann, Hillewaert, Huynh, and Kroll (2013). *High-order CFD methods: current status and perspective*.

Talk outline

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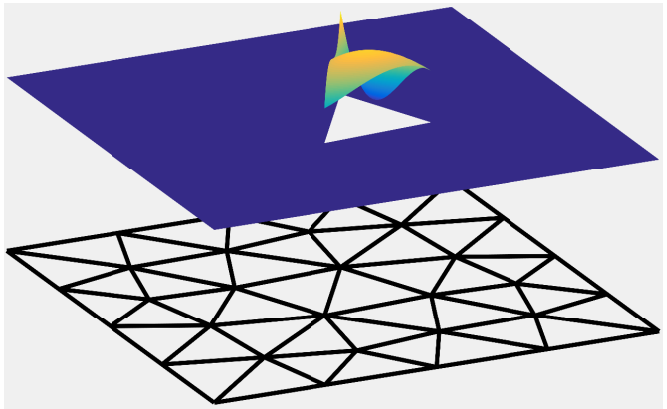
Discontinuous Galerkin methods

Discontinuous Galerkin (DG) methods:

- High order accuracy, geometric flexibility.
- Weak continuity across faces.



- Continuous PDE (example: advection)

$$\frac{\partial u}{\partial t} = \frac{\partial f(u)}{\partial x}, \qquad f(u) = u.$$

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

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

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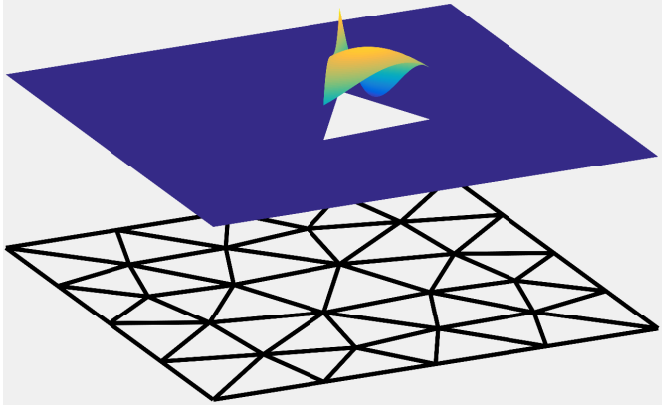
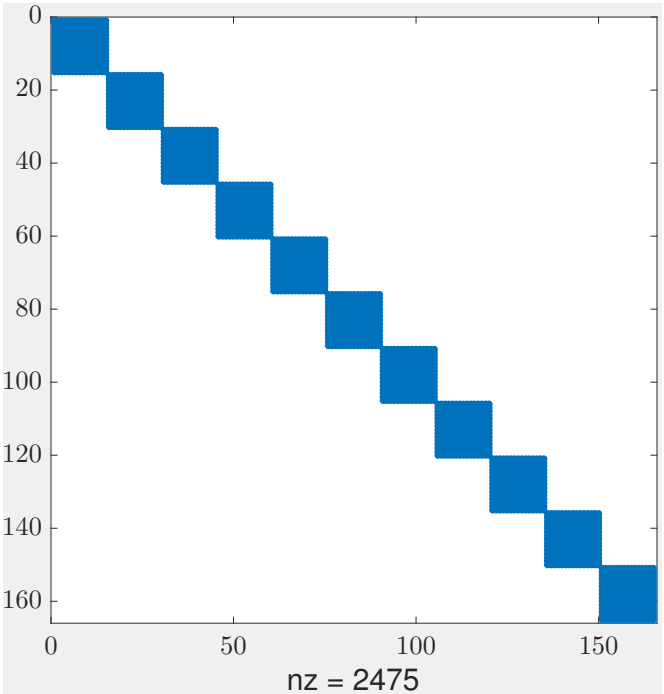


DG in space yields system of ODEs

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

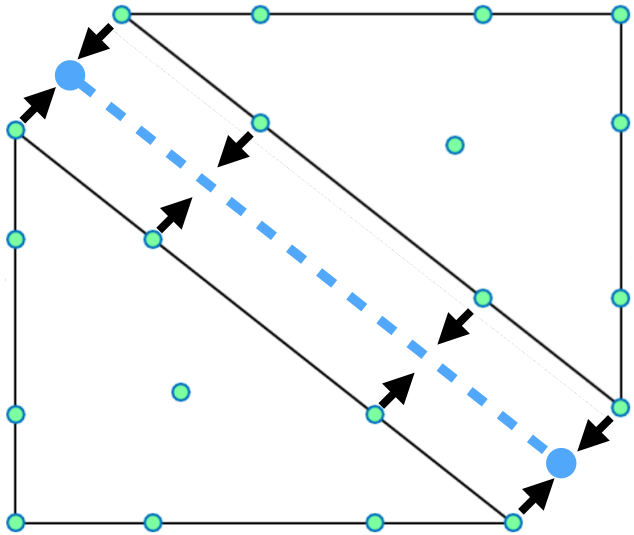
DG mass matrix decouples across elements, inter-element coupling only through $\mathbf{A}$.



Time-domain explicit DG methods

Given initial condition $u(\mathbf{x}, 0)$:

- Compute numerical flux on element faces (non-local).
- Compute RHS of (local) ODE.
- Evolve (local) solution using explicit time integration (RK, AB, etc).



$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{D}_x \mathbf{u} + \sum_{\text{faces}} \mathbf{L}_f \left(\text{flux}\right), \qquad \mathbf{L}_f = \mathbf{M}^{-1}\mathbf{M}_f.$$

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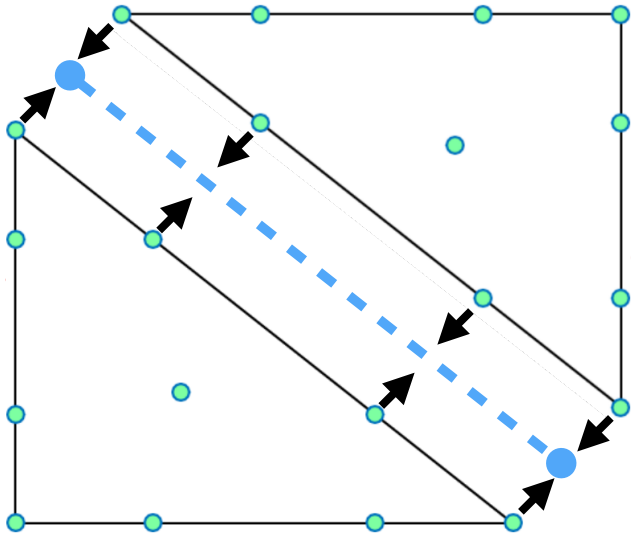

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \underbrace{\mathbf{D}_x\mathbf{u}}_{\text{Volume}} + \underbrace{\sum_{\text{faces}} \mathbf{L}_f\,(\text{flux})}_{\text{Surface}}, \qquad \mathbf{L}_f = \mathbf{M}^{-1}\mathbf{M}_f.$$

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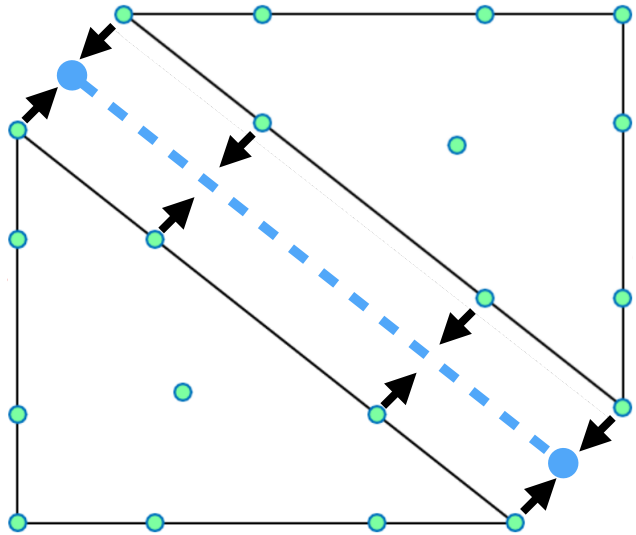

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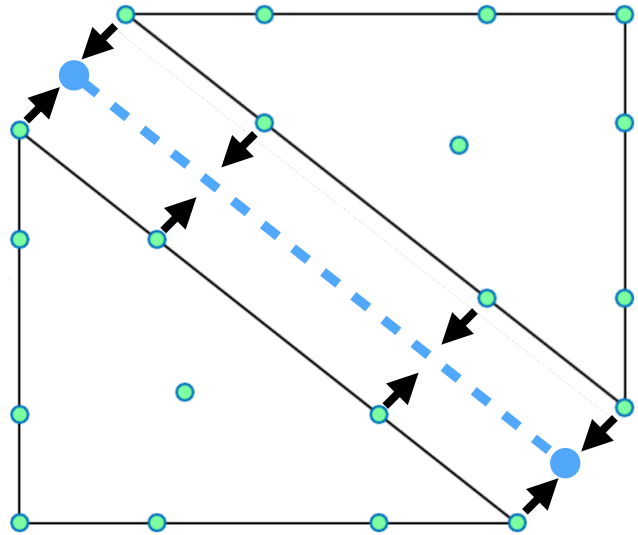

Pros: simple, scalable, and efficient matrix-free implementation.

Cons: explicit and high order methods: both prone to instability. Regularization (slope limiting, artificial viscosity) to avoid blow up!

Must ensure semi-discrete system is inherently *energy stable*!

Semi-discrete energy stability of DG methods

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

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

- Triangulate domain with elements D^k, define $[\![u]\!] = u^+ - u$ on D^k.
- DG formulation: find $u(x) \in P^N(D^k)$ s.t. $\forall v \in P^N(D^k)$

$$\sum_k \int_{D^k} \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} \right) v \, \mathrm{d}x + \frac{1}{2} \int_{\partial D^k} \left([\![u]\!] \, n_x + \tau \, [\![u]\!] \right) v \, \mathrm{d}x = 0.$$

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

$$\sum_k \frac{\partial}{\partial t} \|u\|^2_{D^k} \leq - \sum_k \frac{\tau}{2} \int_{\partial D^k} [\![u]\!]^2 \, \mathrm{d}x.$$

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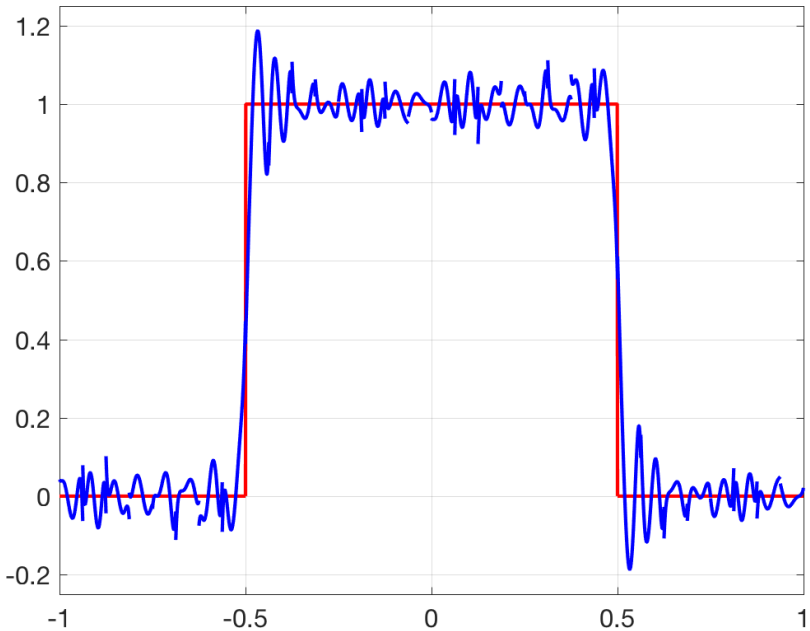
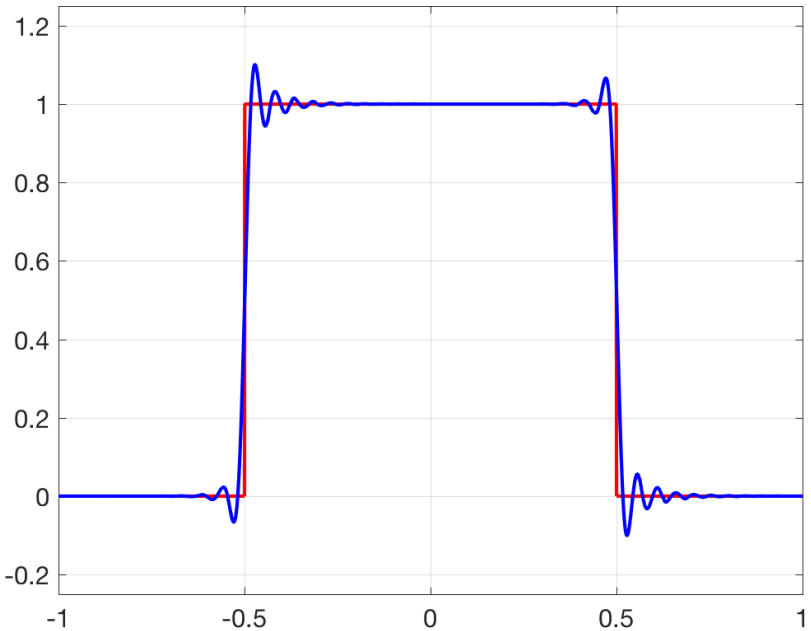
Energy conservative and energy stable DG methods

- Energy estimate: implies solution is non-increasing if $\tau \geq 0$.
- Energy conservative "central" flux when $\tau = 0$.
- Energy stable (i.e. dissipative) "Lax-Friedrichs" flux when $\tau = 1$.



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



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

Entropy stability for nonlinear conservation laws

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

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

- Continuous entropy inequality: convex entropy function $S(\boldsymbol{u})$ and "entropy potential" $\psi(\boldsymbol{u})$.

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

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

Example: mathematical entropy (compressible flow)

- Conservative variables: density, momentum, energy

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

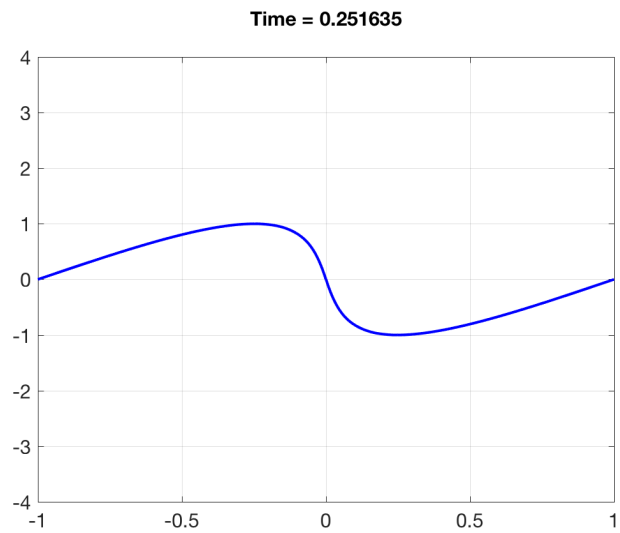
- Physical entropy $s(\boldsymbol{u})$ always increasing; mathematical entropy $S(\boldsymbol{u})$ always decreasing (analogous to energy).

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

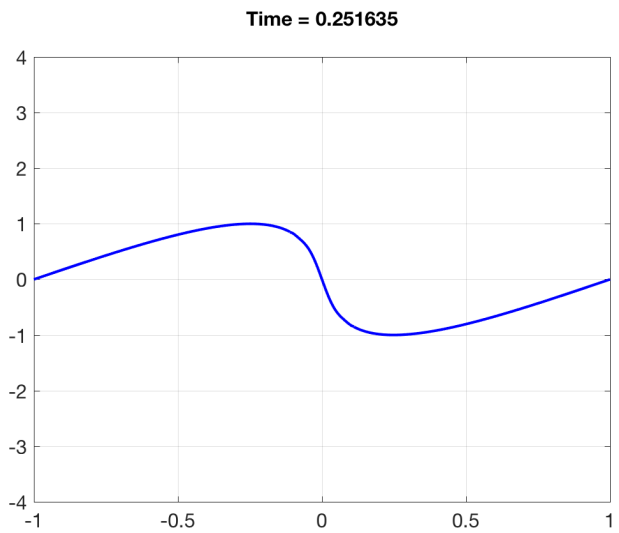
- Entropy variables $\boldsymbol{v}(\boldsymbol{u})$: invertible function of $\boldsymbol{u}$

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

Why are discretizations of nonlinear PDEs unstable?



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



(b) $N = 7, K = 9$ (non-aligned mesh)

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

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

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

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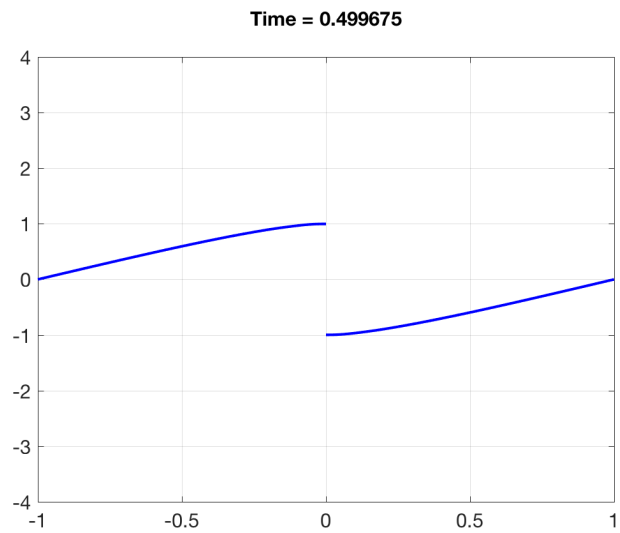

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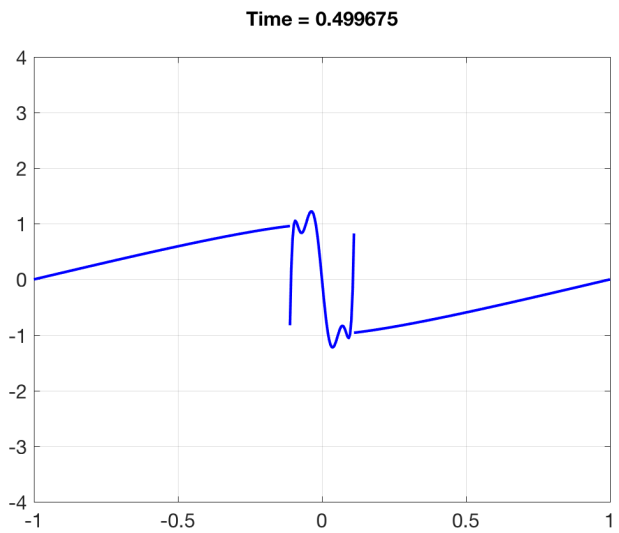

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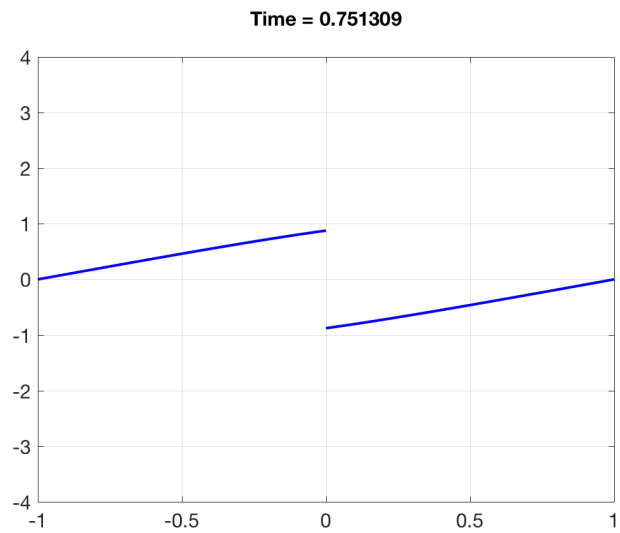

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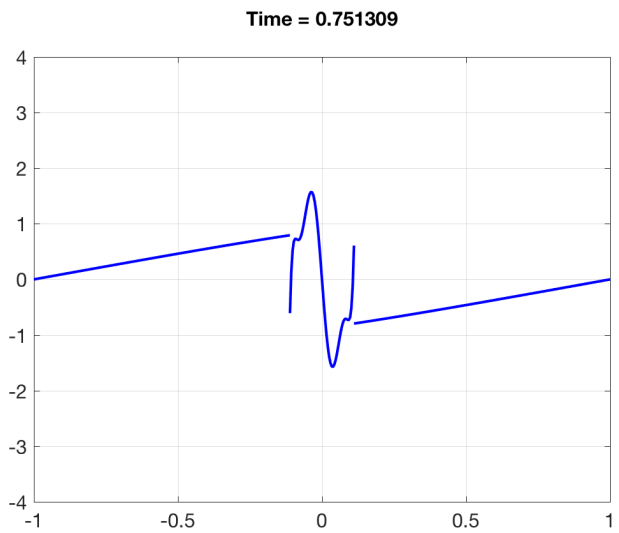

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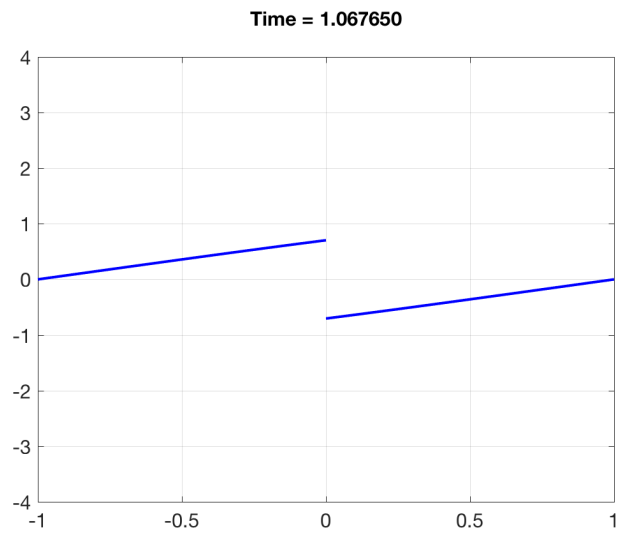

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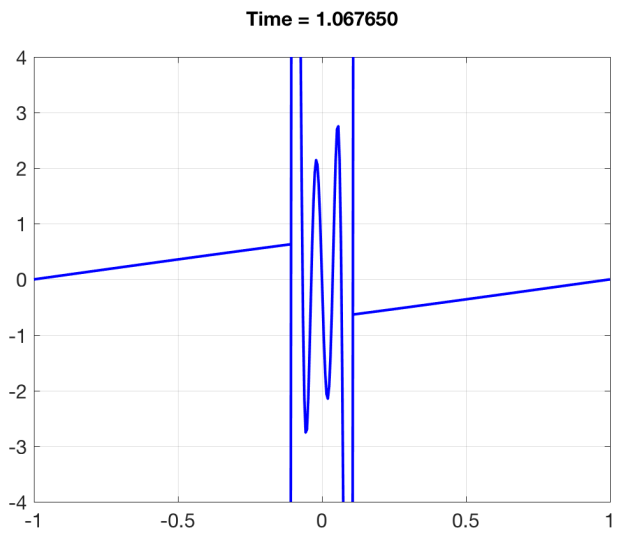

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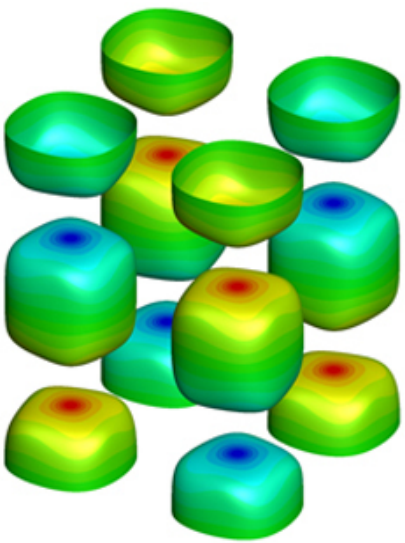
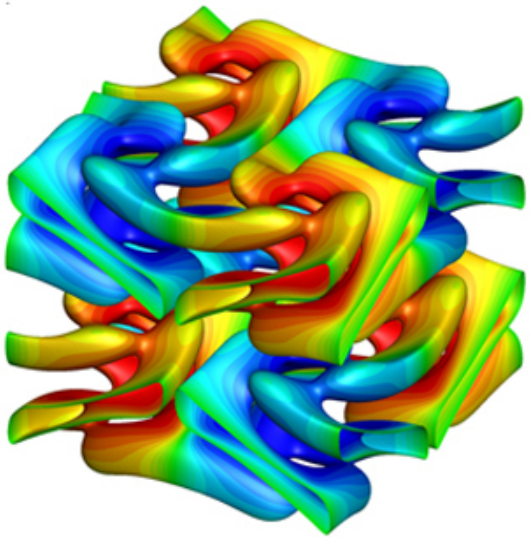
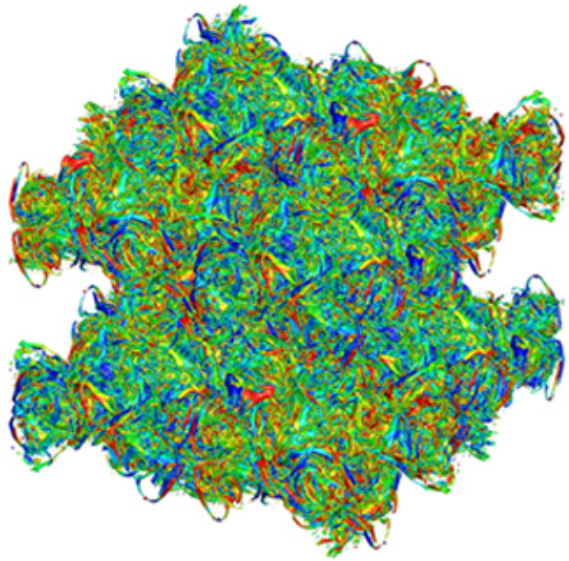
Tradeoff: high order accuracy vs stability

- Asymptotic stability for smooth solutions (not shocks or turbulence!)
- One option: stabilize by regularizing (limiters, filtering, art. viscosity).





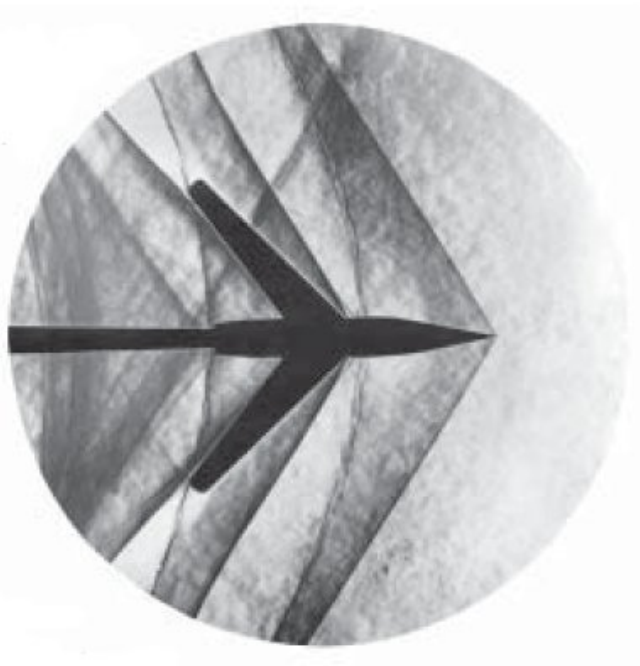


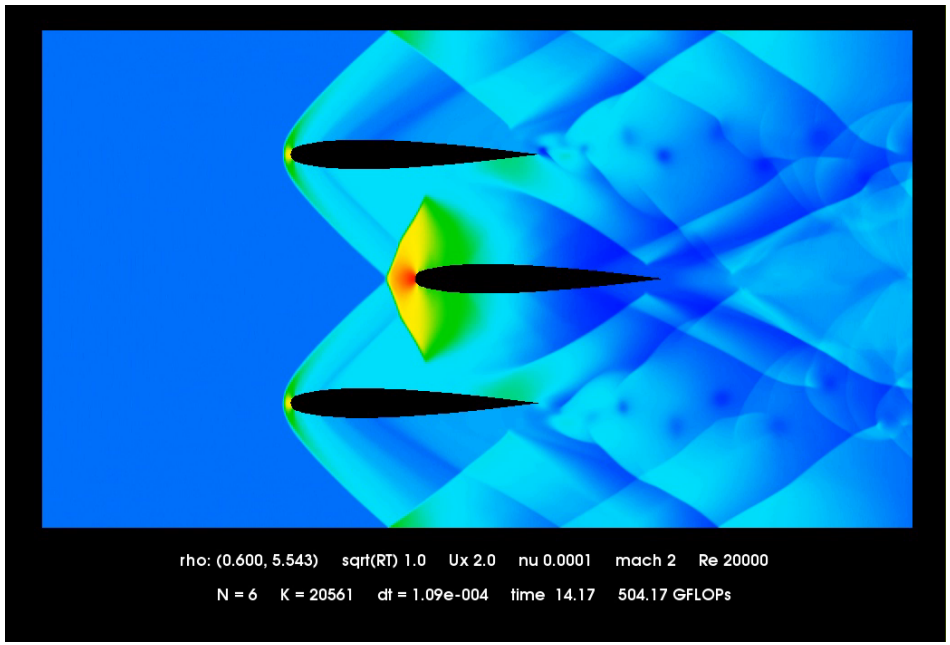
Under-resolved solutions: turbulence (inviscid Taylor-Green vortex).

Figures courtesy of Gregor Gassner, T. Warburton, Coastal Inlets Research Program (CIRP).

Tradeoff: high order accuracy vs stability

- Asymptotic stability for smooth solutions (not shocks or turbulence!)
- One option: stabilize by regularizing (limiters, filtering, art. viscosity).





Under-resolved solutions: shock waves.

Figures courtesy of Gregor Gassner, T. Warburton, Coastal Inlets Research Program (CIRP).

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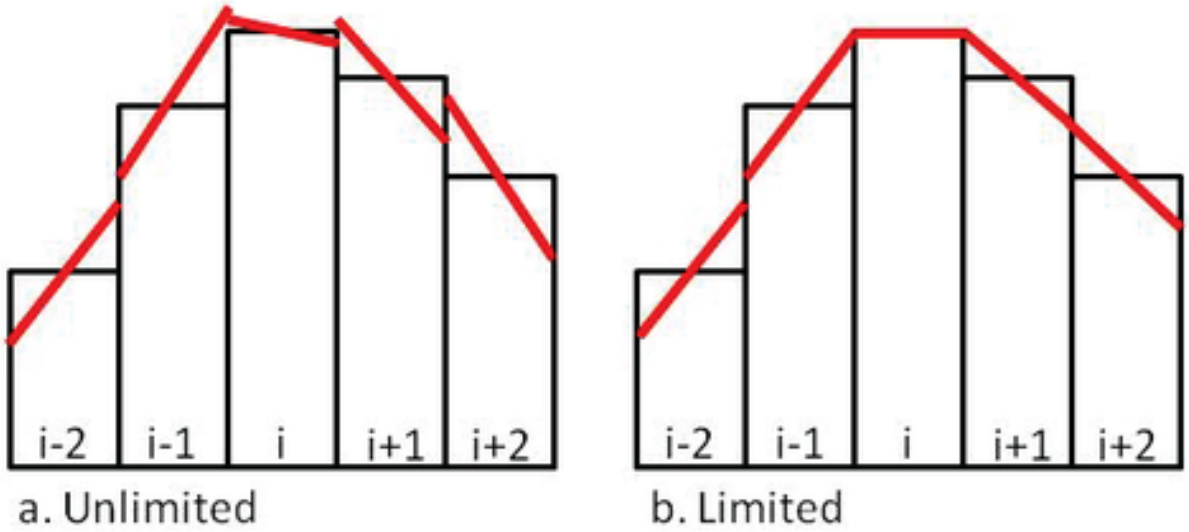

Slope limiting for a finite volume method.

Figures courtesy of Gregor Gassner, T. Warburton, Coastal Inlets Research Program (CIRP).

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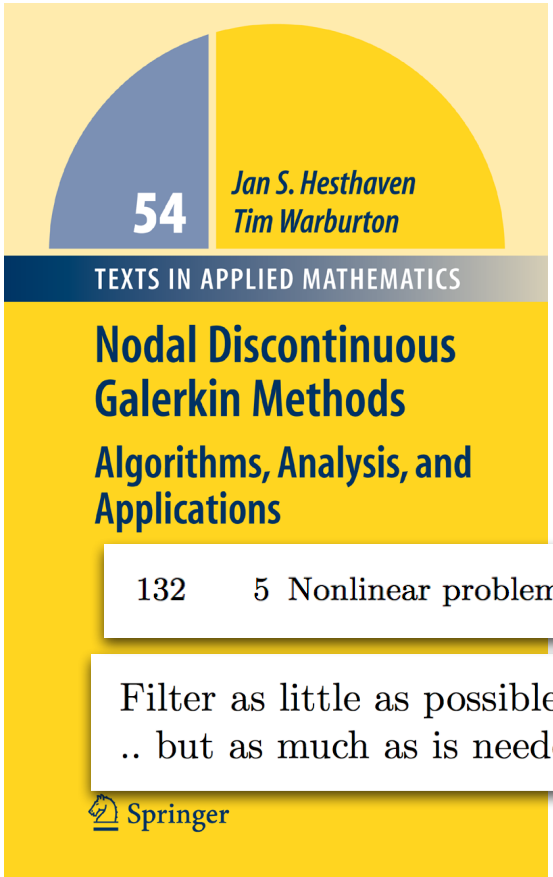

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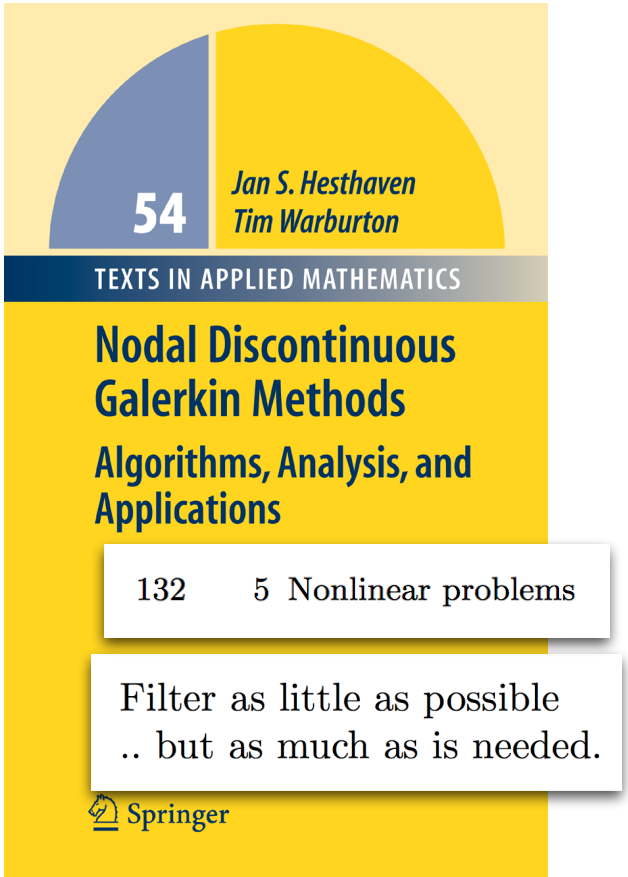
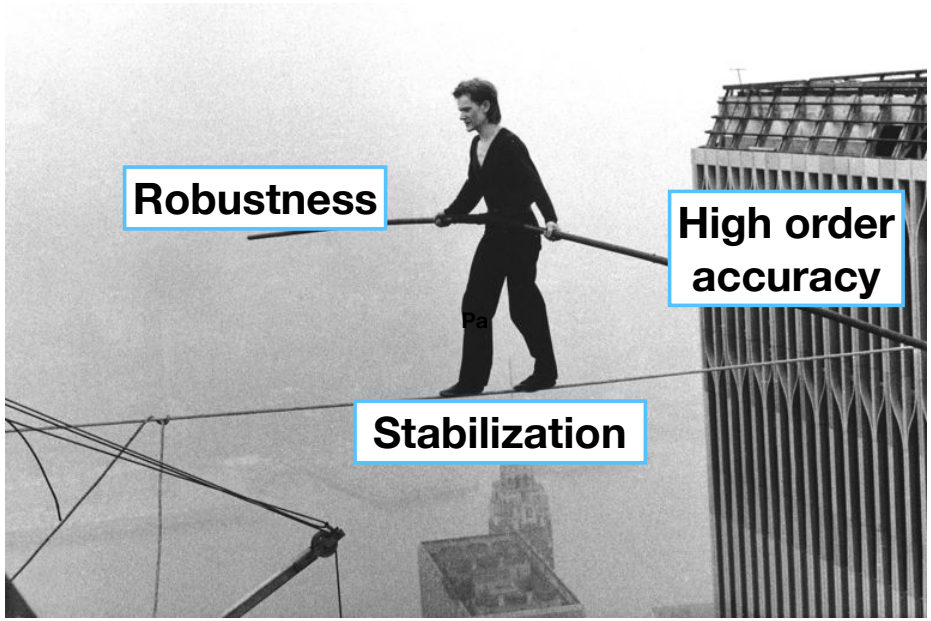


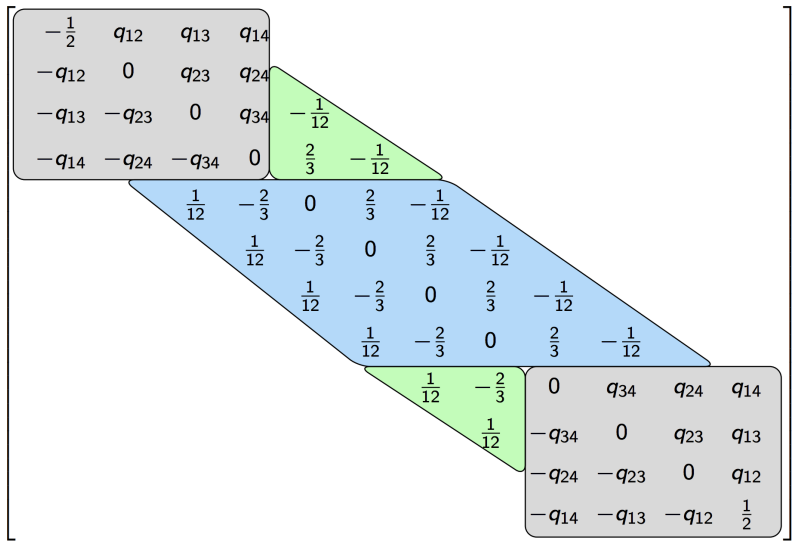


Figures courtesy of Gregor Gassner, T. Warburton, Coastal Inlets Research Program (CIRP).

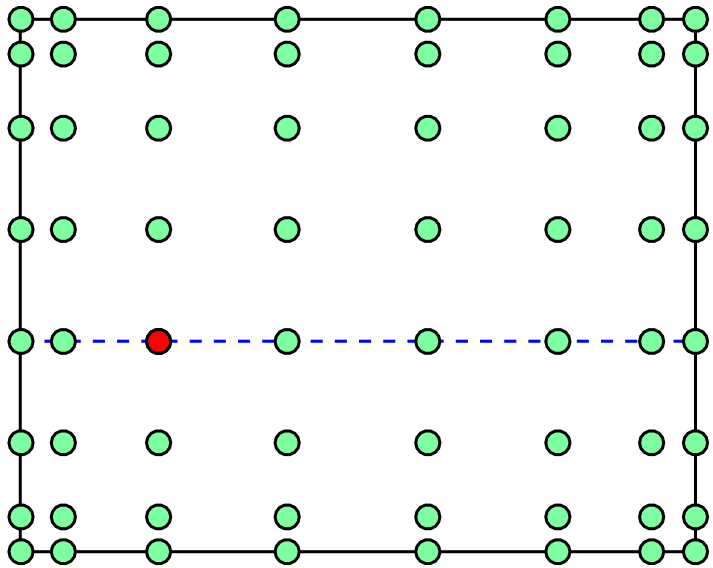
Talk outline

Summation-by-parts (SBP) finite differences

- Finite differences satisfying matrix form of integration by parts.
- Related to nodal "collocation" DG and under-integration.
- Both high order accuracy and a discrete entropy inequality.



(a) 1D matrix ($N = 2$, equispaced)



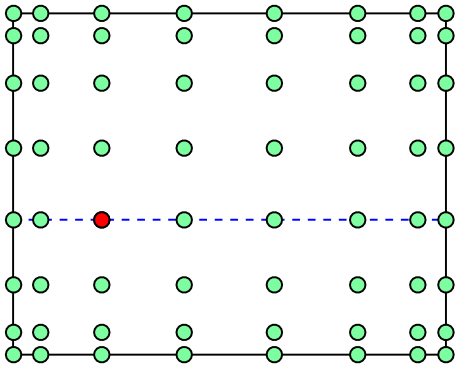
(b) 2D SBP ($N = 7$, GLL nodes)

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.*

Entropy stable SBP discretizations: current/challenges



(a) GLL collocation

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

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Carpenter et al. (2014). *Entropy stable spectral collocation schemes for the NS equations: discontinuous interfaces.*

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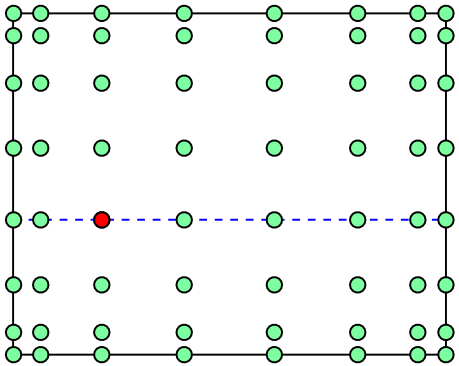

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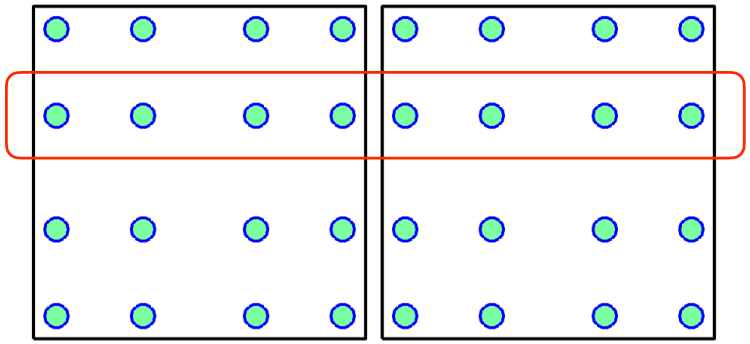

(b) Gauss nodes element coupling

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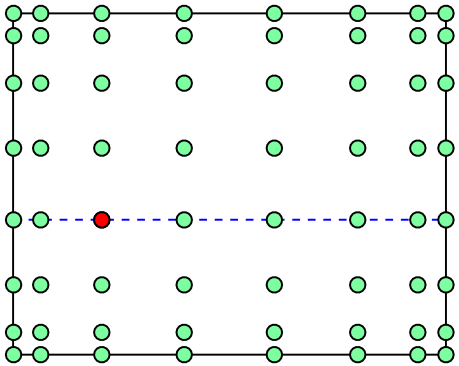

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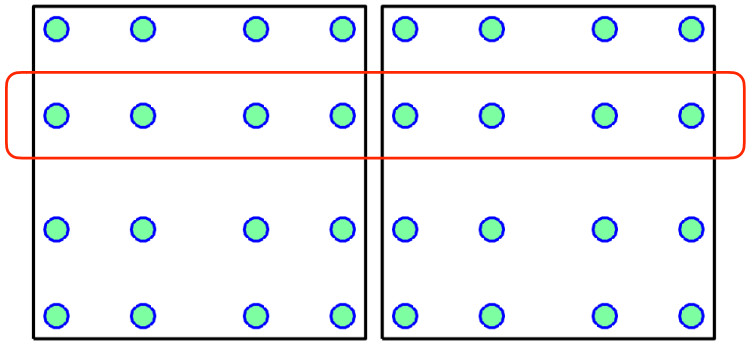

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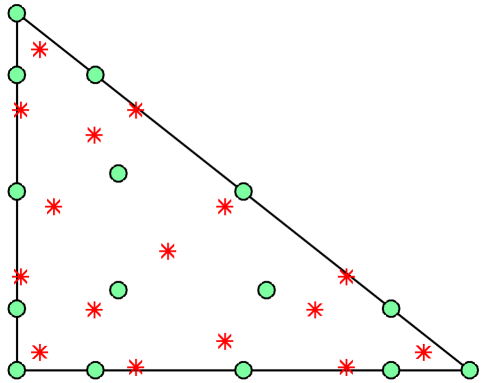

(c) Nodes vs cubature

- (Current) Discrete entropy inequality using high order GLL hexes.
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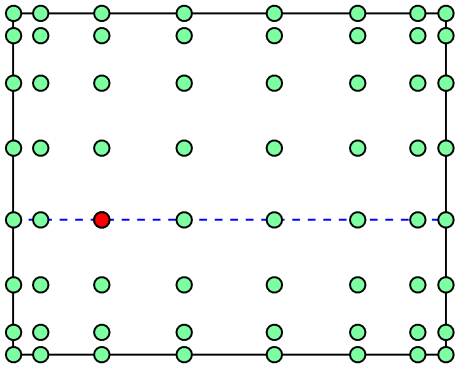
Entropy stable SBP discretizations: current/challenges



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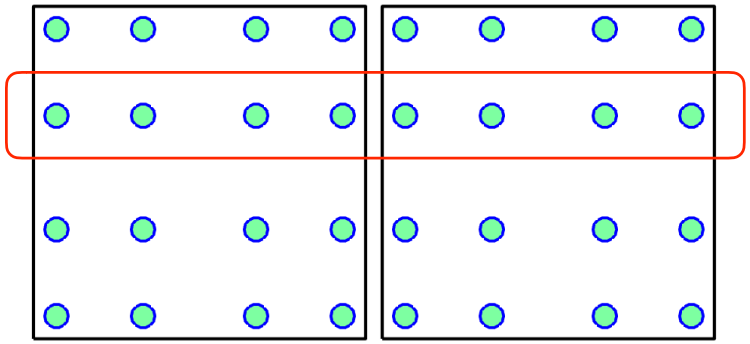

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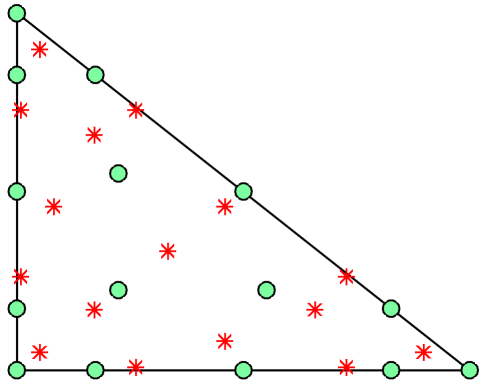

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- Tetrahedra, wedges, pyramids? Over-integration?

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

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

Carpenter et al. (2014). *Entropy stable spectral collocation schemes for the NS equations: discontinuous interfaces.*

Quadrature-based matrices for polynomial bases

- Volume and surface quadratures $(\boldsymbol{x}_i^q, \boldsymbol{w}_i^q)$, $(\boldsymbol{x}_i^f, \boldsymbol{w}_i^f)$, exact for degree $2N$ polynomials. Define diagonal quadrature weight matrices

$$\boldsymbol{W} = \operatorname{diag}\left(\boldsymbol{w}^q\right), \qquad \boldsymbol{W}_f = \operatorname{diag}\left(\boldsymbol{w}^f\right).$$

- Assume some polynomial basis $\phi_1, \ldots, \phi_{N_p}$. Define differentiation matrix $\boldsymbol{D}^i$, interpolation matrices $\boldsymbol{V}_q, \boldsymbol{V}_f$

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

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

$$\boldsymbol{P}_q = \boldsymbol{M}^{-1}\boldsymbol{V}_q^T\boldsymbol{W}, \qquad \boldsymbol{L}_f = \boldsymbol{M}^{-1}\boldsymbol{V}_f^T\boldsymbol{W}_f.$$

Quadrature-based differentiation matrices

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

$$\boldsymbol{D}_q^i = \boldsymbol{V}_q \boldsymbol{D}^i \boldsymbol{P}_q.$$

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

$$\boldsymbol{W}\boldsymbol{D}_q^i + \left(\boldsymbol{W}\boldsymbol{D}_q^i\right)^T = \left(\boldsymbol{V}_f \boldsymbol{P}_q\right)^T \boldsymbol{W}_f \mathrm{diag}\left(\boldsymbol{n}_i\right) \boldsymbol{V}_f \boldsymbol{P}_q.$$

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

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

- $\boldsymbol{D}_q^i$ leads to generalized SBP methods; complicated interface terms.

A "decoupled" block SBP operator

- Approx. derivatives also using boundary traces (compact coupling).
- On an element D^k with unit normal vector $\boldsymbol{n}$: approximate derivative w.r.t. the ith coordinate.

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

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

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

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

Differentiation using decoupled SBP operators

- Note: $\boldsymbol{D}_N^i$ is not a differentiation matrix on its own.
- $\boldsymbol{D}_N^i$ produces a high order approximation of $f\frac{\partial g}{\partial x}$ at $\boldsymbol{x} = [\boldsymbol{x}^q, \boldsymbol{x}^f]$.

$$f\frac{\partial g}{\partial x} \approx \begin{bmatrix} \boldsymbol{P}_q & \boldsymbol{L}_f \end{bmatrix} \operatorname{diag}(\boldsymbol{f})\, \boldsymbol{D}_N \boldsymbol{g}, \qquad \boldsymbol{f}_i, \boldsymbol{g}_i = f(\boldsymbol{x}_i), g(\boldsymbol{x}_i).$$

- Equivalent to solving variational problem for $u(\boldsymbol{x}) \approx f\frac{\partial g}{\partial x}$

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

- $\boldsymbol{D}_N^i \mathbf{1} = 0$ holds (necessary for discrete entropy conservation).

Talk outline

Burgers' equation: energy stable formulations

- 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 $u(x) = \sum_j \widehat{\boldsymbol{u}}_j \phi(x)$. Find $\widehat{\boldsymbol{u}}$ such that

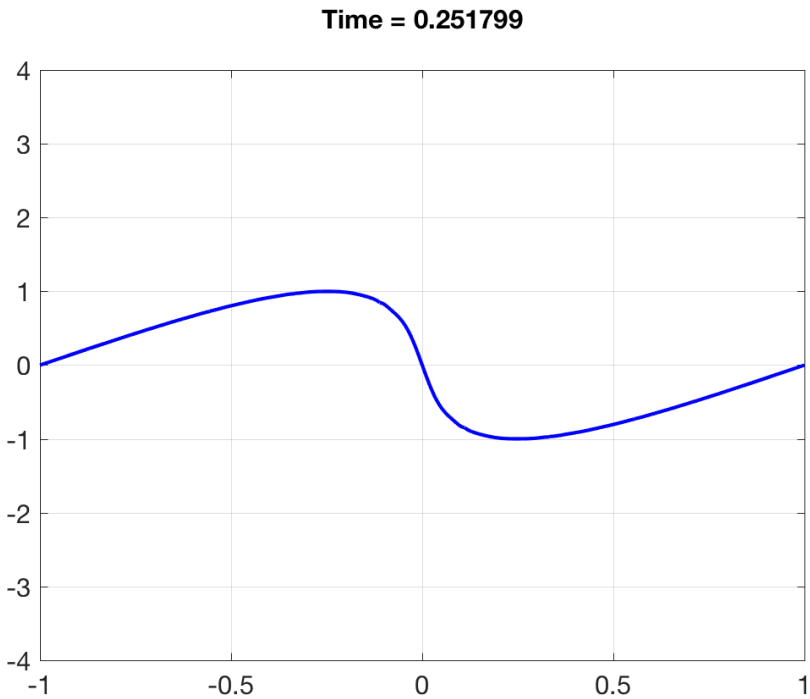
$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{V}_q \\ \boldsymbol{V}_f \end{bmatrix} \widehat{\boldsymbol{u}}, \qquad \boldsymbol{f}^* = \boldsymbol{f}^*(u^+, u) = \text{numerical flux}$$

$$\frac{\mathrm{d}\widehat{\boldsymbol{u}}}{\mathrm{d}t} + \frac{1}{3}\begin{bmatrix} \boldsymbol{P}_q & \boldsymbol{L}_f \end{bmatrix}\left(\boldsymbol{D}_N\left(\boldsymbol{u}^2\right) + \mathrm{diag}\left(\boldsymbol{u}\right)\boldsymbol{D}_N\boldsymbol{u}\right) + \boldsymbol{L}_f(\boldsymbol{f}^*) = 0.$$

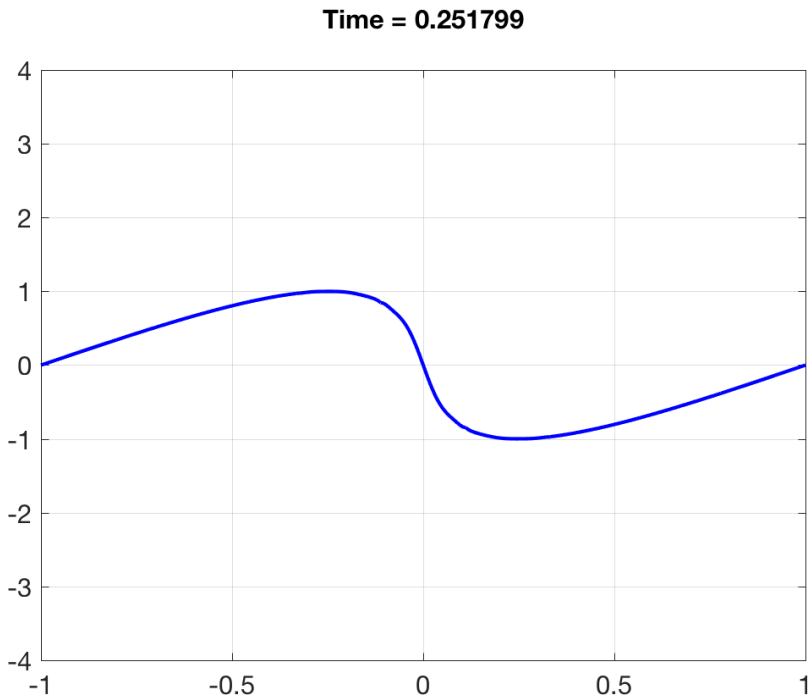
- Energy estimate: multiply by $\widehat{\boldsymbol{u}}^T\boldsymbol{M}$, use SBP, sum over D^k

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

Burgers' equation: energy stable shock solution

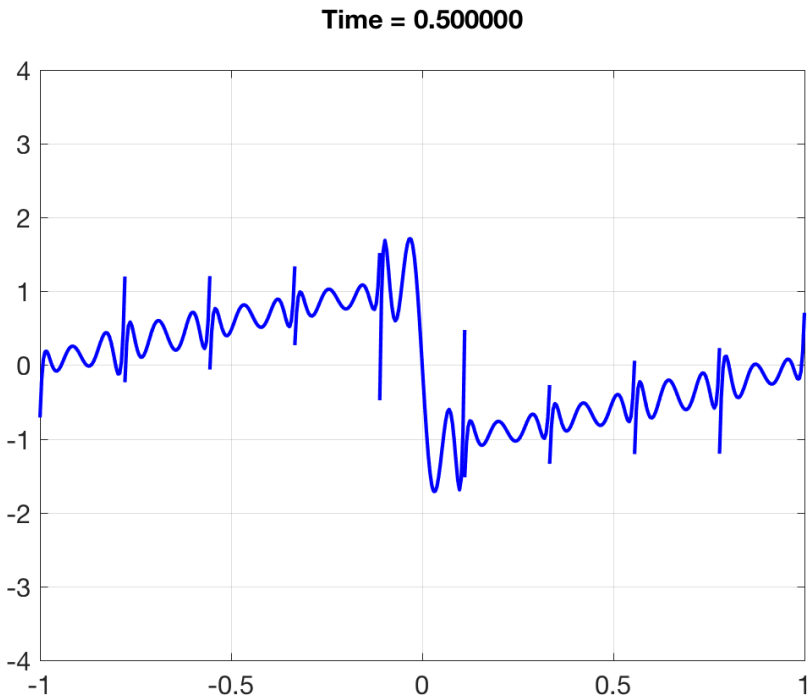


(a) $\tau = 0$



(b) $\tau = 1$

Burgers' equation: energy stable shock solution



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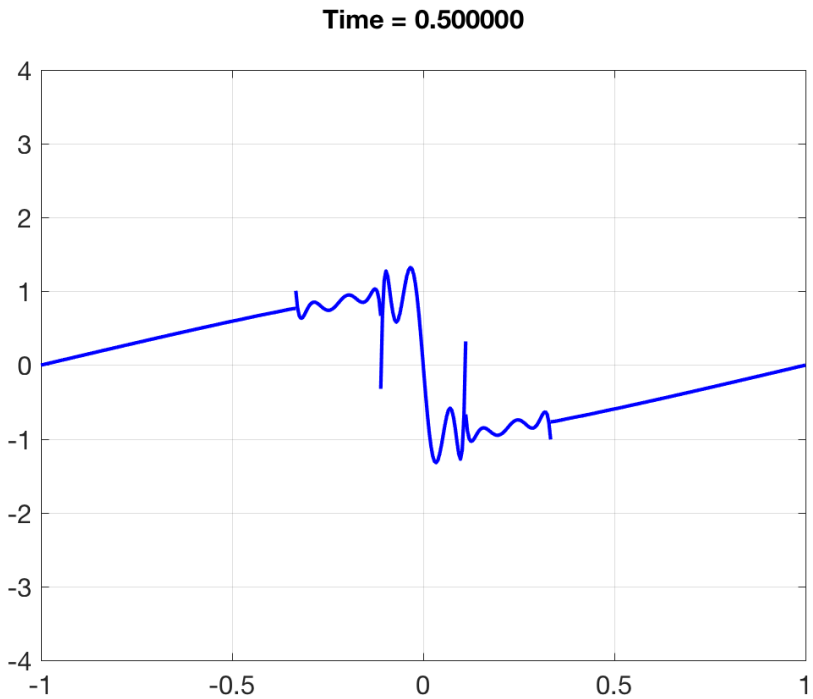

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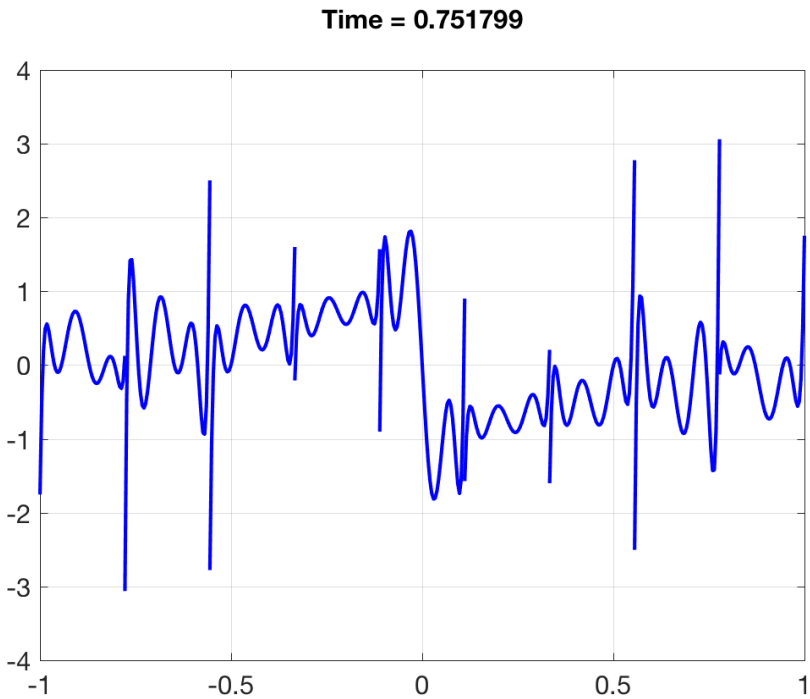

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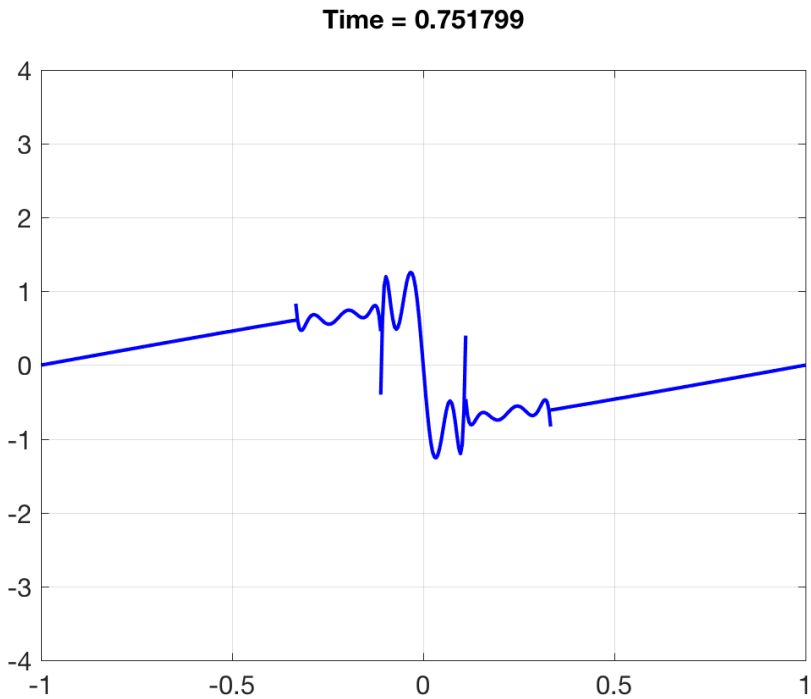

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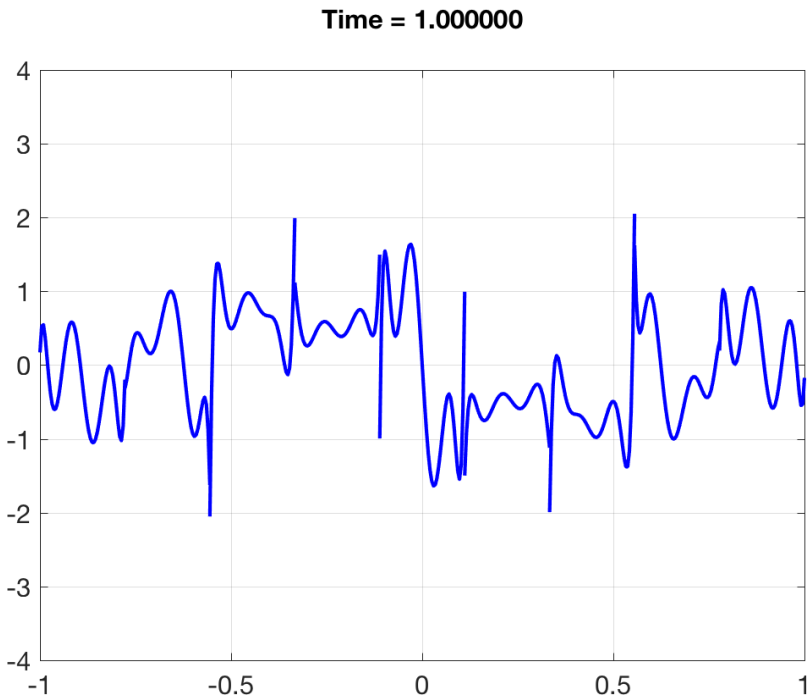

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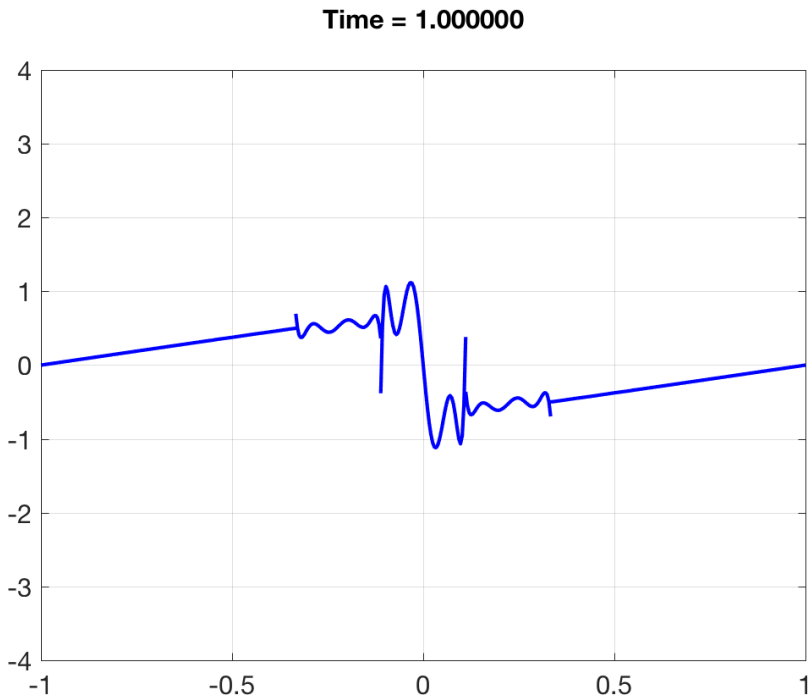

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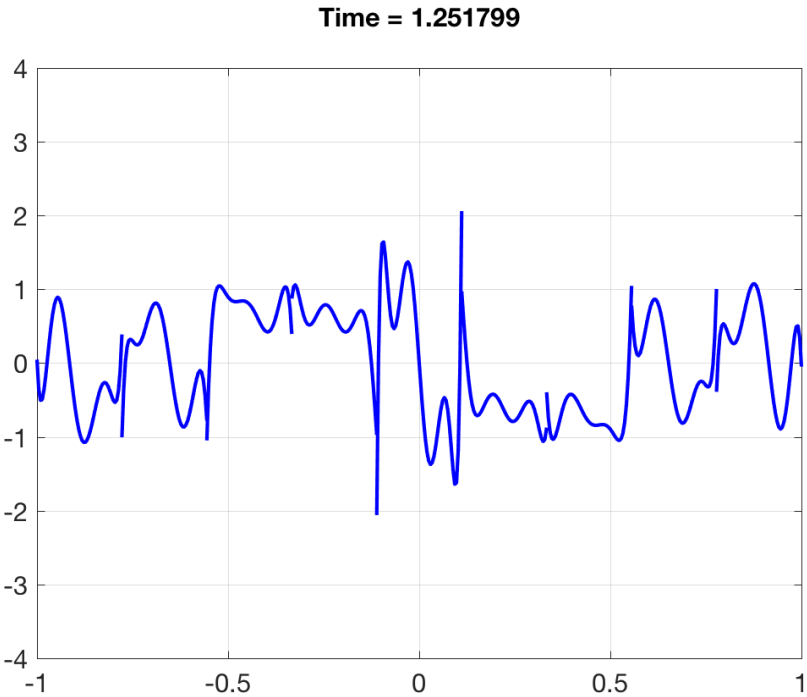

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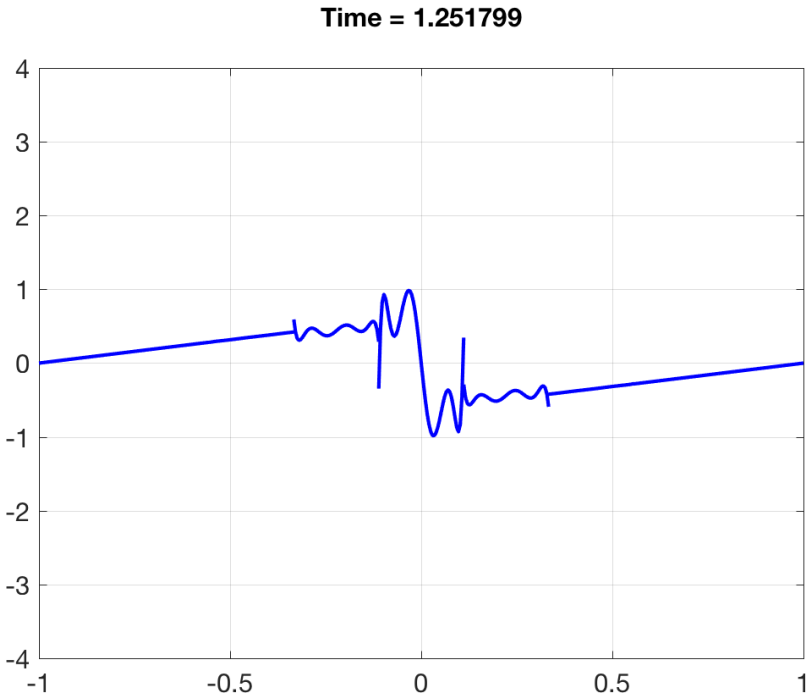

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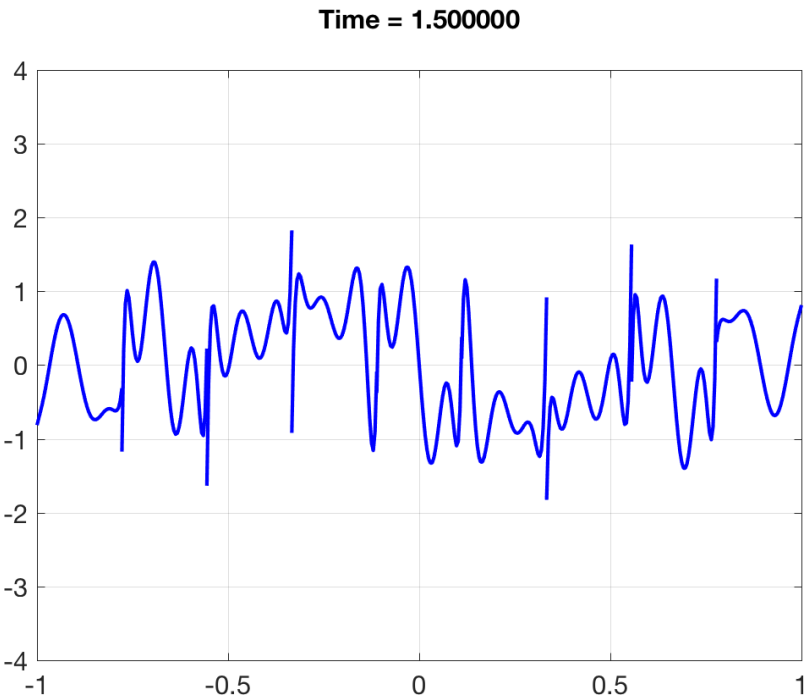
Burgers' equation: energy stable shock solution



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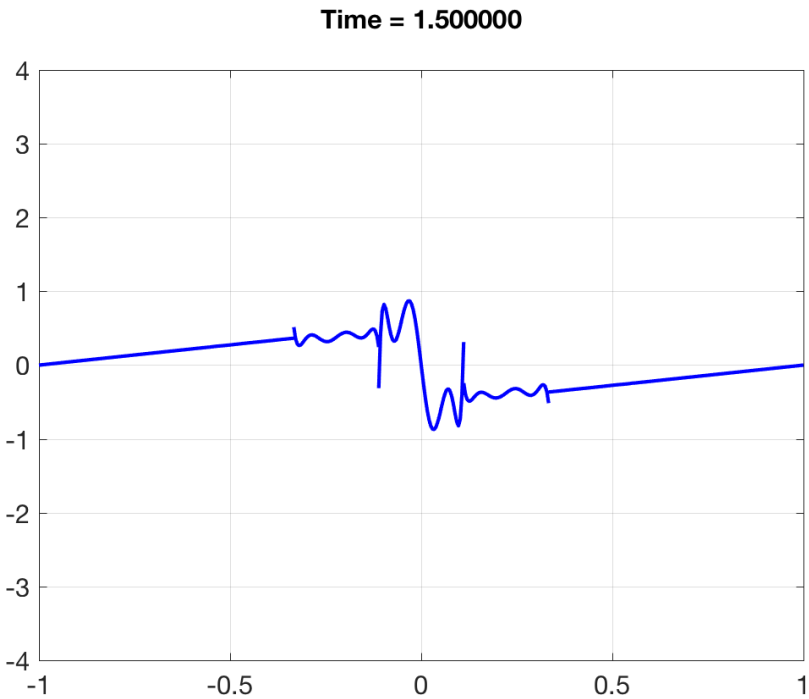

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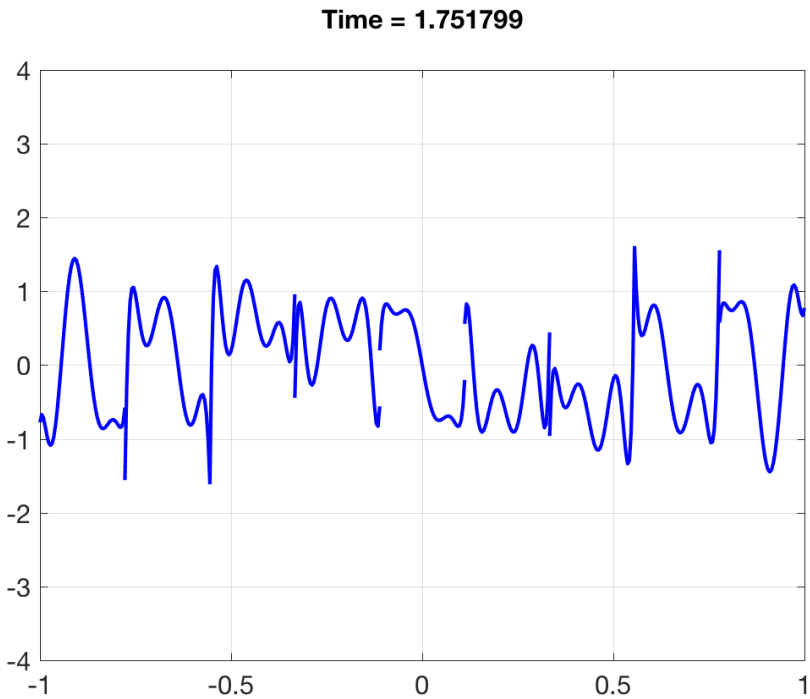
Burgers' equation: energy stable shock solution



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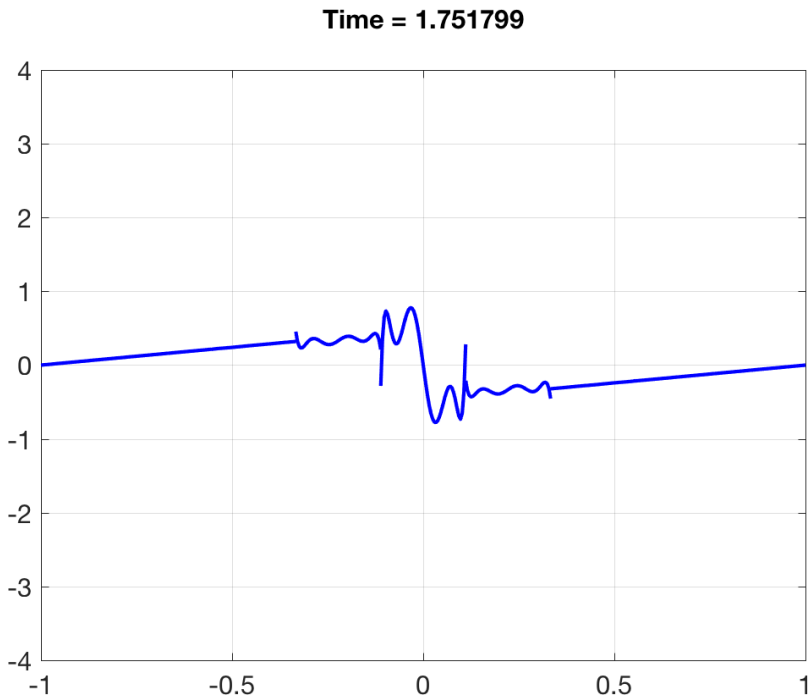
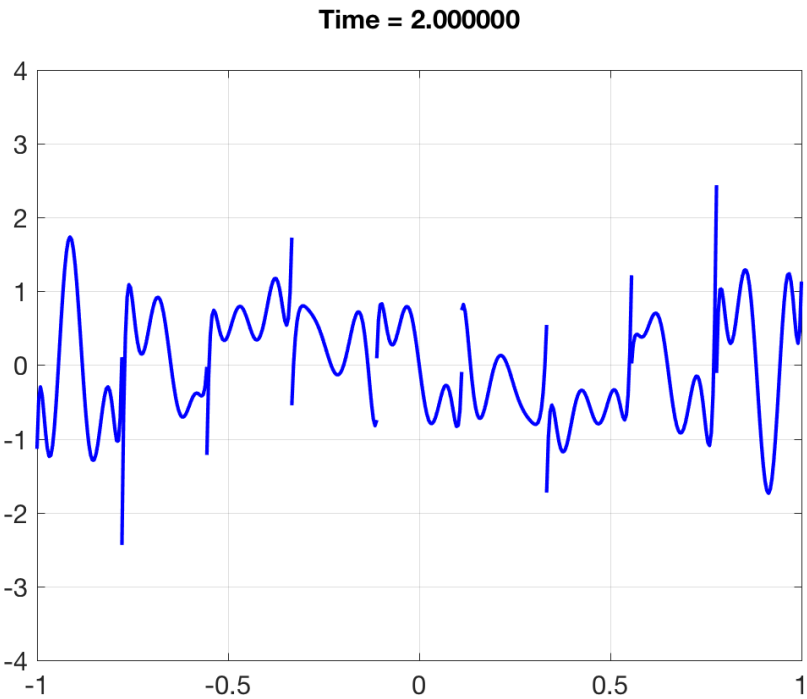
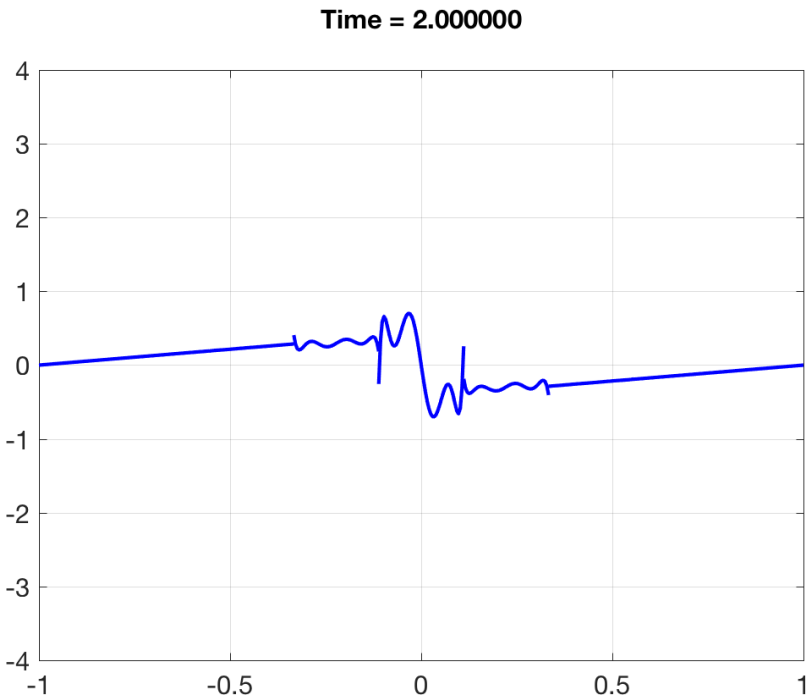


(b) $\tau = 1$

Burgers' equation: energy stable shock solution



(a) $\tau = 0$



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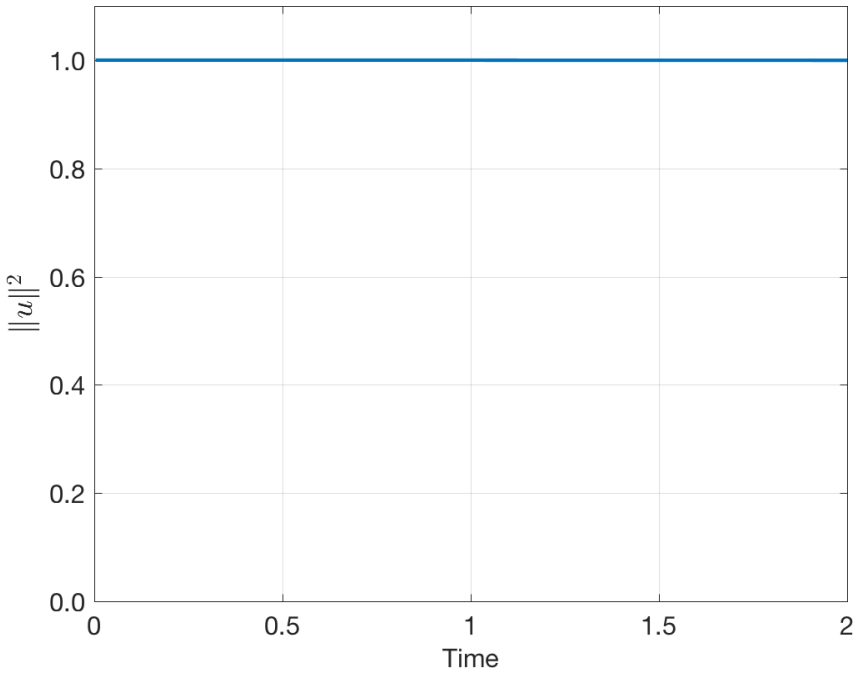
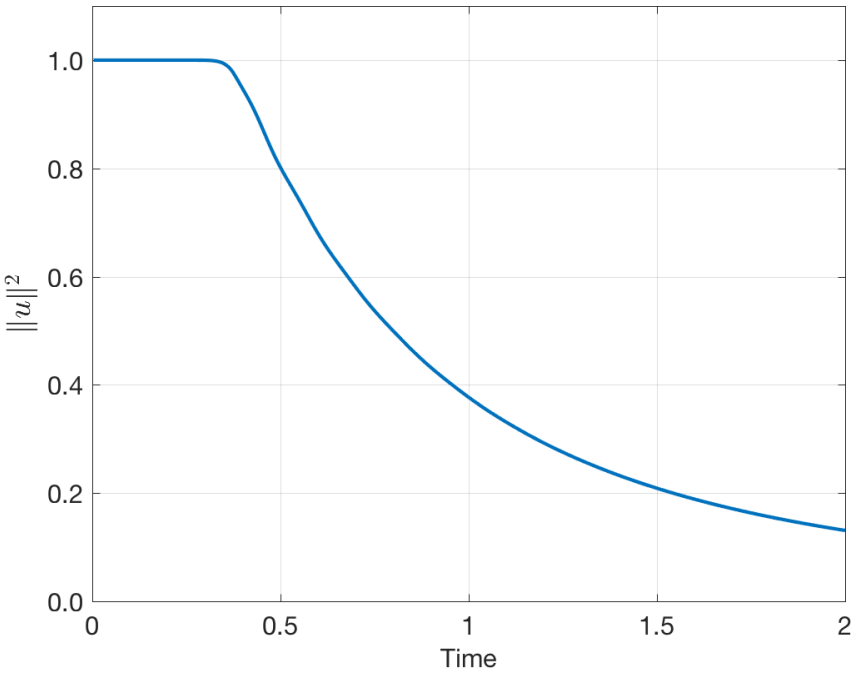
Burgers' equation: energy stable shock solution



(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

$$\begin{aligned} \boldsymbol{f}_S(\boldsymbol{u}, \boldsymbol{u}) &= \boldsymbol{f}(\boldsymbol{u}), && \text{(consistency)} \\ \boldsymbol{f}_S(\boldsymbol{u}, \boldsymbol{v}) &= \boldsymbol{f}_S(\boldsymbol{v}, \boldsymbol{u}), && \text{(symmetry)} \\ (\boldsymbol{v}_L - \boldsymbol{v}_R)^T \boldsymbol{f}(\boldsymbol{u}_L, \boldsymbol{u}_R) &= \psi_L - \psi_R, && \text{(conservation).} \end{aligned}$$

- Example: entropy conservative flux for Burgers' equation

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

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

Tadmor, Eitan (1987). *The numerical viscosity of entropy stable schemes for systems of conservation laws. I.*

Flux differencing: entropy conservative finite volume fluxes

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Tadmor, Eitan (1987). *The numerical viscosity of entropy stable schemes for systems of conservation laws. I.*

Flux differencing: recovering split formulations

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

- Flux differencing: let $u_L = u(x), u_R = u(y)$

$$\frac{\partial f(u)}{\partial x} \Longrightarrow 2\frac{\partial f_S\left(u(x), u(y)\right)}{\partial x}\bigg|_{y=x}$$

- Recovering the Burgers' split formulation

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

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

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

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

- Logarithmic mean and "inverse temperature" β

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

Chandreshekar (2013), *Kinetic energy preserving and entropy stable FV schemes for comp. Euler and NS equations.*

Flux differencing: implementational details

- Define $\boldsymbol{F}_S$ as evaluation of $\boldsymbol{f}_S$ at all combinations of quadrature points

$$(\boldsymbol{F}_S)_{ij} = (u(\boldsymbol{x}_i), u(\boldsymbol{x}_j)), \qquad \boldsymbol{x} = \left[\boldsymbol{x}^q, \boldsymbol{x}^f\right]^T.$$

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

$$2\frac{\partial f_S\left(u(x), u(y)\right)}{\partial x}\bigg|_{y=x} \Longrightarrow \left[\begin{array}{cc} \boldsymbol{P}_q & \boldsymbol{L}_f \end{array}\right] \mathrm{diag}(2\boldsymbol{D}_N\boldsymbol{F}_S).$$

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

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

Flux differencing: avoiding the chain rule

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

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

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

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

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

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Modifying the conservative variables

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

$$\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(P_N \boldsymbol{v}(\boldsymbol{u}_h)\right).$$

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

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

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

Shi and Shu (2017). *On local conservation of numerical methods for conservation laws*.

A discretely entropy conservative DG method

Theorem (Chan 2018)

Let $\boldsymbol{u}_h(\boldsymbol{x}) = \sum_j \widehat{\boldsymbol{u}}_j \phi_j(\boldsymbol{x})$ *and* $\widetilde{\boldsymbol{u}} = \boldsymbol{u}(P_N \boldsymbol{v})$. *Let* $\widehat{\boldsymbol{u}}$ *locally solve*

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

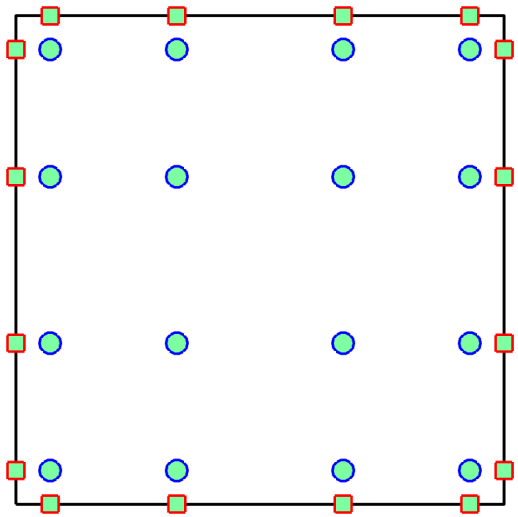
Assuming continuity in time, $\boldsymbol{u}_h(\boldsymbol{x})$ *satisfies the quadrature form of*

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

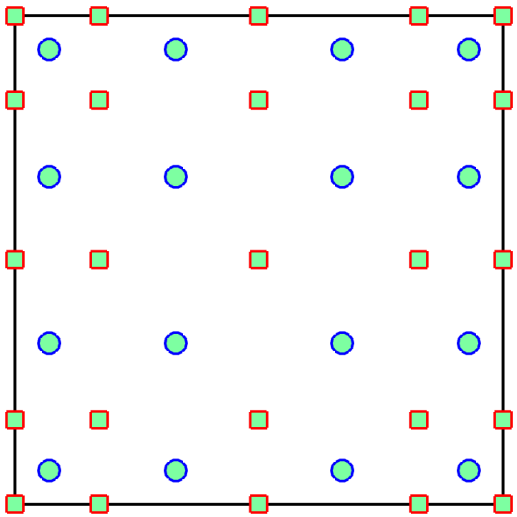
- Can modify interface flux (e.g. Lax-Friedrichs) for entropy dissipation.

Chan (2018). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods.*

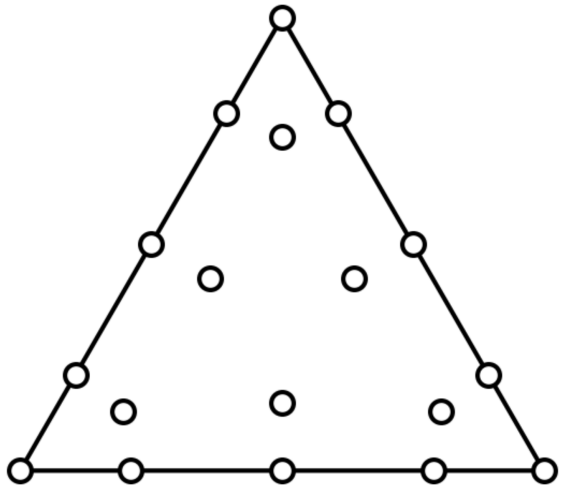
Unifying (some) finite difference SBP formulations



(a) Generalized SBP



(b) Staggered-grid SBP



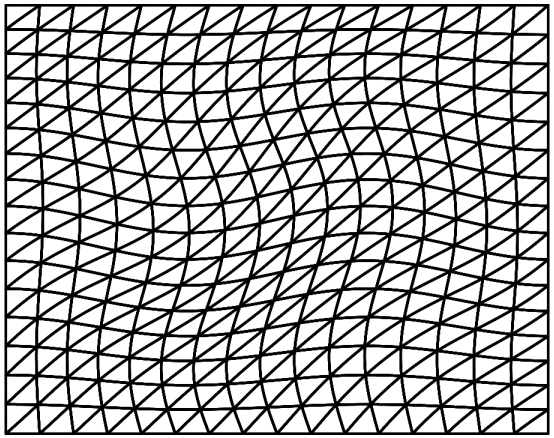
(c) Triangular SBP

- Specific basis and quadratures recover many existing discretizations (DG-SEM, Gauss collocation, staggered grid, dense norm, etc).
- Recovers existing (and new) interface coupling terms (SBP-SATs).
- Setting $\boldsymbol{P}_q = \boldsymbol{I}$ recovers non-basis SBP finite differences on simplices.

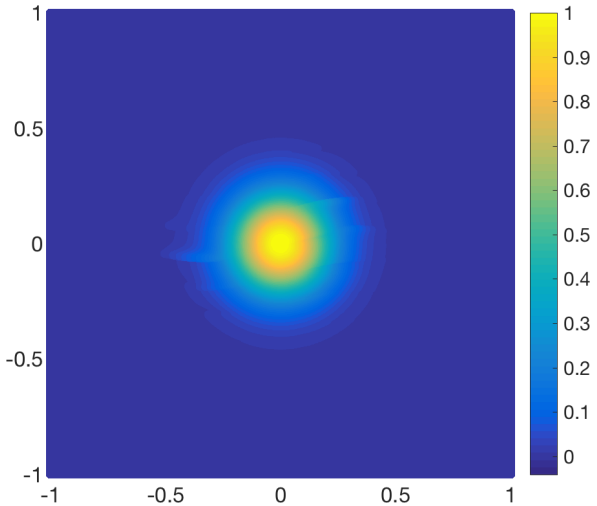
Parsani et al. (2016). *ES staggered grid disc. spectral collocation methods of any order for the comp. NS eqns.*

Crean, Hicken, et al. (2018). *Entropy-stable SBP discretization of the Euler equations on general curved elements.*

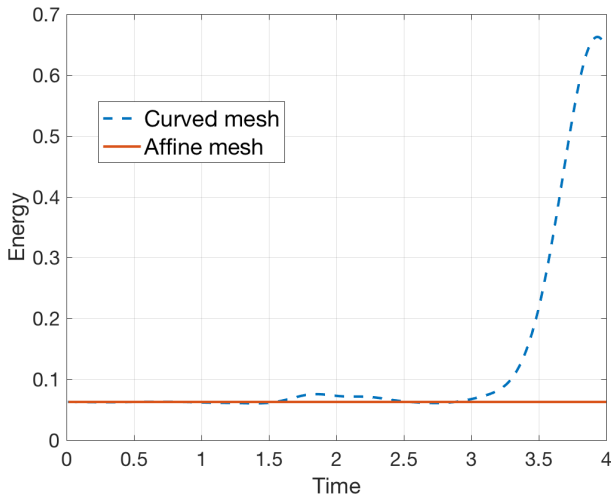
Curved meshes and stability



(a) Curved mesh



(b) Aliased solution



(c) Energy growth

- Necessary for high order accuracy on curved geometries, but can produce "aliasing" instabilities and energy growth.
- Geometric terms $J, \boldsymbol{G}_{ij}$ vary spatially over each element

$$\frac{\partial u}{\partial x_i} = \sum_{j=1}^{d} \boldsymbol{G}_{ij} \frac{\partial u}{\partial \widehat{x}_j}, \qquad \boldsymbol{G}_{ij} = \frac{\partial \widehat{x}_j}{\partial x_i}, \qquad J = \frac{1}{\det(\boldsymbol{G})}.$$

Curved meshes: geometric terms

- Rewrite derivatives in split form with scaled geometric terms

$$J\frac{\partial u}{\partial x_i} = \frac{1}{2}\sum_{j=1}^{d}\left(J\boldsymbol{G}_{ij}\frac{\partial u}{\partial \widehat{x}_j} + \frac{\partial\left(J\boldsymbol{G}_{ij}u\right)}{\partial \widehat{x}_j}\right), \qquad \sum_{j=1}^{d}\frac{\partial\left(J\boldsymbol{G}_{ij}\right)}{\partial \widehat{x}_j} = 0.$$

- Define physical matrices in terms of reference matrices $\widehat{\boldsymbol{D}}_N^j$

$$\boldsymbol{D}_N^i = \frac{1}{2}\sum_{i=1}^{d}\left(\text{diag}\left(J\boldsymbol{G}_{ij}\right)\widehat{\boldsymbol{D}}_N^j + \widehat{\boldsymbol{D}}_N^j\text{diag}\left(J\boldsymbol{G}_{ij}\right)\right).$$

- Proof of discrete entropy conservation requires $\boldsymbol{D}_N^i\mathbf{1} = 0$. Must ensure geometric terms satisfy geometric conservation law (GCL).

$$\boldsymbol{D}_N^i\mathbf{1} = 0 \Longrightarrow \sum_{j=1}^{d}\widehat{\boldsymbol{D}}_N^j\left(J\boldsymbol{G}_{ij}\right) = 0.$$

Thomas and Lombard (1979). Geometric Conservation Law and Its Application to Flow Computations on Moving Grids.

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

Curved meshes: weighted mass matrices

- Weighted mass matrix $\boldsymbol{M}_J$ on D^k, weighted L^2 projection $\boldsymbol{P}_q^k$

$$(\boldsymbol{M}_J)_{ij} = \int_{\widehat{D}} \phi_j \phi_i J \, \mathrm{d}\widehat{\boldsymbol{x}}, \qquad \boldsymbol{P}_q^k = (\boldsymbol{M}_J)^{-1} \boldsymbol{V}_q^T \boldsymbol{W} \mathrm{diag}(\boldsymbol{J}).$$

- Avoid $\boldsymbol{M}_J^{-1}$: generalized mass lumping, weight-adjusted mass matrix

$$\boldsymbol{M}_J \approx \boldsymbol{M}\boldsymbol{M}_{1/J}^{-1}\boldsymbol{M}, \qquad \left(\boldsymbol{M}\boldsymbol{M}_{1/J}^{-1}\boldsymbol{M}\right)^{-1} = \boldsymbol{M}^{-1}\boldsymbol{M}_{1/J}\boldsymbol{M}^{-1}$$

- Low-storage matrix-free application of $\boldsymbol{M}_{1/J}$ using quadrature.
- For discrete entropy conservation, use weight-adjusted projection

$$\widetilde{P}_N^k u = P_N \left(\frac{1}{J} P_N (uJ) \right).$$

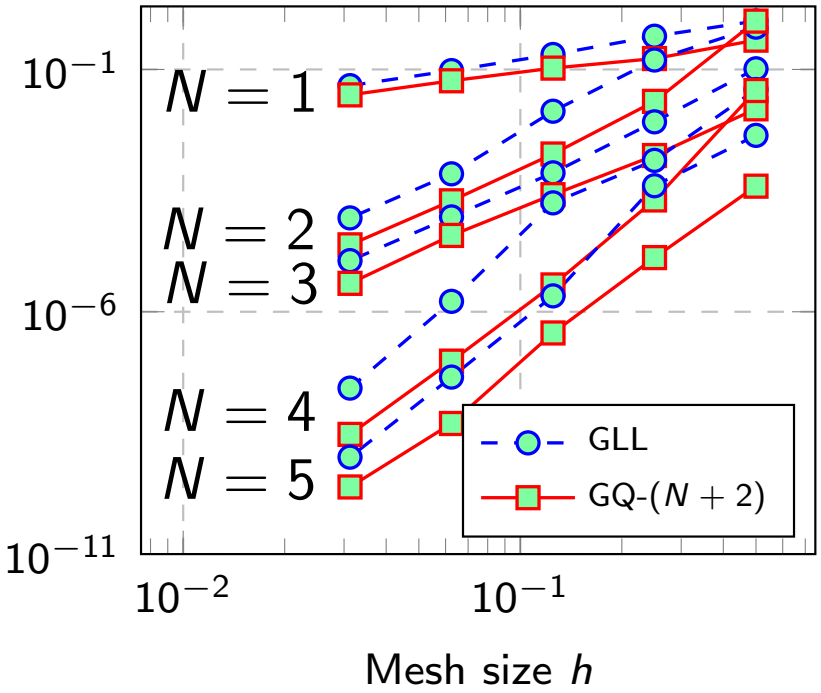
Chan, Wilcox (in preparation). *On discretely entropy stable weight-adjusted DG methods: curvilinear meshes*.

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

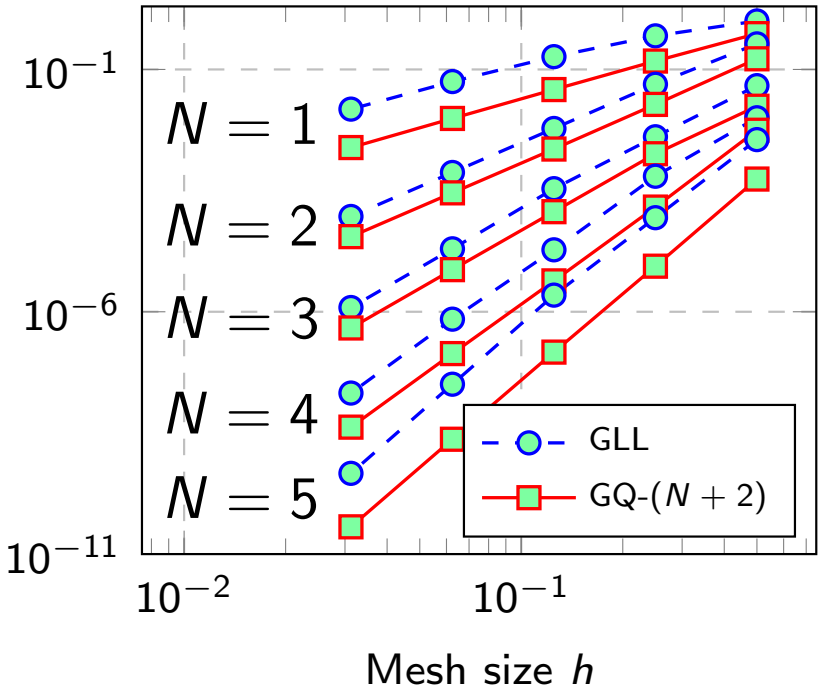
Talk outline

1D compressible Euler equations

- Inexact Gauss-Legendre-Lobatto (GLL) vs Gauss (GQ) quadratures.
- Entropy conservative (EC) and Lax-Friedrichs (LF) fluxes.
- No additional stabilization, filtering, or limiting.



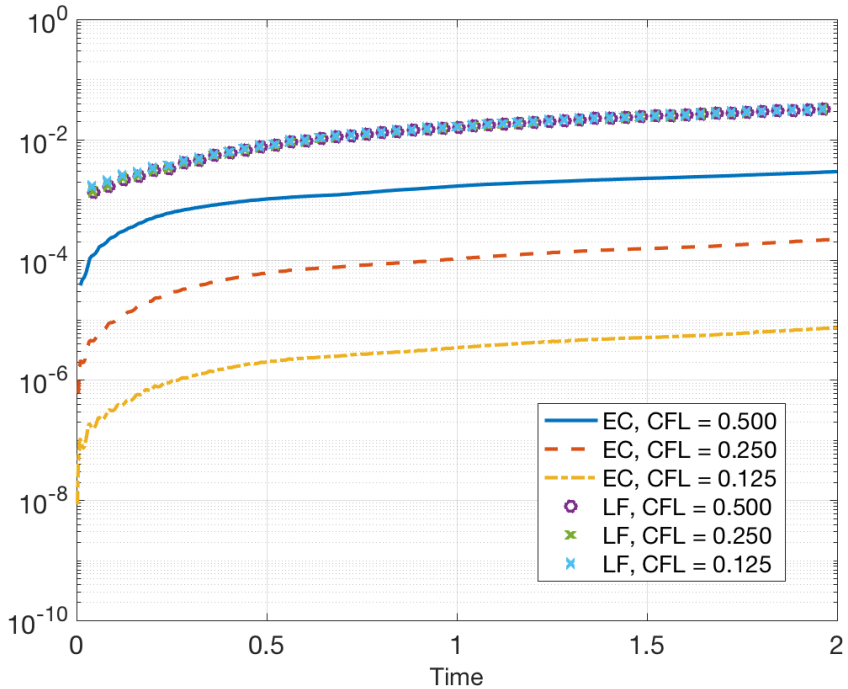
(a) Entropy conservative flux



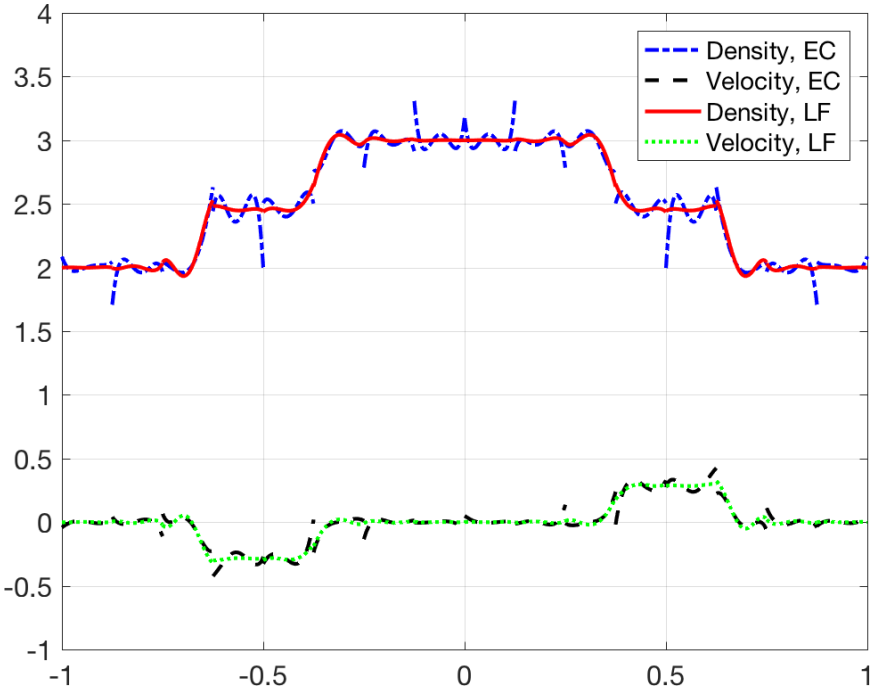
(b) With Lax-Friedrichs penalization

Conservation of entropy: fully discrete schemes

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



(a) $\Delta S(\boldsymbol{u})$ for various Δt

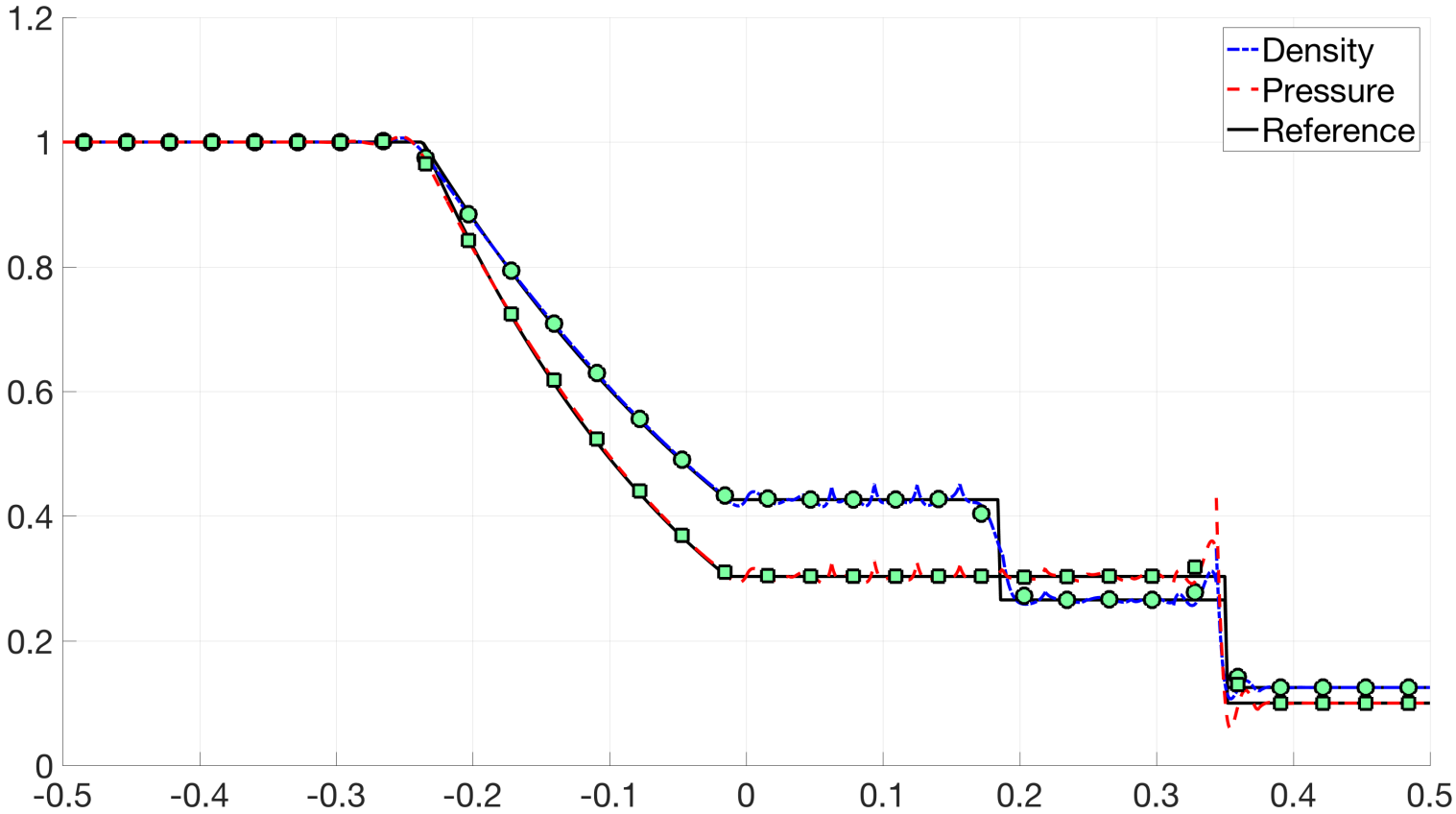


(b) $\rho(x), u(x)$ $(N = 4, K = 16)$

Solution and change in entropy $\Delta S(\boldsymbol{u})$ 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

- Circles are cell averages.
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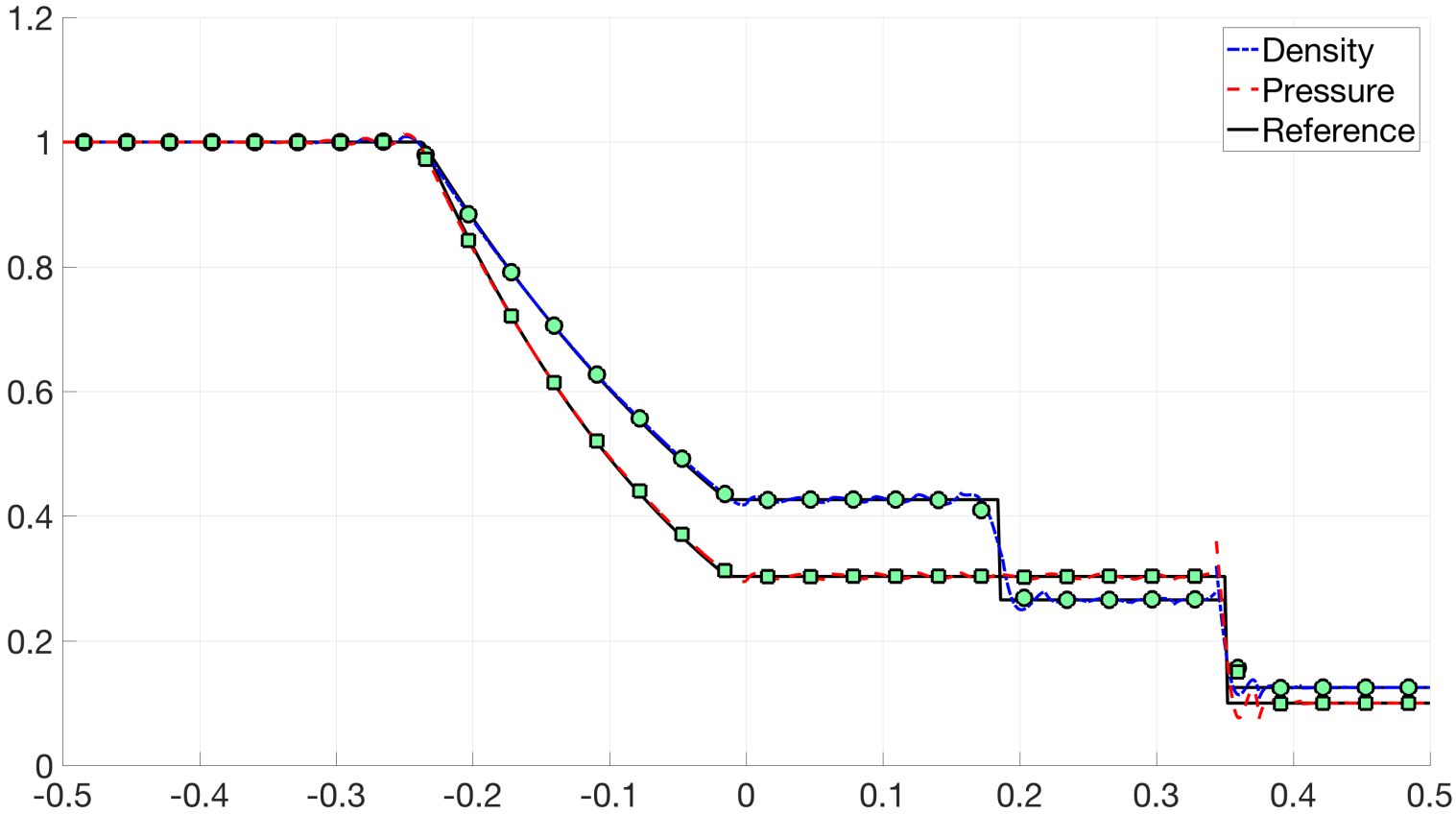
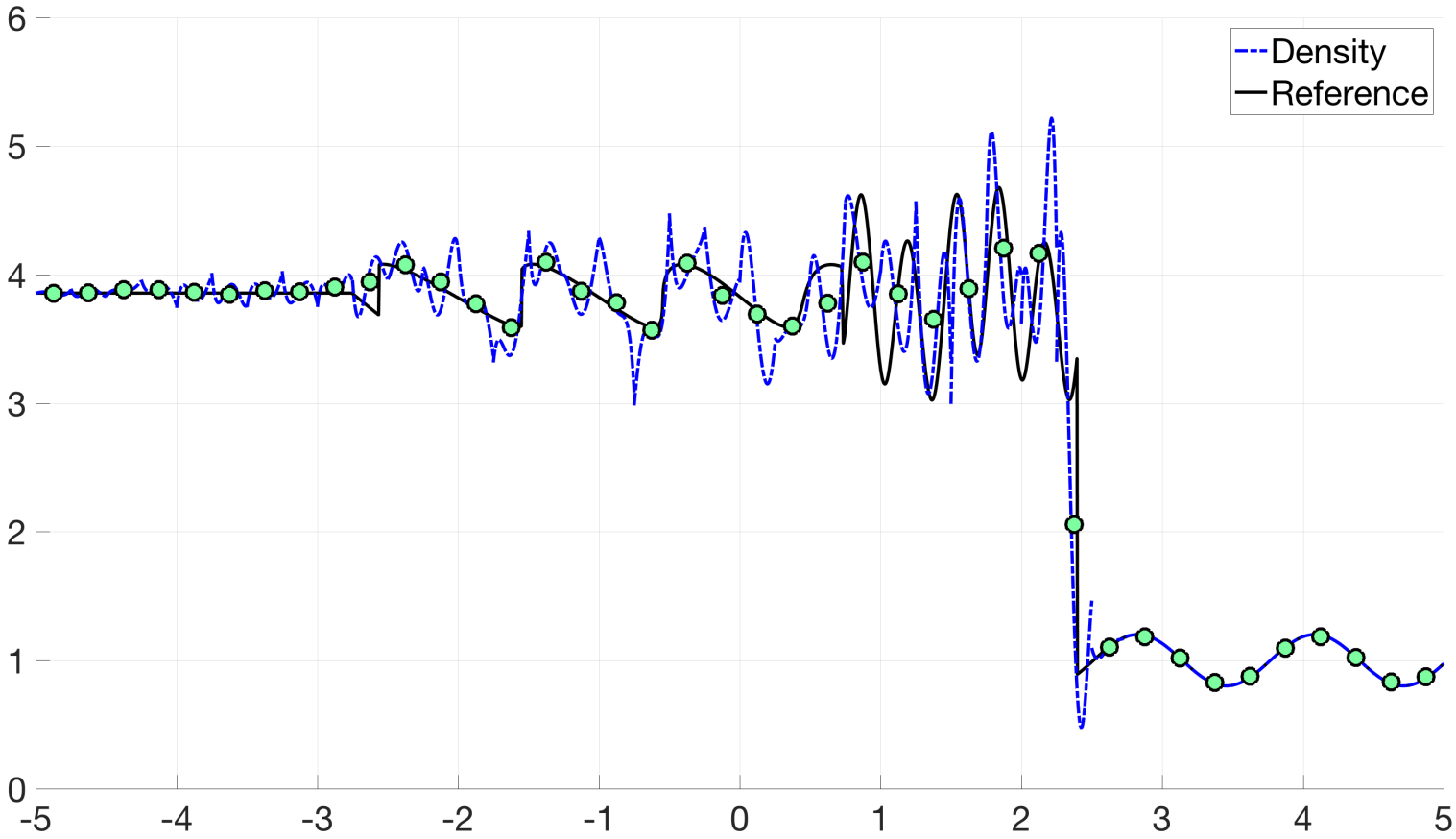


$N = 4, K = 32$, $(N+2)$ point Gauss quadrature.

1D sine-shock interaction

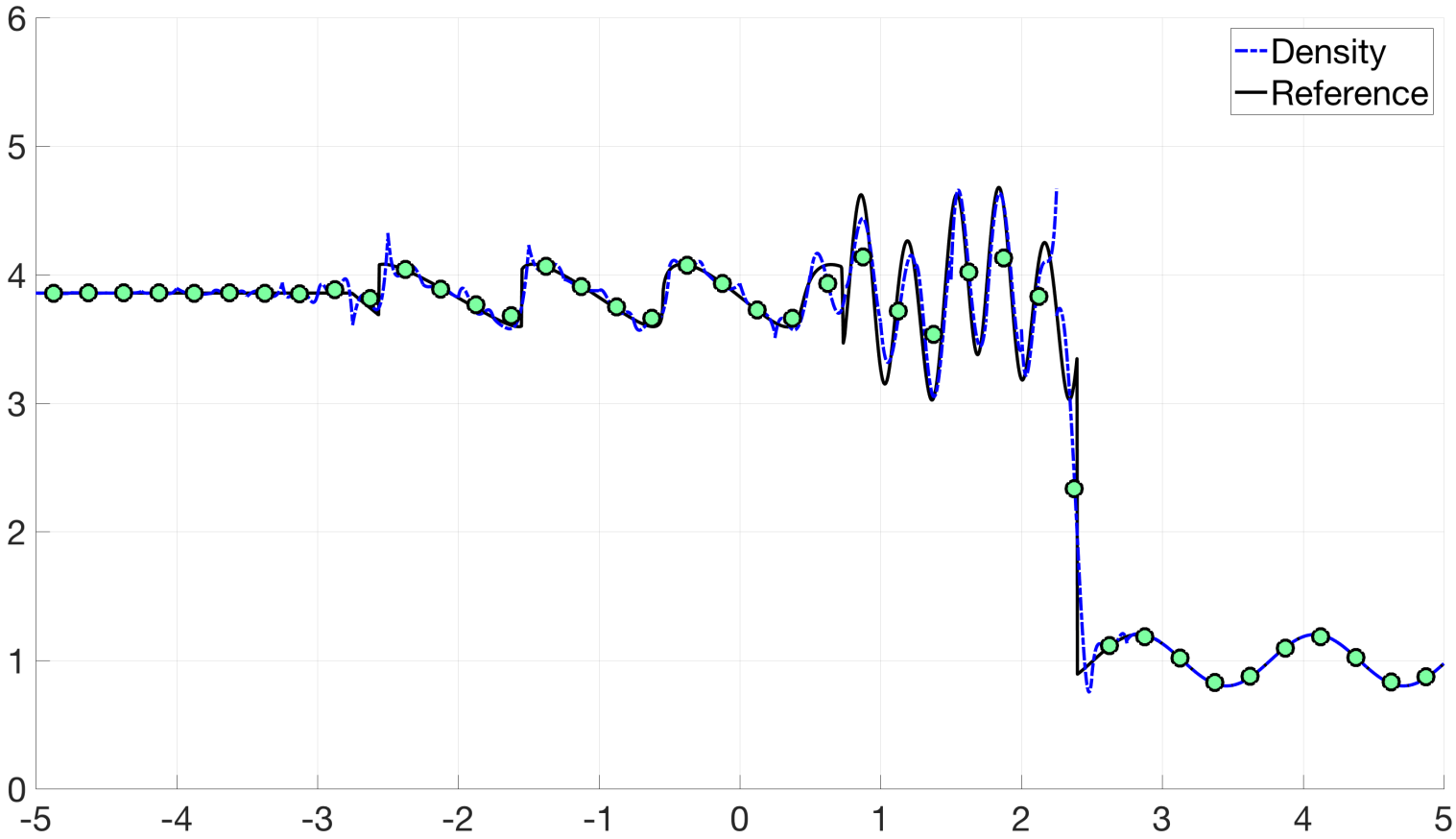
- GQ-$(N+2)$ needs smaller CFL (.05 vs .125) for stability.



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

1D sine-shock interaction

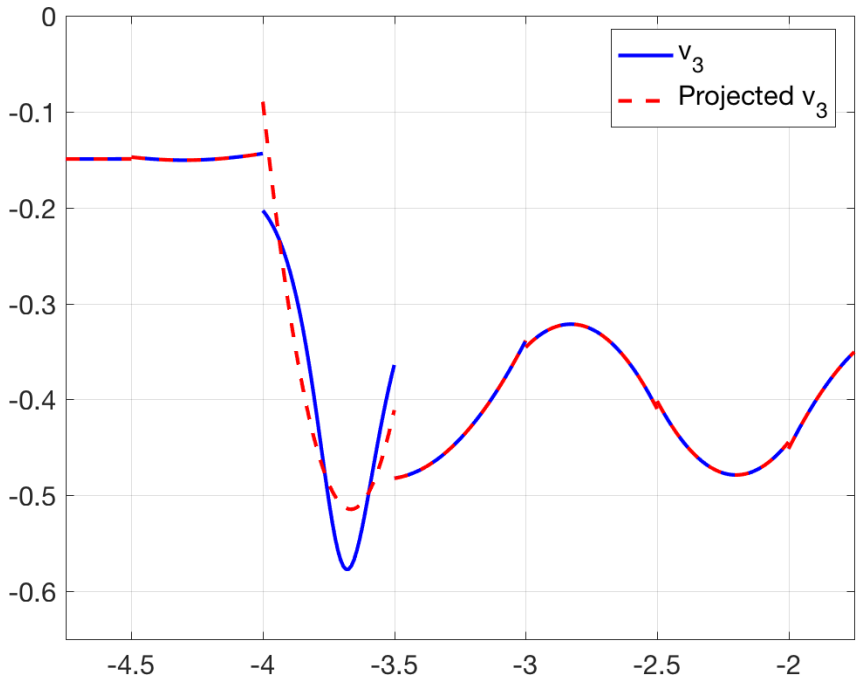
- GQ-$(N+2)$ needs smaller CFL (.05 vs .125) for stability.



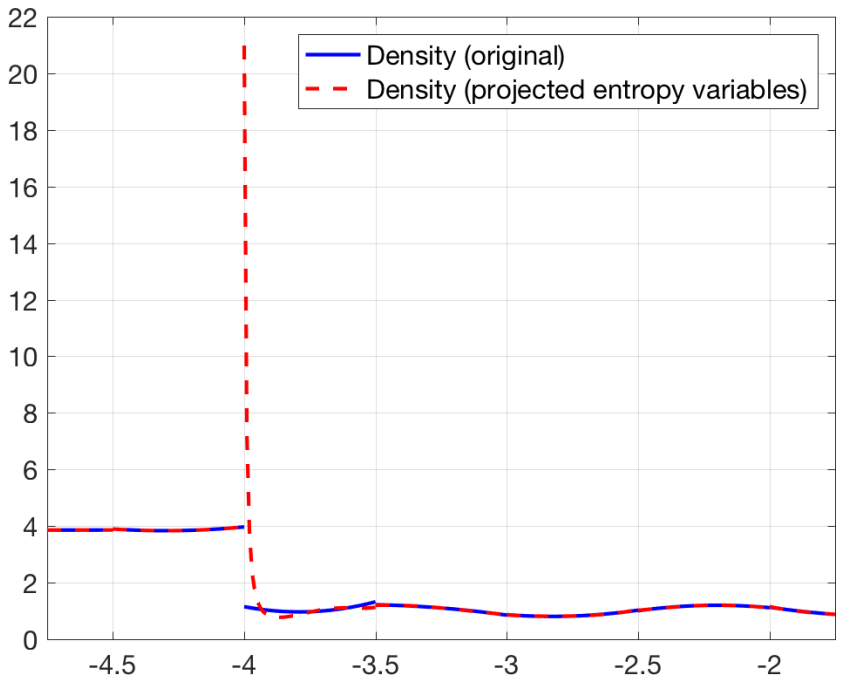
$N = 4, K = 40, CFL = .05$, $(N+2)$ point Gauss quadrature.

On CFL restrictions

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



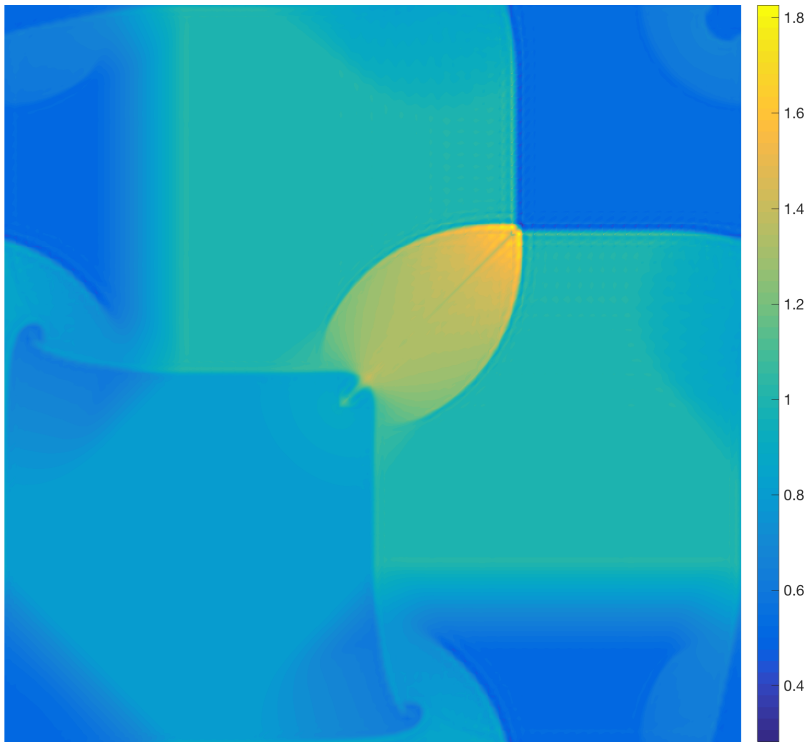
(a) $v_3(x), (P_N v_3)(x)$



(b) $\rho(x), \rho((P_N \boldsymbol{v})(x))$

2D Riemann problem

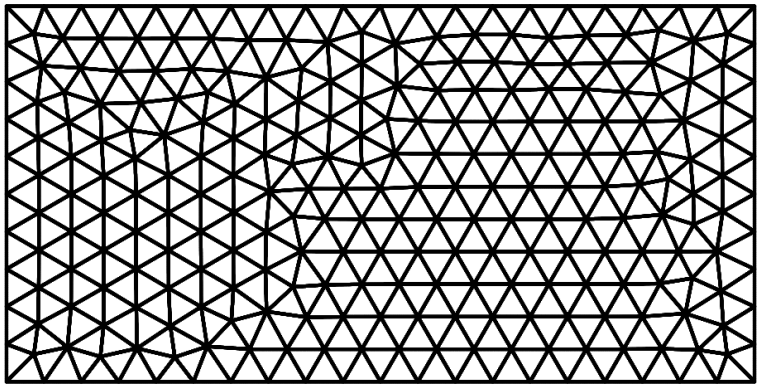
- Uniform 64×64 mesh: $N = 3$, CFL .125, Lax-Friedrichs stabilization.
- No limiting or artificial viscosity required to maintain stability!
- Periodic on larger domain ("natural" boundary conditions unstable).



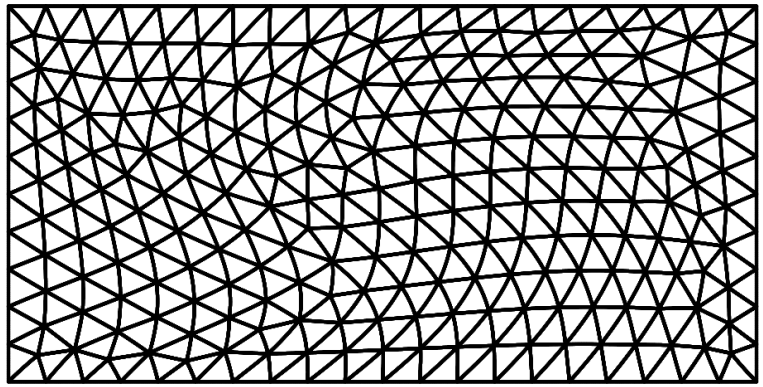
(a) $\Omega = [-1, 1]^2$

(b) $\Omega = [-.5, .5]^2$, 32×32 elements

2D smooth isentropic vortex



(a) Affine mesh



(b) Curved mesh

Figure: Example of affine and warped meshes (corresponding to $h = 1$).

- All experiments utilize weight-adjusted mass matrices.
- Modified conservative variables $\widetilde{\boldsymbol{u}} = \boldsymbol{u}(\widetilde{\boldsymbol{v}})$, $\widetilde{\boldsymbol{v}} = \widetilde{P}_N^k \boldsymbol{v}(\boldsymbol{u}_h)$ defined using weight-adjusted projection $\widetilde{P}_N^k$.

2D smooth isentropic vortex

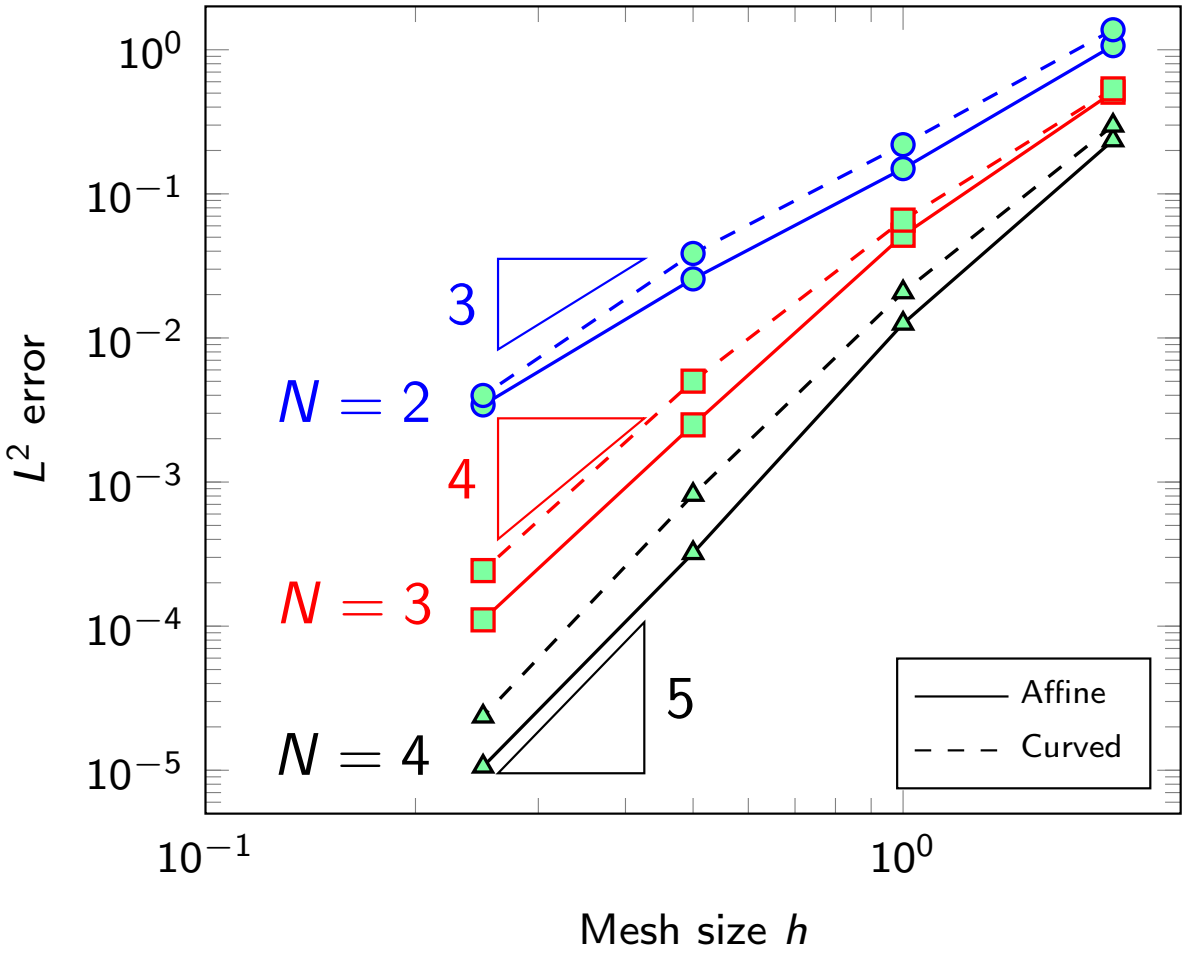
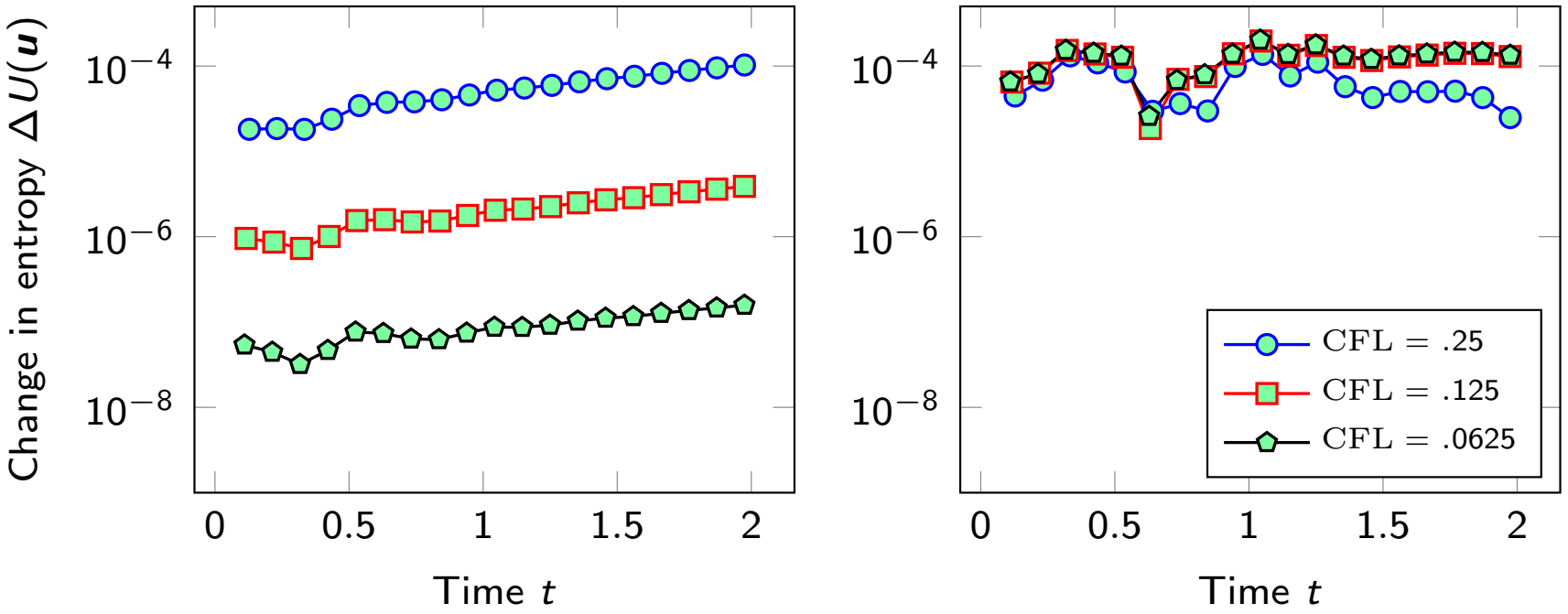


Figure: L^2 errors at $T = 5$ for the 2D isentropic vortex on affine, curved meshes.

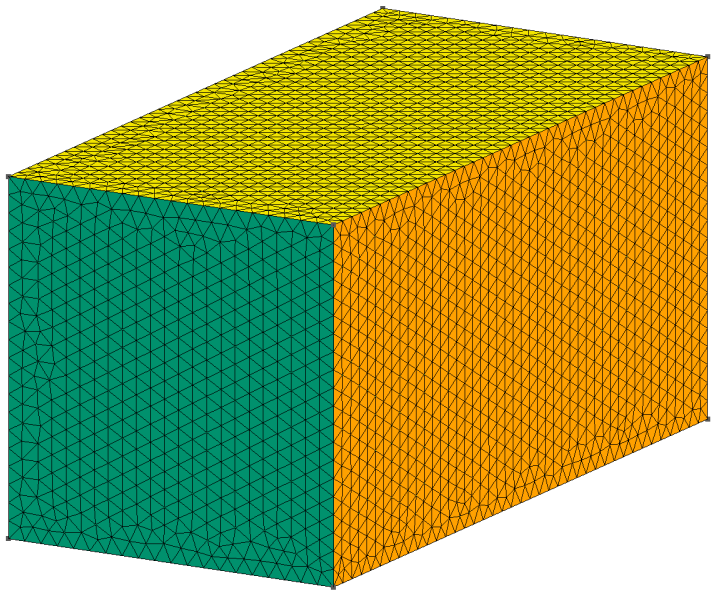
2D curved meshes: conservation of entropy



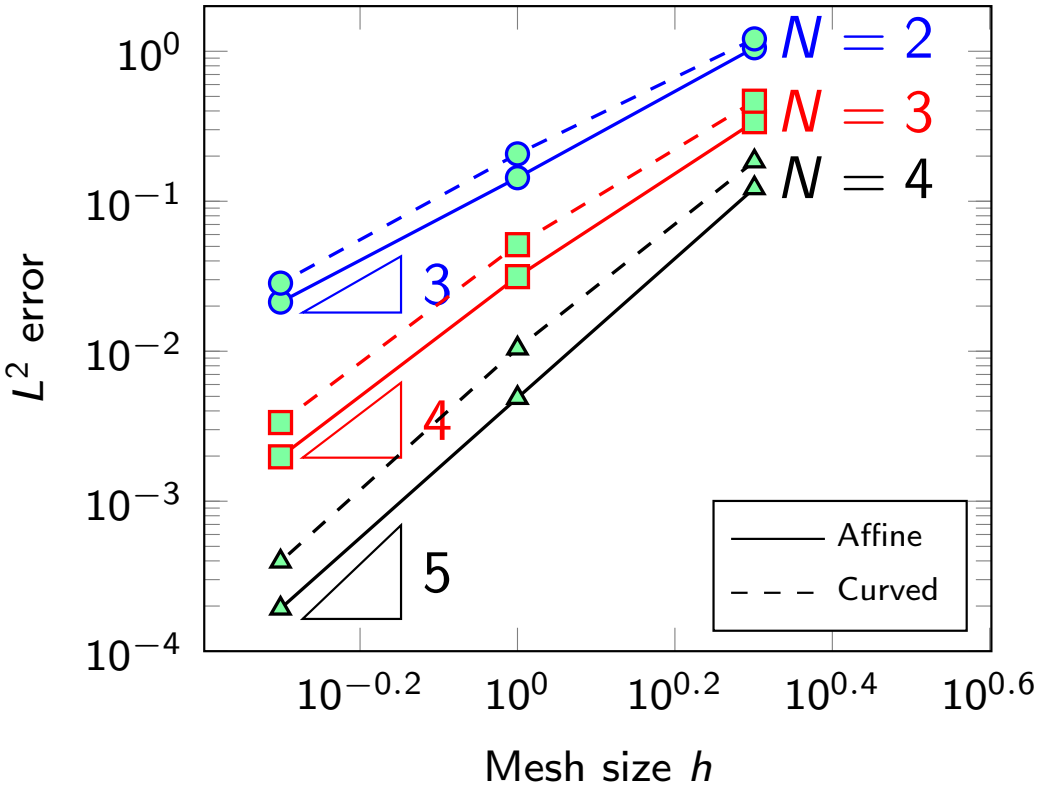
(a) With weight-adjusted projection (b) Without weight-adjusted projection

Figure: Change in entropy under an entropy conservative flux with $N = 4$. In both cases, the spatial formulation tested with $\widetilde{\boldsymbol{v}} = P_N \boldsymbol{v}(\boldsymbol{u})$ is $O\left(10^{-14}\right)$.

3D isentropic vortex



(a) Affine mesh for $h = 1/2$



(b) L^2 errors

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

Taylor-Green vortex

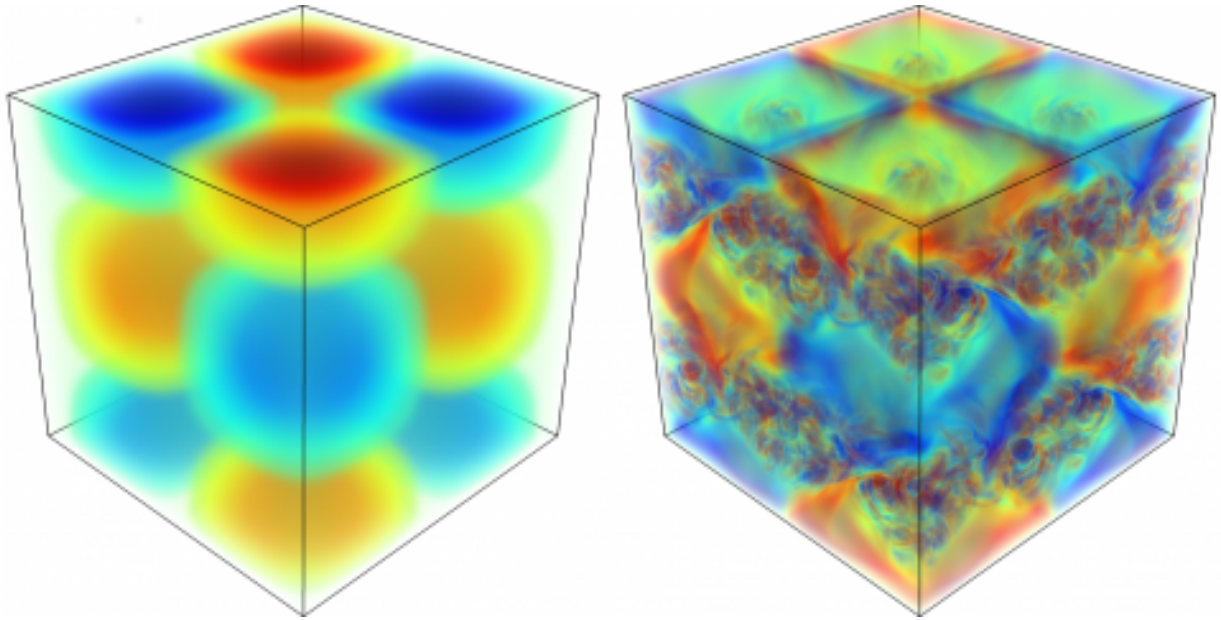
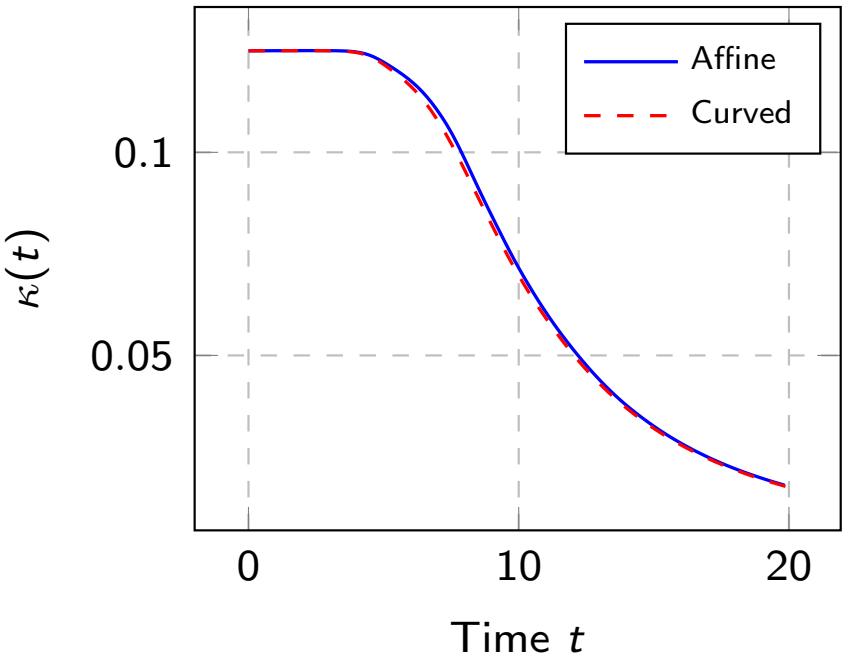


Figure: Isocontours of z-vorticity for Taylor-Green at $t = 0, 10$ seconds.

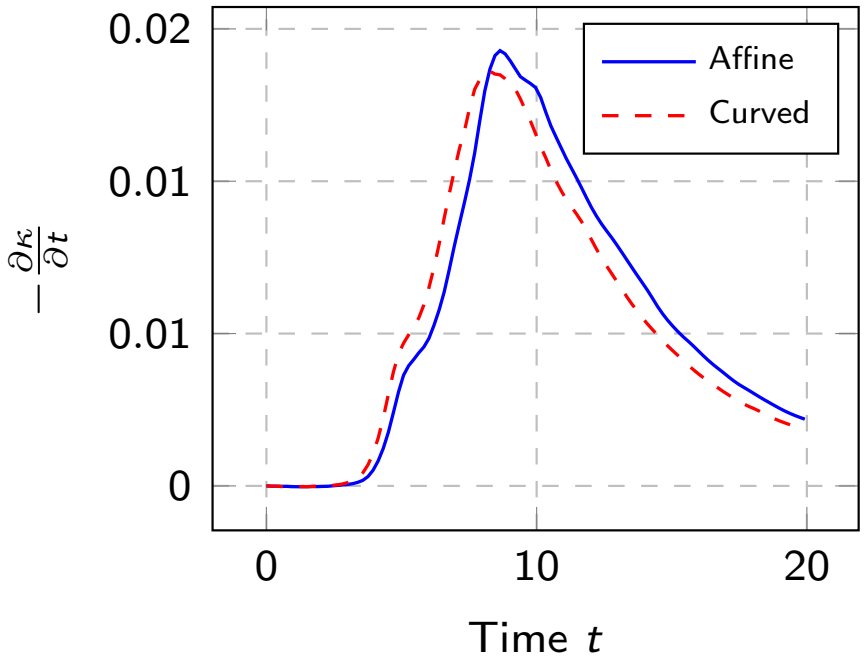
- Simple turbulence-like behavior (generation of small scales).
- Inviscid Taylor-Green: tests robustness w.r.t. under-resolved solutions.

`https://how4.cenaero.be/content/bs1-dns-taylor-green-vortex-re1600`.

Taylor-Green vortex: kinetic energy dissipation rate



(a) Kinetic energy



(b) Kinetic energy dissipation rate

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

Summary and future work

- Discretely stable time-domain high order discontinuous Galerkin methods: provable semi-discrete stability, excellent GPU efficiency.[1]
- Additional work required: strong shocks, positivity preservation.
- Currently: hybrid meshes, continuous FEM, regularization (limiting, artificial viscosity), multi-GPU (with Lucas Wilcox).
- This work is supported by DMS-1719818.

Thank you! Questions?

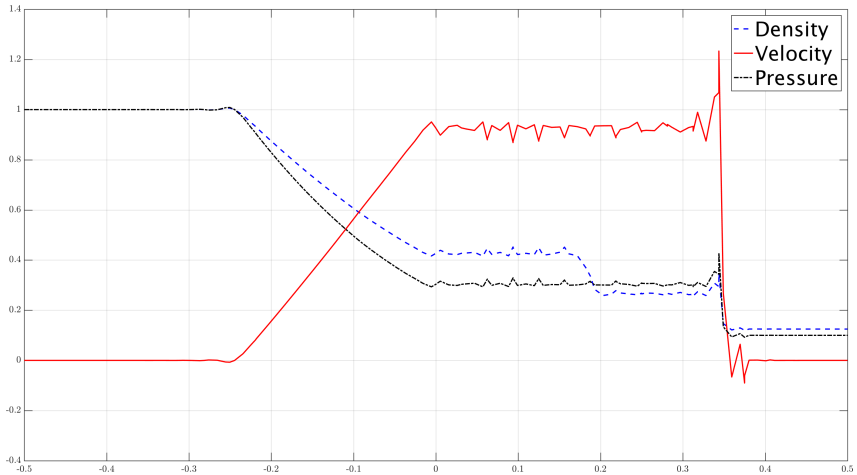
[1] Extra slides on GPU efficiency available!

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

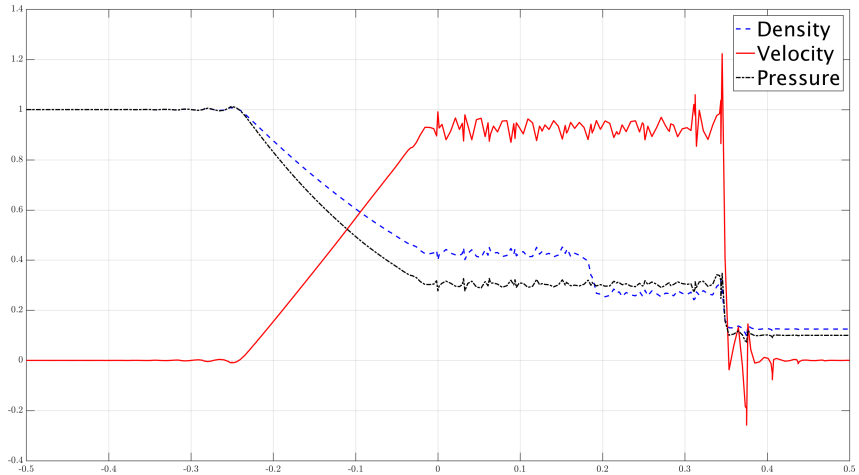
Chan (2017). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods.*

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.

High order DG on many-core (GPU) architectures

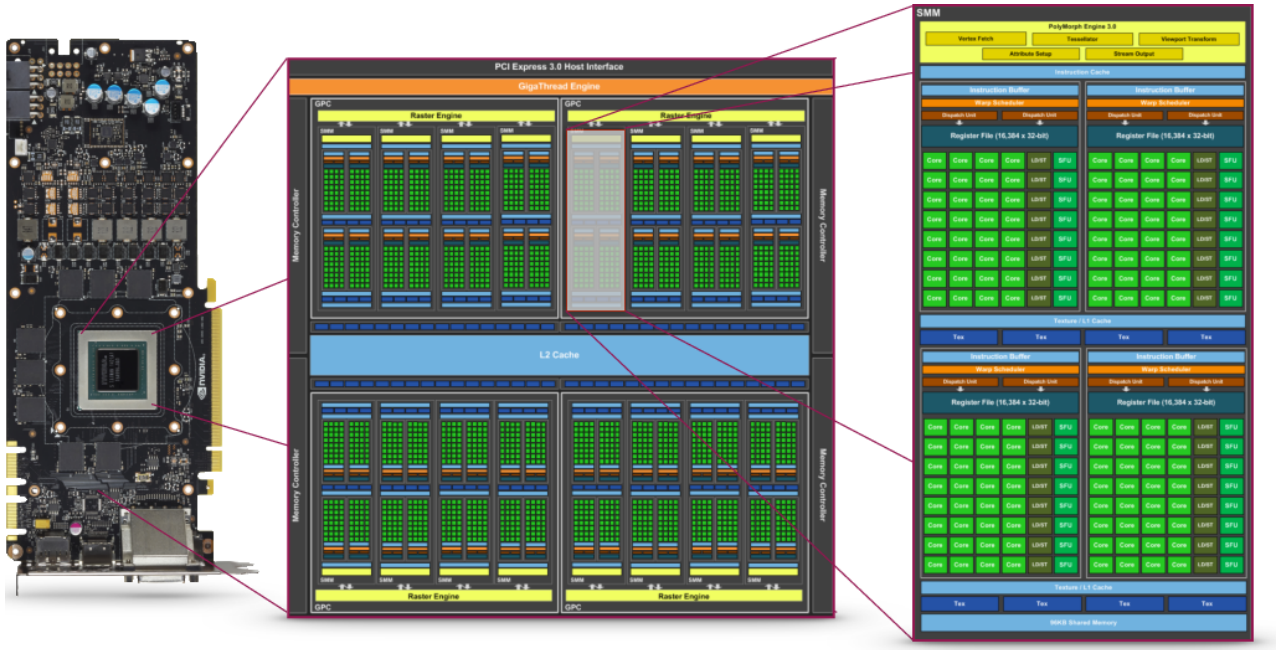


Figure: NVIDIA Maxwell GM204 GPU: 16 cores, 4 SIMD clusters of 32 units.

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

Klockner, Warburton, Bridge, Hesthaven 2009, Nodal discontinuous Galerkin methods on graphics processors.

High order DG on many-core (GPU) architectures

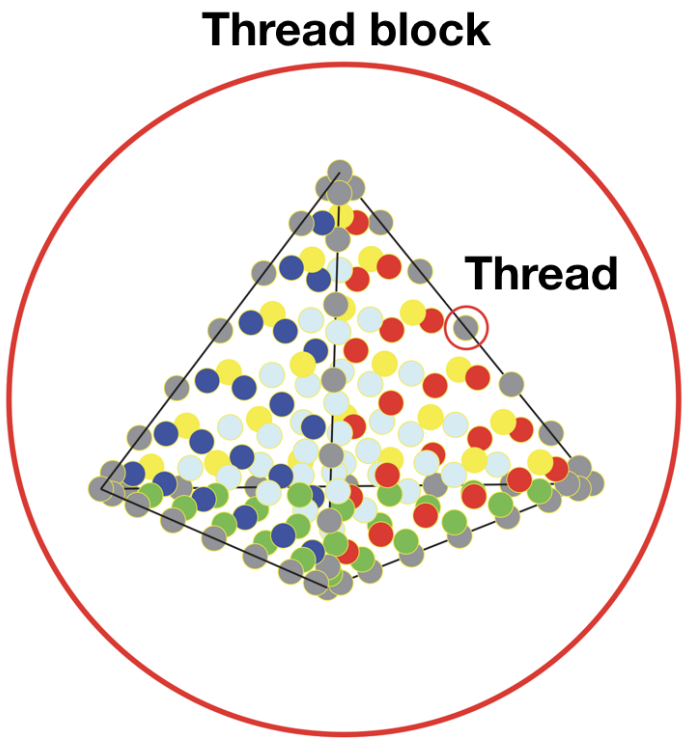


Figure: Thread blocks process elements, threads process degrees of freedom.

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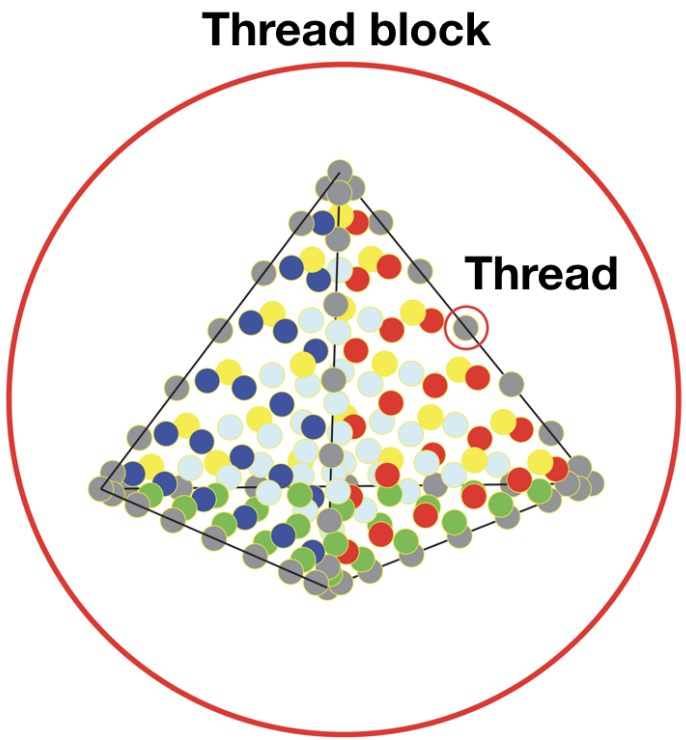

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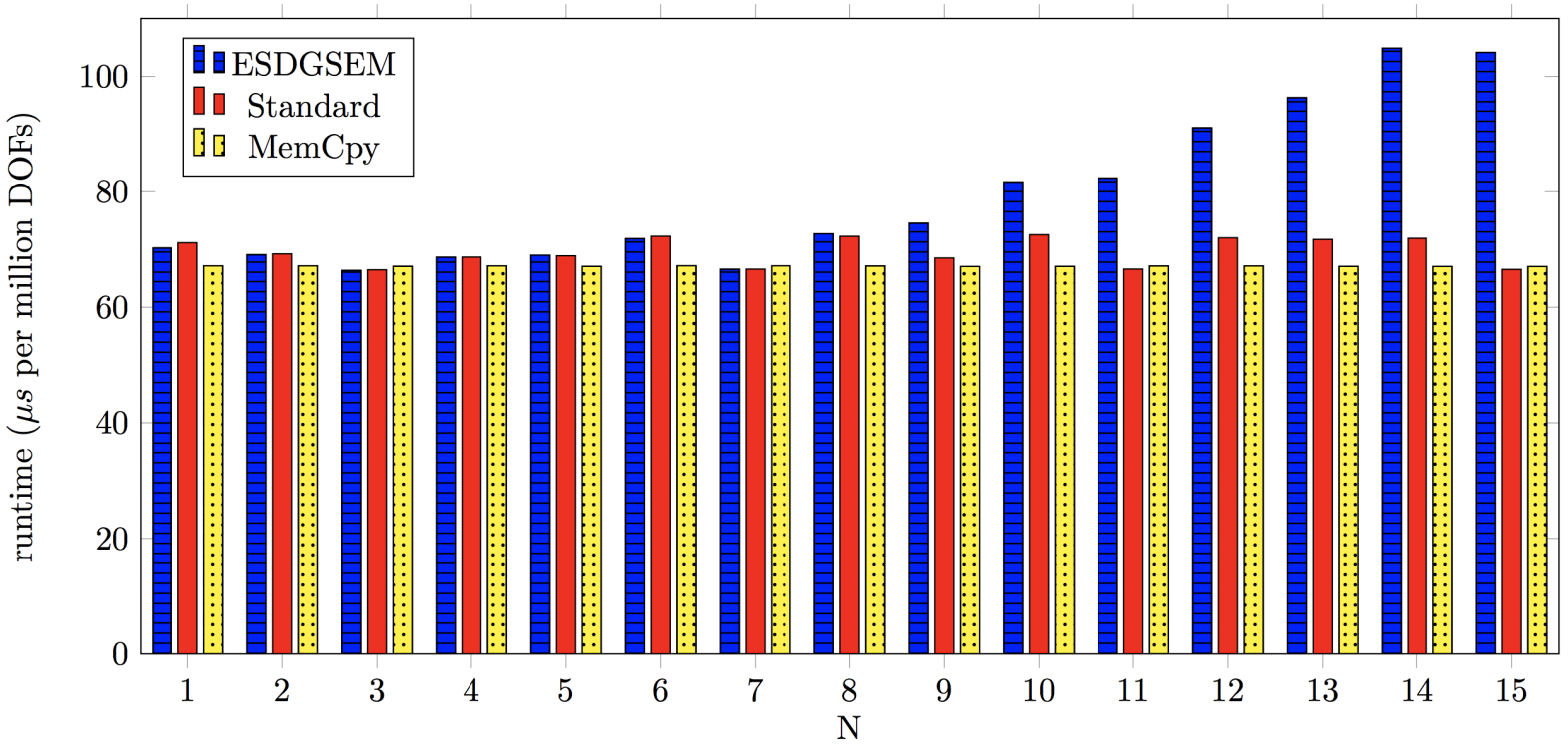
Implementing high order entropy stable DG on GPUs

- "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*.