# Entropy stable discontinuous Galerkin methods using arbitrary bases and quadratures

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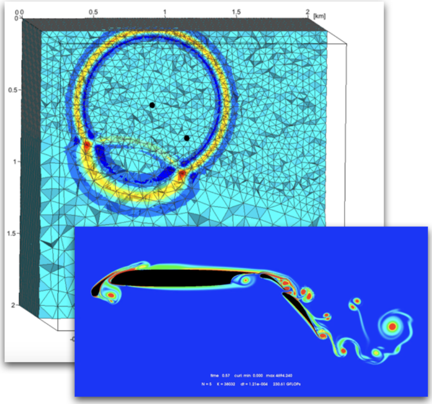
# High order methods for time-dependent hyperbolic PDEs

- 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.

Goal: address instability of high order methods!

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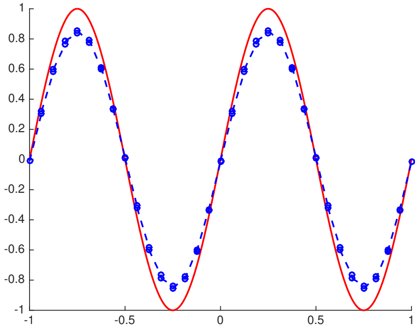


**Fine** linear approximation.

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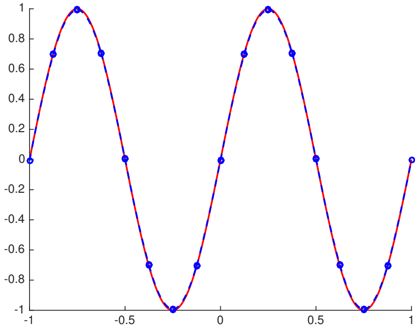


**Coarse** quadratic approximation.

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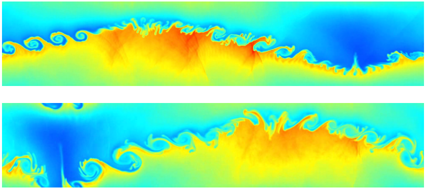

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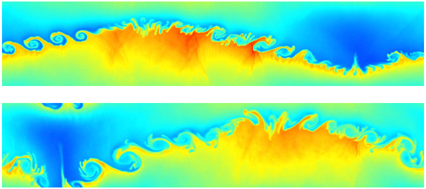

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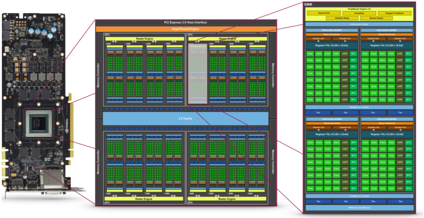

A graphics processing unit (GPU).

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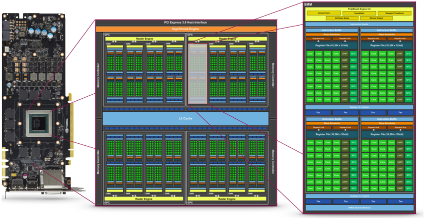

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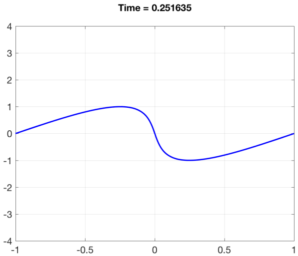
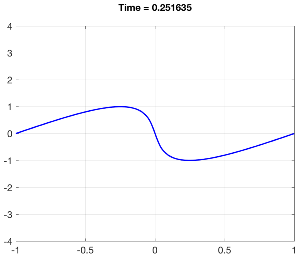
# Why are discretizations of nonlinear PDEs so unstable?




(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.

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

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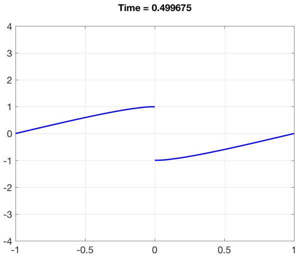


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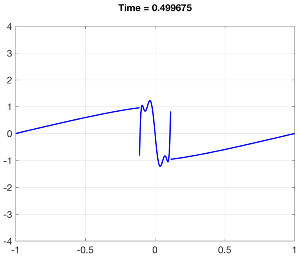


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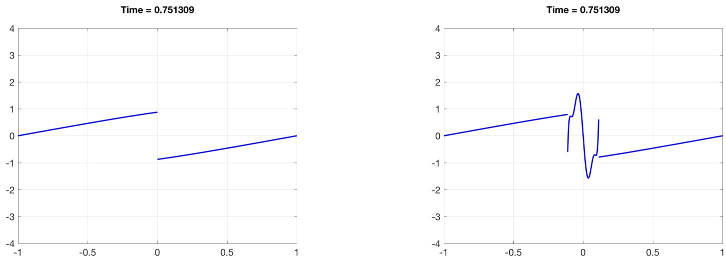


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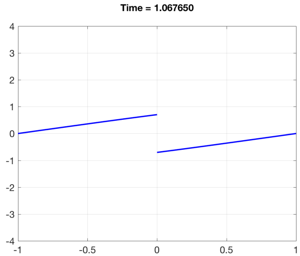


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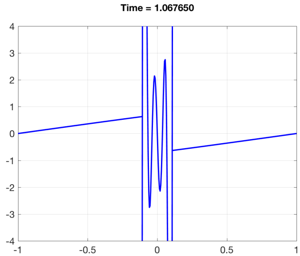


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# Entropy stability for nonlinear conservation laws

- Analogue of energy for nonlinear systems of conservation laws

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

- Weak solutions satisfy a continuous entropy inequality: convex entropy function $S(\boldsymbol{u})$ and "entropy potential" $\psi(\boldsymbol{u})$.

$$\int_\Omega \boldsymbol{v}^T \left( \frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} \right) = 0, \qquad \boldsymbol{v} = \frac{\partial S}{\partial \boldsymbol{u}}$$

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

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

# Example: mathematical entropy (compressible flow)

- Burgers': square entropy $S(\boldsymbol{u}) = u^2/2$, entropy variables $\boldsymbol{v}(\boldsymbol{u}) = u$.
- Shallow water: entropy is total energy, convex if $h > 0$.

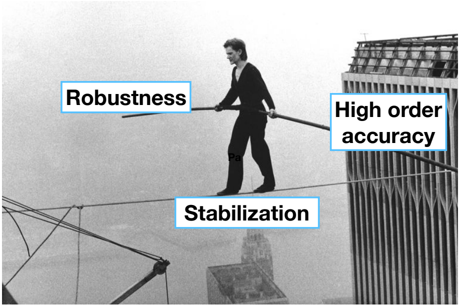
$$S(\boldsymbol{u}) = \frac{1}{2}hu^2 + \frac{1}{2}gh^2 + ghb, \qquad \boldsymbol{v}(\boldsymbol{u}) = \begin{bmatrix} g(h+b) - \frac{u^2}{2} \\ u \end{bmatrix}.$$

- Compressible Euler equations: physical entropy $s(\boldsymbol{u})$ always increases; mathematical entropy $S(\boldsymbol{u})$ always decreases.

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

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

# Why discretely entropy stable (ES) schemes?




- Existing discrete stability theory: regularization, viscosity, TVD, etc.
- Can result in a balancing act between high order accuracy, stability, and robustness.
- Goal: aim for stability independently of artificial viscosity, limiters, and quadrature accuracy.

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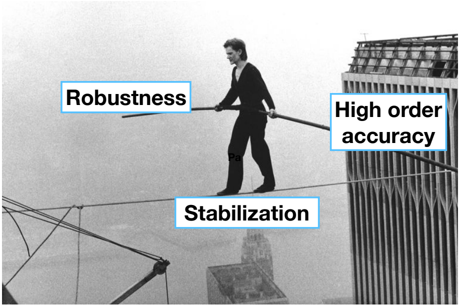


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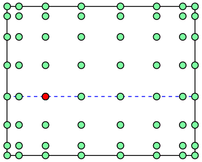
# Talk outline

1. Summation by parts methods
2. Entropy stable formulations and flux differencing
3. Numerical experiments

# Talk outline

# Overview of entropy stable high order SBP schemes



(a) GLL collocation

- Discrete entropy inequality for SBP schemes (e.g. GLL collocation).
- GSBP (e.g. Gauss collocation): higher accuracy, but require non-compact coupling conditions between neighboring elements.
- Tetrahedra, wedges, pyramids: over-integration?

Goals: entropy stability, compact coupling, arbitrary basis/quadrature.

Fisher and Carpenter (2013), Gassner, Winters, and Kopriva (2016), Chen and Shu (2017), Crean, Hicken, et al. (2018).

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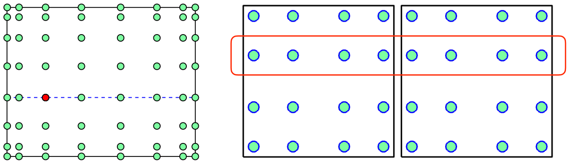

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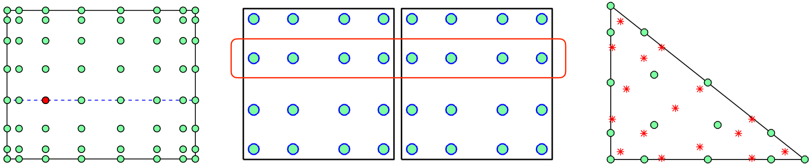

(a) GLL collocation (b) Gauss nodes coupling (c) Nodes vs cubature

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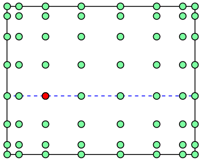

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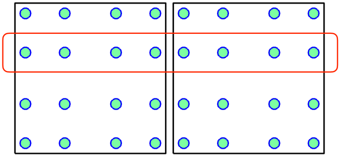
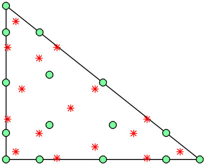


(b) Gauss nodes coupling



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# 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 $2N-1$ (volume) and $2N$ (surface). Define diagonal weight matrices

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

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- Useful operators: quadrature-based $L^2$ projection and lifting matrices

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

- $\boldsymbol{D}_q^i = \boldsymbol{V}_q \boldsymbol{D}^i \boldsymbol{P}_q$: evaluates $i$th derivative of $L^2$ projection at $\boldsymbol{x}_i^q$.

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# A "decoupled" block SBP operator

- Decoupled SBP: improve approx. by incorporating boundary points:

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

- $\boldsymbol{D}_N^i$ 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 $u \approx f\frac{\partial g}{\partial x}$

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

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

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

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

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

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

$$\boldsymbol{Q}_N^i = \begin{bmatrix} \boldsymbol{W} & \\ & \boldsymbol{W}_f \end{bmatrix} \boldsymbol{D}_N^i, \qquad \boldsymbol{Q}_N^i + \left(\boldsymbol{Q}_N^i\right)^T = \begin{bmatrix} 0 & \\ & \boldsymbol{W}_f \boldsymbol{n}_i \end{bmatrix}$$

# Talk outline

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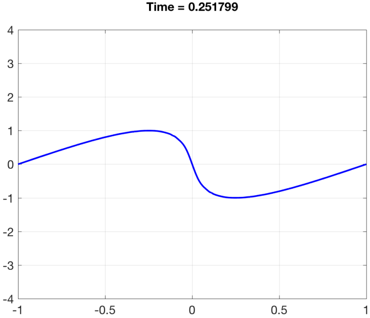
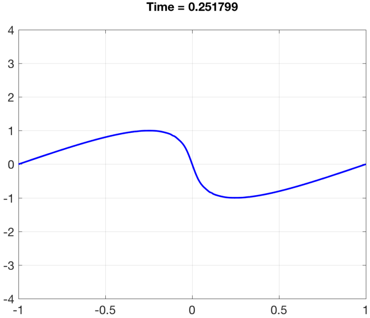



(a) Energy conservative




(b) Energy stable

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

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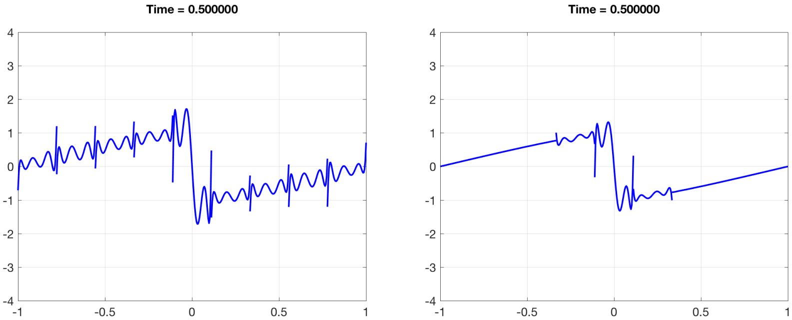


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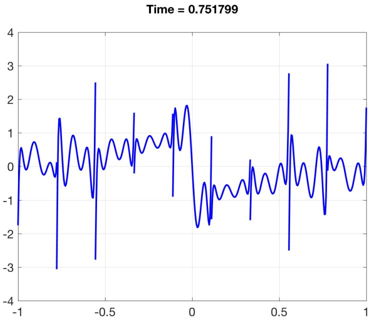


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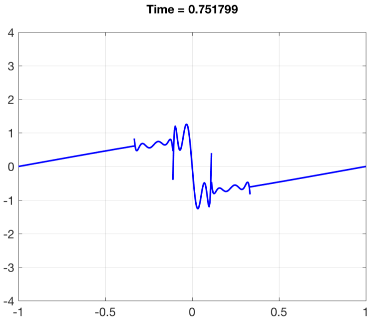


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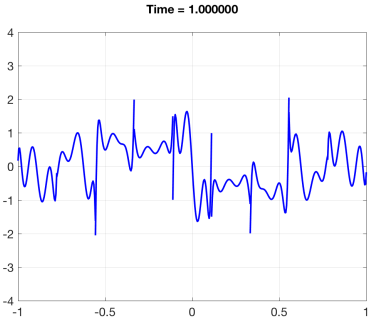


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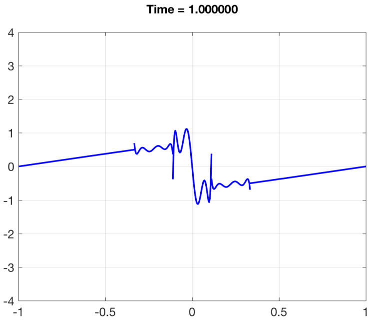


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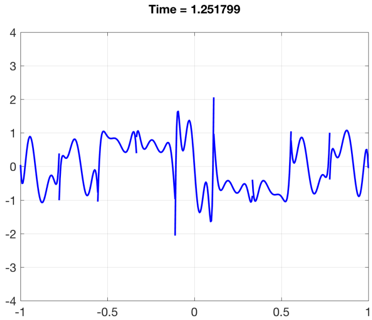


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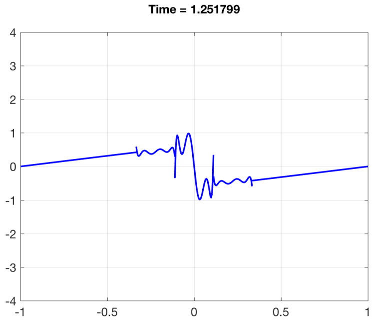


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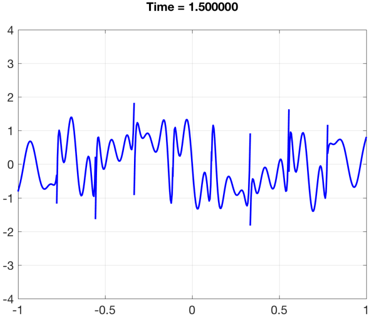


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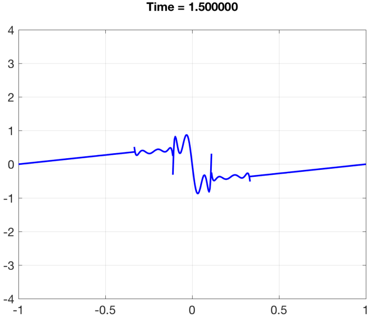


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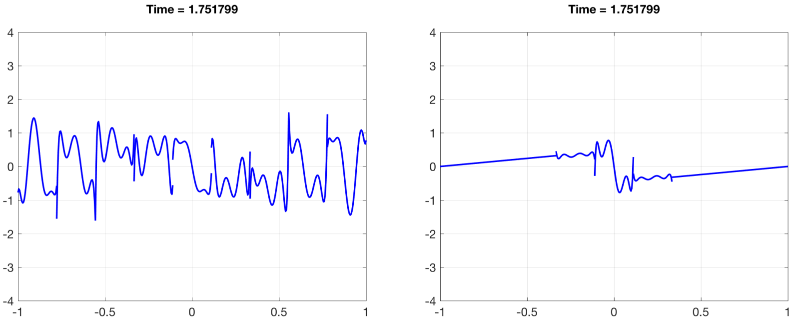


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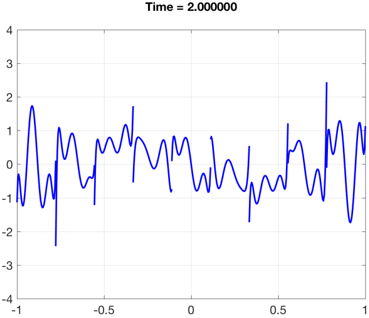


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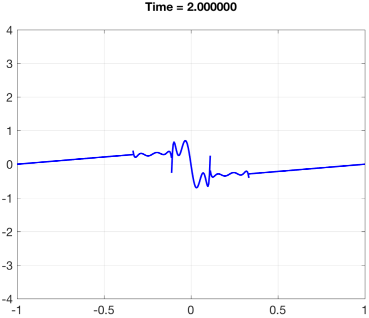


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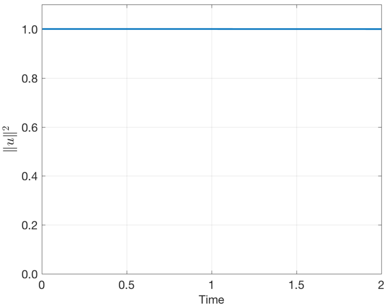


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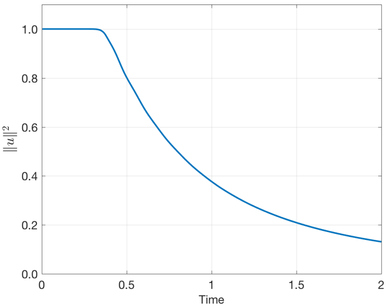


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# Flux differencing: entropy conservative finite volume fluxes

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

$$\boldsymbol{f}_S(\boldsymbol{u},\boldsymbol{u}) = \boldsymbol{f}(\boldsymbol{u}), \qquad \boldsymbol{f}_S(\boldsymbol{u},\boldsymbol{v}) = \boldsymbol{f}_S(\boldsymbol{v},\boldsymbol{u}), \qquad \text{(consistency, symmetry)}$$
$$\left(\boldsymbol{v}_L - \boldsymbol{v}_R\right)^T \boldsymbol{f}\left(\boldsymbol{u}_L,\boldsymbol{u}_R\right) = \psi_L - \psi_R, \qquad \text{(conservation).}$$

- Flux differencing for Burgers' equation: let $u_L = u(x), u_R = u(y)$

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

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- Beyond split formulations: mass flux for compressible Euler

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

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# Flux differencing: implementational details

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

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

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

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

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

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

# 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* $\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(P_N \boldsymbol{v}\right)$. *Let* $\widehat{\boldsymbol{u}}$ *locally solve*

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

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

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

- Need to modify $\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(P_N \boldsymbol{v}\right)$ for projected entropy variables $P_N \boldsymbol{v}$!
- Add interface dissipation (e.g. Lax-Friedrichs) for entropy inequality.

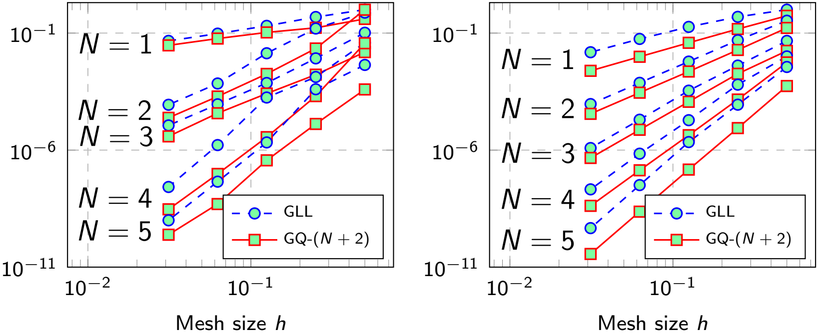
Parsani et al. (2016). *ES staggered grid disc. spectral collocation methods of any order for the comp. NS eqns.*

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

# 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.

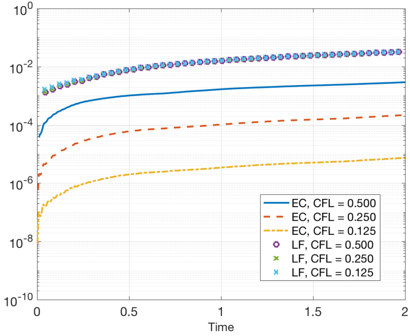



(a) Entropy conservative flux

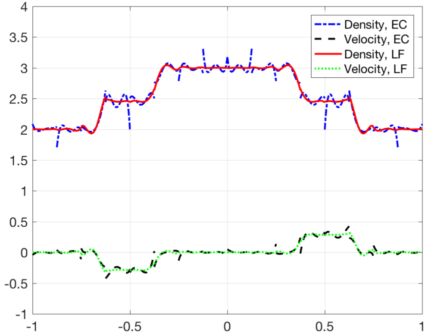
(b) With Lax-Friedrichs penalization

# 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 $\Delta t$

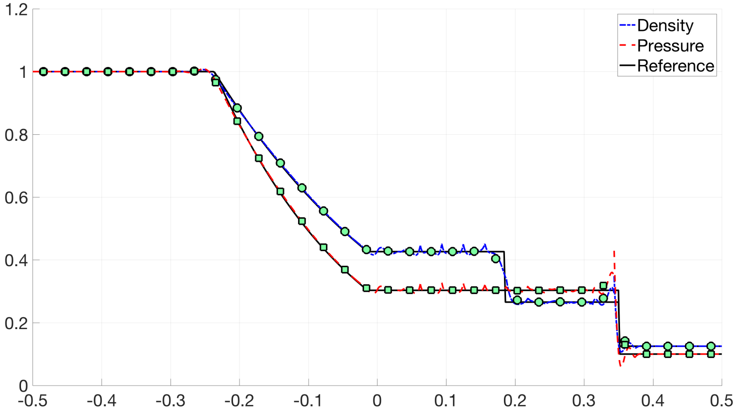



(b) $\rho(x), u(x)$ $(N = 4, K = 16)$

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

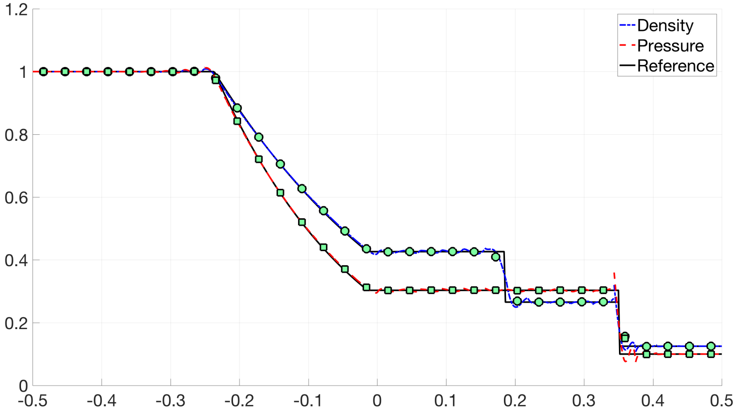
- Circles are cell averages.
- CFL of .125 used for both GLL-$(N+1)$and GQ-$(N+2)$.




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

# 1D Sod shock tube

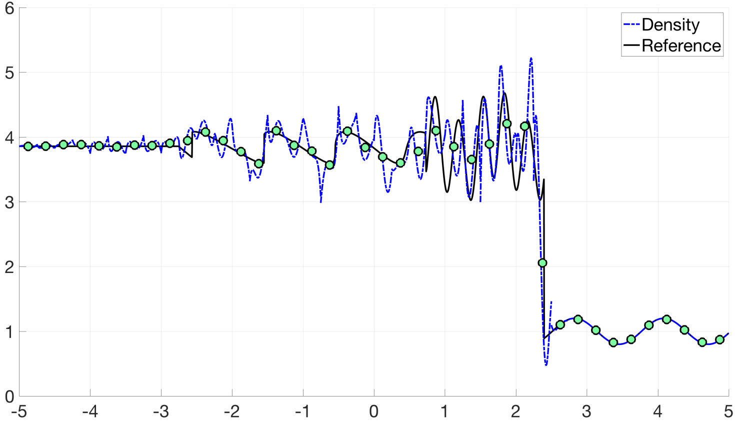
- Circles are cell averages.
- CFL of .125 used for both GLL-$(N+1)$and GQ-$(N+2)$.




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

# 1D sine-shock interaction

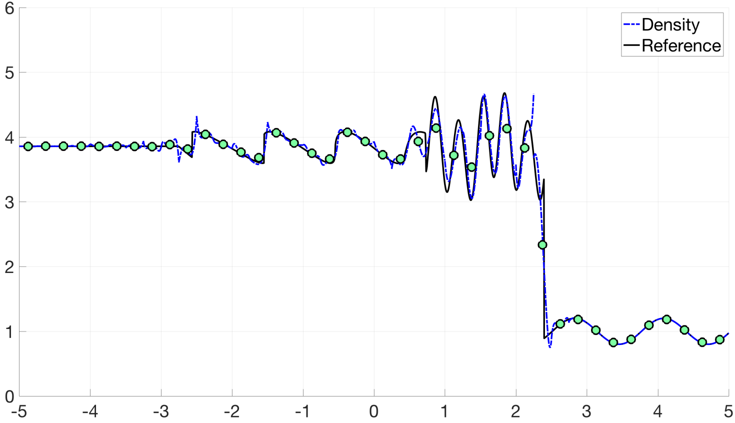
- GQ-$(N+2)$ needs smaller CFL (.05 vs .125) for stability.




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

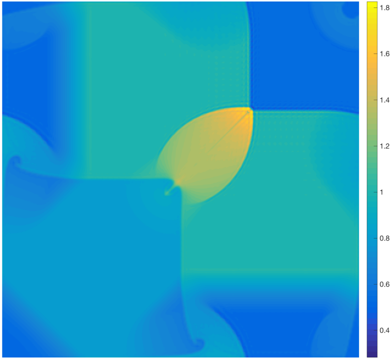
# 1D sine-shock interaction

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




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

# 2D Riemann problem

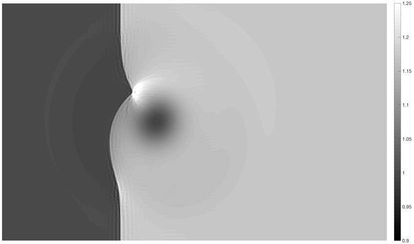



(a) $\Omega = [-1,1]^2$

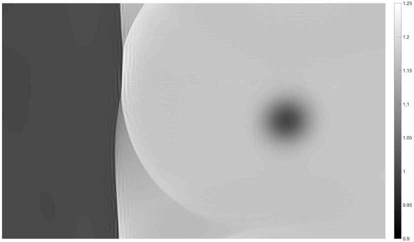

(b) $\Omega = [-.5,.5]^2$, $32 \times 32$ elements

- Uniform $64 \times 64$ 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).

# 2D shock-vortex interaction




(a) $t = .3$




(b) $t = .7$

- Vortex passing through a shock on a periodic domain (matrix dissipation, degree $N = 3$ approximation, mesh size $h = 1/128$).
- Entropy stable wall boundary conditions for GSBP still needed.

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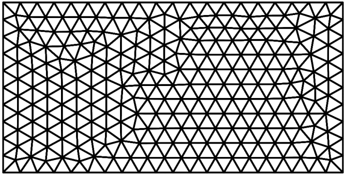
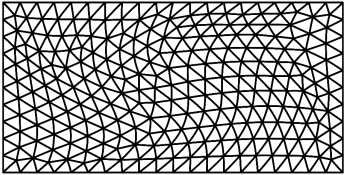
Winters, Derigs, Gassner, Walch (2017). *A uniquely defined entropy stable matrix dissipation operator for high Mach number ideal MHD and compressible Euler simulations.*

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



(a) Affine mesh



(b) Curved mesh

Figure: Example of an affine and warped 2D mesh (corresponding to $h = 1$).

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

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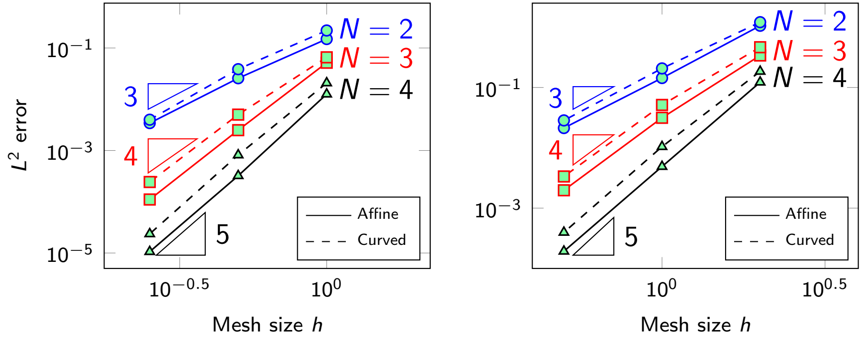
Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.
Kopriva (2006). Metric identities and the discontinuous spectral element method on curvilinear meshes.
Chan, Hewett, and Warburton (2016). *Weight-adjusted discontinuous Galerkin methods: 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.

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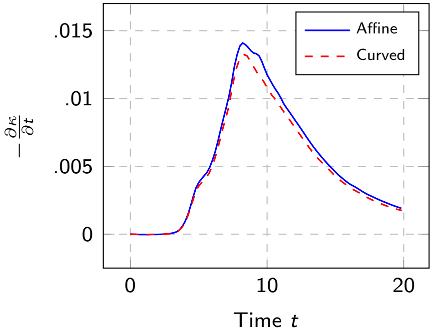
Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.

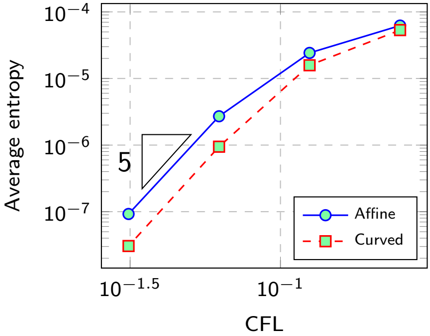
Kopriva (2006). Metric identities and the discontinuous spectral element method on curvilinear meshes.

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

# 3D inviscid Taylor-Green vortex: KE dissipation rate




(a) KE dissipation rate ($N = 3$, $h = \pi/8$)




(b) $\int_\Omega U(\boldsymbol{u}) \to 0$ without dissipation

- Kinetic energy dissipation rate: good agreement with literature.
- $\int_\Omega U(\boldsymbol{u}) \to 0$ as $\mathrm{CFL} \to 0$ for entropy conservative scheme.

# Summary and future work

- Discretely stable time-domain high order discontinuous Galerkin methods: provable semi-discrete stability
- Challenges: strong shocks, positivity, computational cost.
- Current work: Gauss collocation (with DCDR Fernandez, M. Carpenter), adaptivity + hybrid meshes, multi-GPU (with L. Wilcox).
- This work is supported by DMS-1719818 and DMS-1712639.

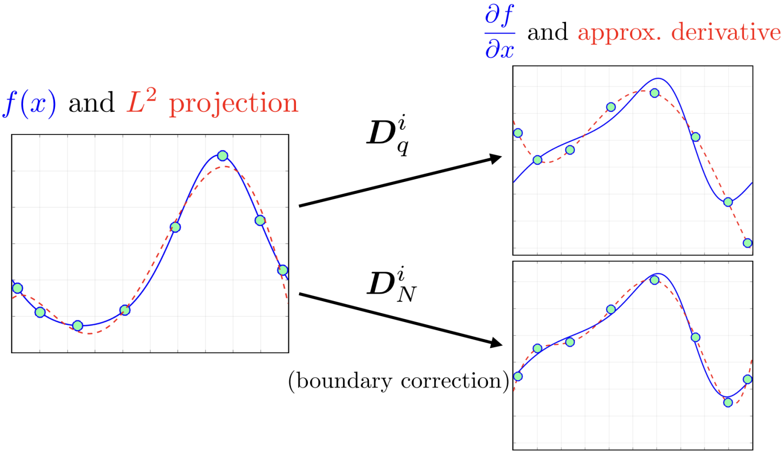
Thank you! Questions?

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

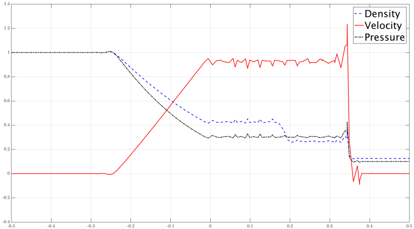
Chan (2017). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods.*

# Additional slides

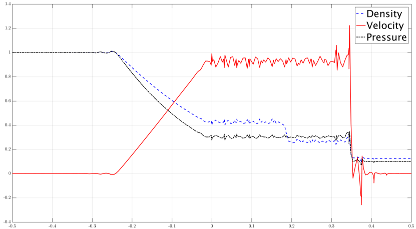
# Accuracy of $D_N^i$



# Over-integration is ineffective without $L^2$ projection




(a) Degree $N$ GLL, $(N+1)$ points

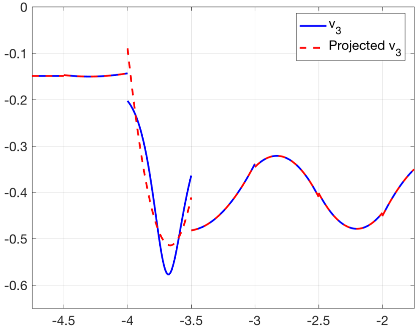



(b) Degree $N$ GLL, $(N+4)$ points

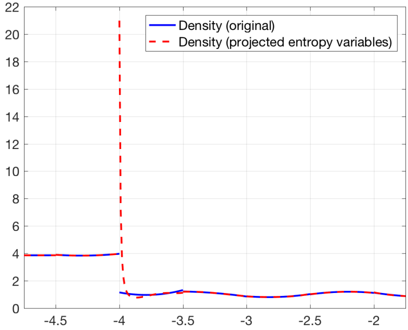
Figure: Sod shock tube for $N = 4$ and $K = 32$ elements. Over-integrating by increasing the number of quadrature points does not improve solution quality.

# On CFL restrictions

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

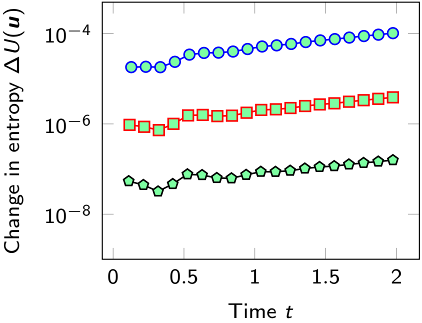



(a) $v_3(x), \left(P_N v_3\right)(x)$

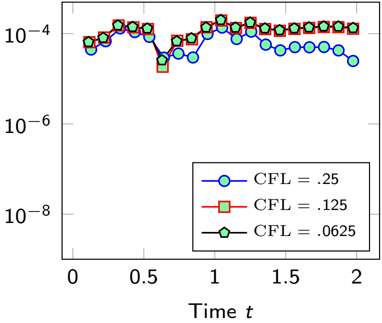



(b) $\rho(x), \rho\left(\left(P_N \boldsymbol{v}\right)(x)\right)$

# 2D curved meshes: conservation of entropy




(c) With weight-adjusted projection




(d) 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 $O\left(10^{-14}\right)$.