Discretely entropy stable discontinuous Galerkin methods for nonlinear conservation laws

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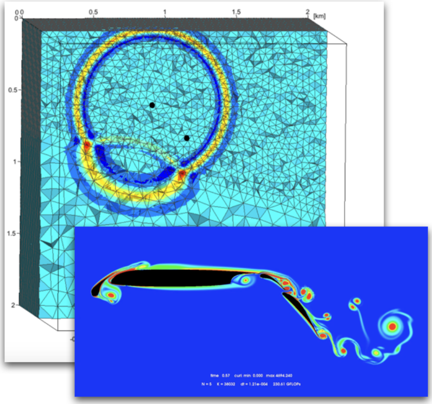
- Accurate resolution of propagating waves and vortices.
- High order: low numerical dissipation and dispersion.
- High order approximations: more accurate per unknown.
- Many-core architectures (efficient explicit time-stepping).



Figures courtesy of T. Warburton, A. Modave.

Goal: address instability of high order methods!

High order methods for time-dependent hyperbolic PDEs

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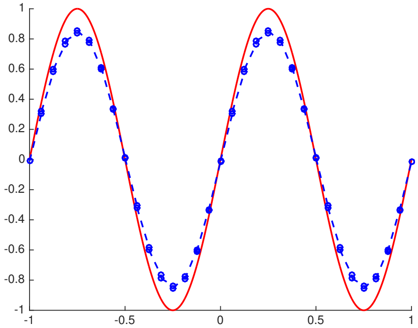

Fine linear approximation.

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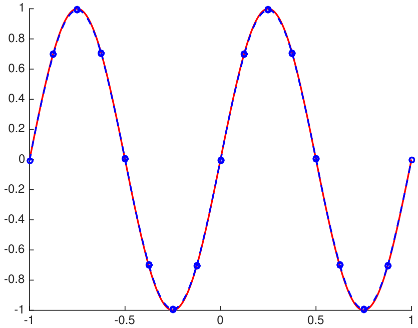

Coarse quadratic approximation.

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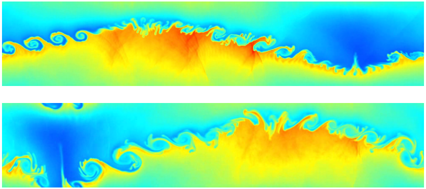

Figure from Per-Olof Persson.

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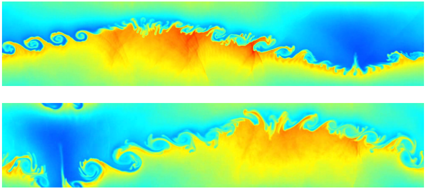

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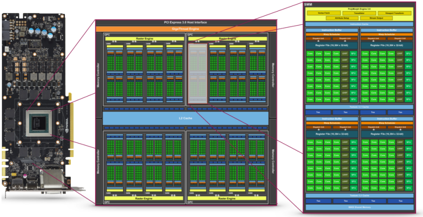

A graphics processing unit (GPU).

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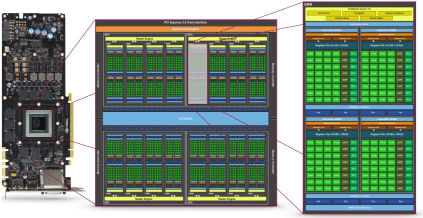

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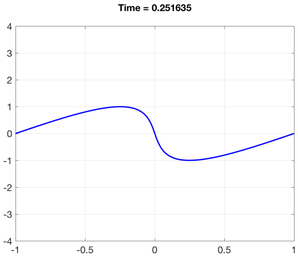
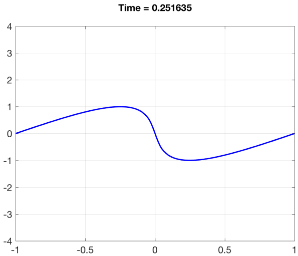
Why are discretizations of nonlinear PDEs so unstable?



(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 $\frac{\partial}{\partial x} f(u)$?

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

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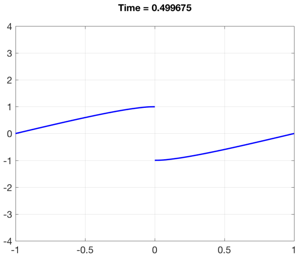

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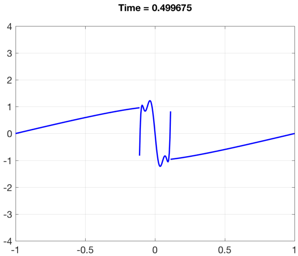

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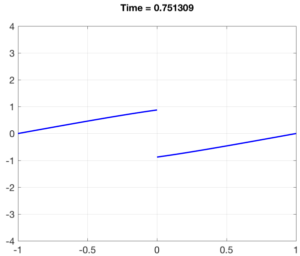

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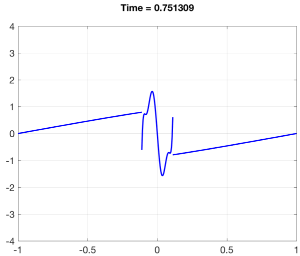

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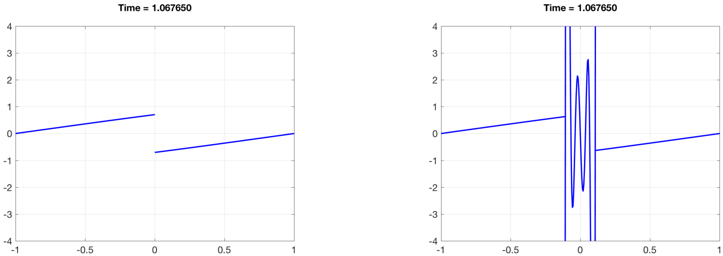

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Entropy stability for nonlinear conservation laws

- 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.

Examples of entropy functions

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

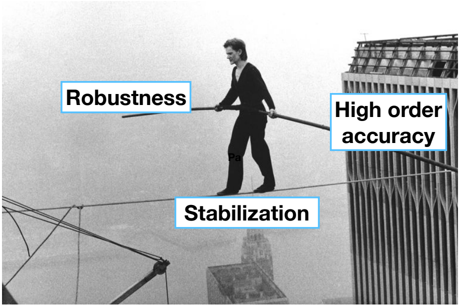
$$S(\boldsymbol{u}) = \frac{1}{2}hu^2 + \frac{1}{2}gh^2 + ghb, \qquad \boldsymbol{v}(\boldsymbol{u}) = \begin{bmatrix} g(h+b) - \frac{u^2}{2} \\ u \end{bmatrix}.$$

- 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.
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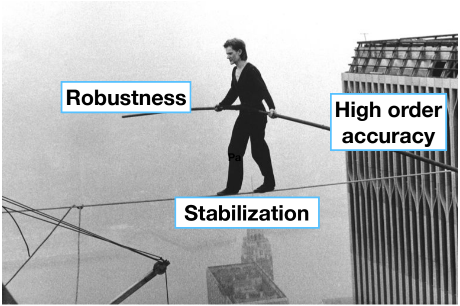

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Talk outline

1 DG as summation by parts finite differences

2 Entropy stable formulations through flux differencing

3 Numerical experiments: triangular and tetrahedral meshes

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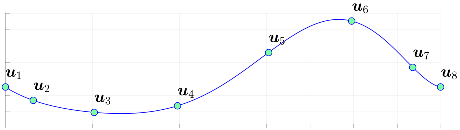
Entropy stable schemes in a nutshell



- Collocate solution at Gauss-Legendre-Lobatto nodes

$$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}+\boldsymbol{D}\boldsymbol{f}(\boldsymbol{u})=0 \quad\Longrightarrow\quad \frac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t}+\sum_j \boldsymbol{D}_{ij}\boldsymbol{f}\left(\boldsymbol{u}_i\right)=0, \qquad \boldsymbol{D}_{ij}=\left.\frac{\partial \ell_j}{\partial x}\right|_{x=x_i}.$$

- Flux differencing: recover above form if $\boldsymbol{f}_S(\boldsymbol{u}_i,\boldsymbol{u}_j)=\frac{1}{2}\left(\boldsymbol{u}_i+\boldsymbol{u}_j\right)$.

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- Semi-discrete entropy equality (add dissipation for inequality)

$$\boldsymbol{M}\frac{\mathrm{d}S(\boldsymbol{u})}{\mathrm{d}t}+\boldsymbol{1}^T\boldsymbol{B}\left(\boldsymbol{v}^T\boldsymbol{f}(\boldsymbol{u})-\psi(\boldsymbol{u})\right)=0.$$

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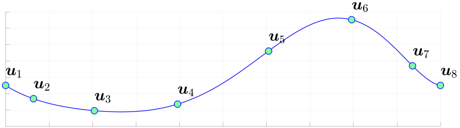

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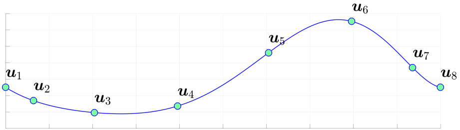

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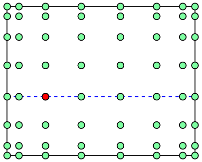

(a) GLL collocation

- SBP finite difference schemes: semi-discrete entropy inequality. Includes DG-SEM (Gauss-Legendre-Lobatto collocation) methods.
- Generalized SBP (e.g. Gauss collocation): higher accuracy, but requires non-compact coupling conditions b/w neighboring elements.
- Tetrahedra, wedges, pyramids: how to address over-integration?

My focus: entropy stability, compact couplings, arbitrary quadratures.

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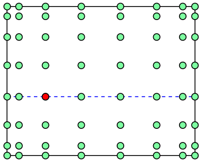

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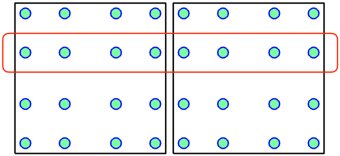

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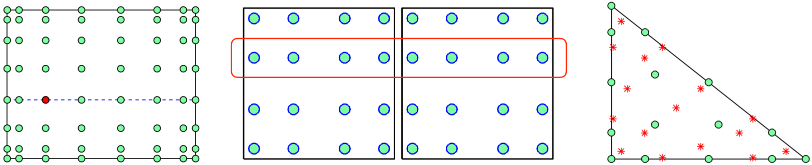

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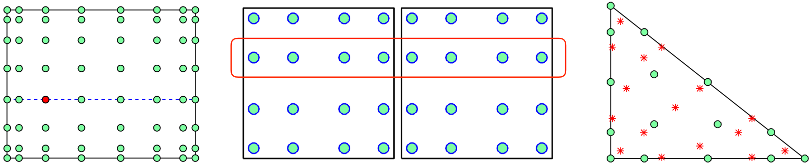

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Making DG look like FD: quadrature-based matrices

- 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

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$$\boldsymbol{W}\boldsymbol{D}_q^i + \left(\boldsymbol{W}\boldsymbol{D}_q^i\right)^T = (\boldsymbol{V}_f \boldsymbol{P}_q)^T \boldsymbol{W}_f \operatorname{diag}(\boldsymbol{n}_i) \boldsymbol{V}_f \boldsymbol{P}_q, \qquad \text{(SBP property)}.$$

A "decoupled" block SBP operator

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

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

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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 $u \approx f\frac{\partial g}{\partial x}$

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

- $\boldsymbol{Q}_N^i = \operatorname{diag}\left(\begin{bmatrix}\boldsymbol{w}^q & \boldsymbol{w}_f\end{bmatrix}\right) \boldsymbol{D}_N^i$ also satisfies an SBP property

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

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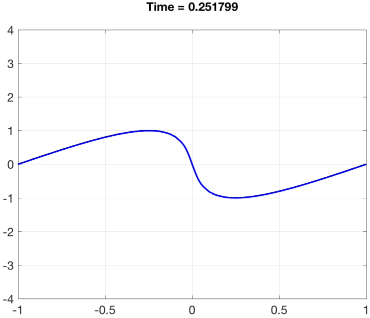
Talk outline

1 DG as summation by parts finite differences

2 Entropy stable formulations through flux differencing

3 Numerical experiments: triangular and tetrahedral meshes

Split form of Burgers': $\frac{\partial u}{\partial t} + \frac{1}{3}\left(\frac{\partial u^2}{\partial x} + u\frac{\partial u}{\partial x}\right) = 0$



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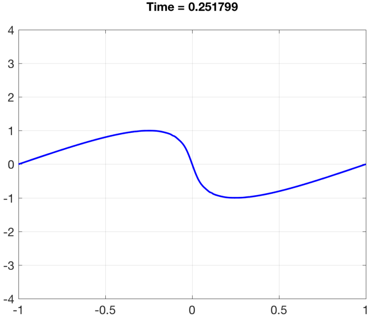

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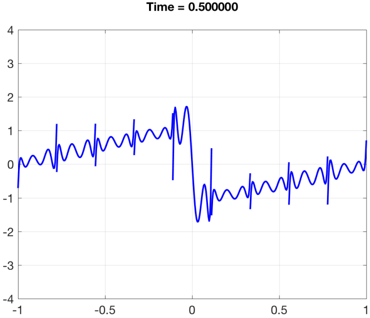

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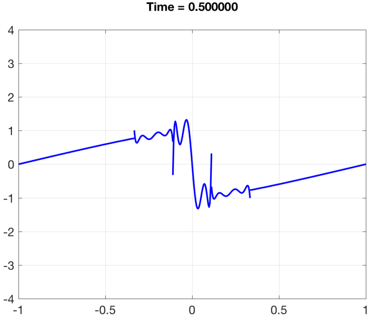

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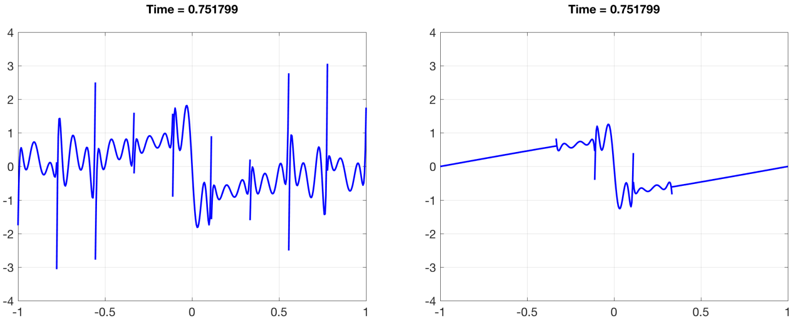

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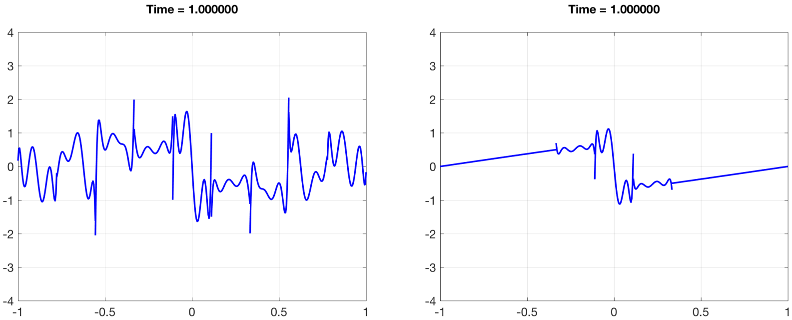

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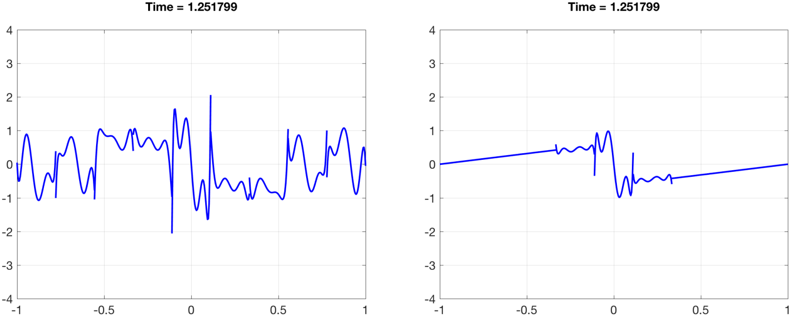

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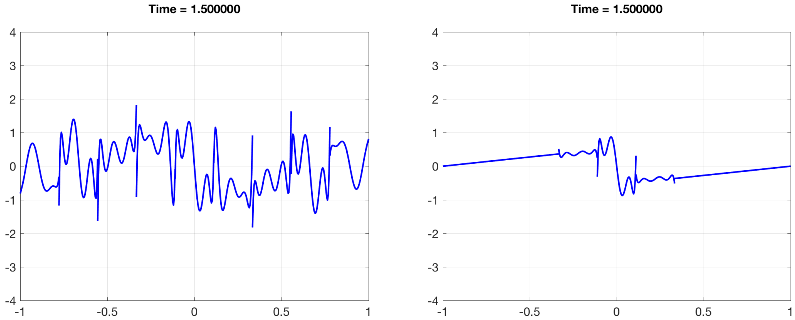

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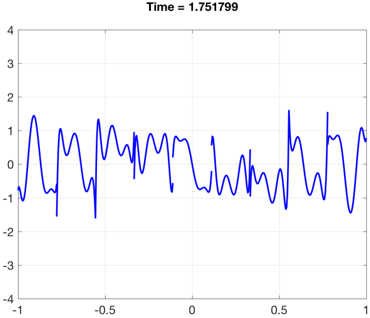

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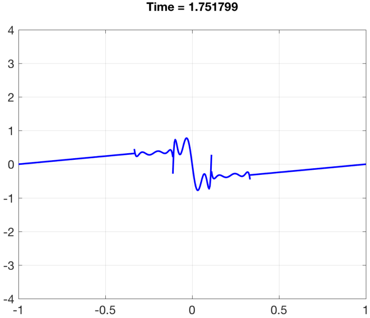

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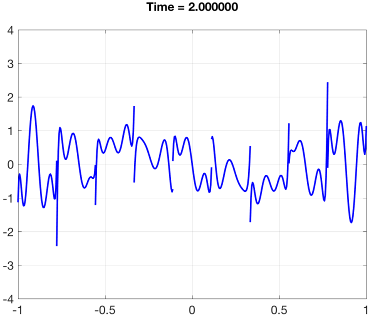

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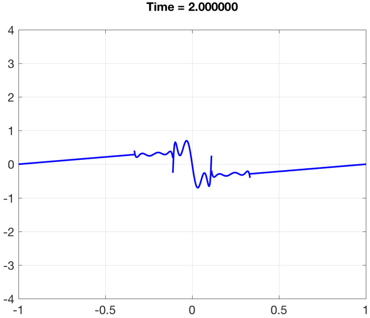

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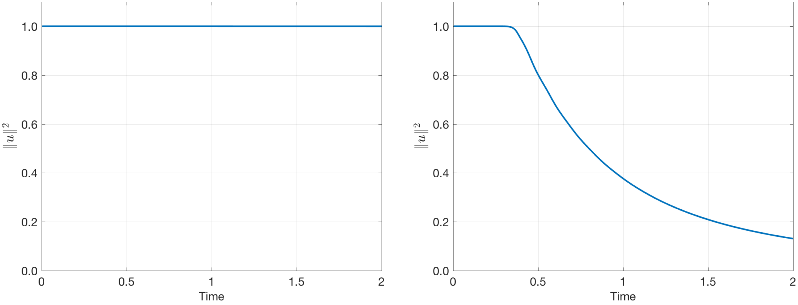

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Flux differencing: entropy conservative finite volume fluxes

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

$$\boldsymbol{f}_S(\boldsymbol{u},\boldsymbol{u}) = \boldsymbol{f}(\boldsymbol{u}), \qquad \boldsymbol{f}_S(\boldsymbol{u},\boldsymbol{v}) = \boldsymbol{f}_S(\boldsymbol{v},\boldsymbol{u}), \qquad \text{(consistency, symmetry)}$$

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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.

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

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

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

A discretely entropy conservative DG method

Theorem (Chan 2018)

Let $\boldsymbol{u}_h(\boldsymbol{x},t) = \sum_j \widehat{\boldsymbol{u}}_j(t)\phi_j(\boldsymbol{x})$ *and* $\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(\begin{bmatrix}\boldsymbol{V}_q\\ \boldsymbol{V}_f\end{bmatrix}\boldsymbol{P}_q\boldsymbol{v}\right)$. *Let* $\widehat{\boldsymbol{u}}$ *locally solve*

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

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

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

- Uses $\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(P_N\boldsymbol{v}\right)$ in terms of L^2 projected entropy variables $P_N\boldsymbol{v}$!
- Add interface dissipation (e.g. Lax-Friedrichs) for entropy inequality.

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

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Talk outline

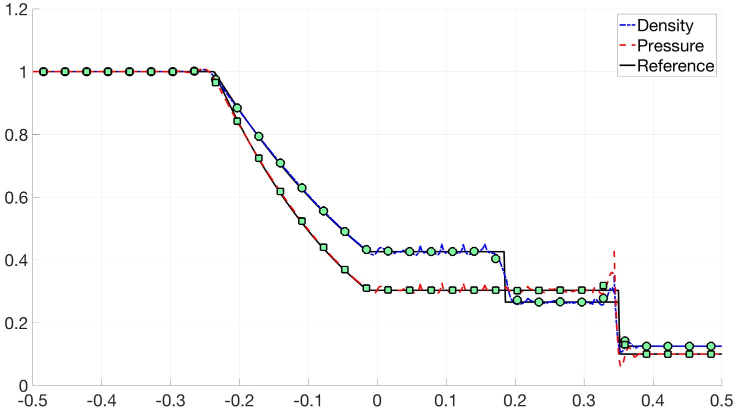
1 DG as summation by parts finite differences

2 Entropy stable formulations through flux differencing

3 Numerical experiments: triangular and tetrahedral meshes

1D Sod shock tube

- Circles are cell averages. No limiting or artificial viscosity applied.
- CFL of .125 used for both GLL-$(N+1)$and GQ-$(N+2)$.



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

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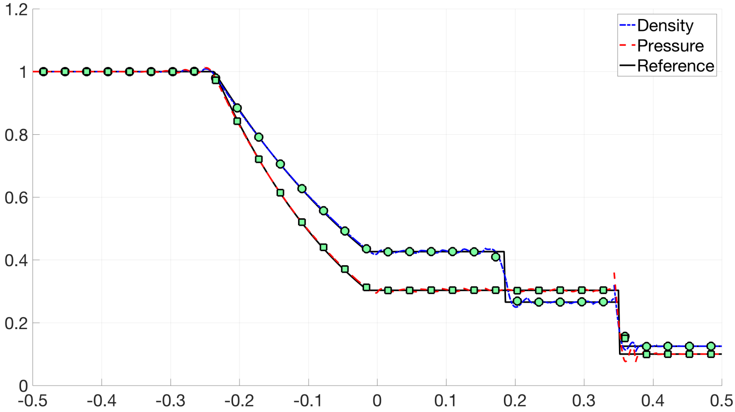
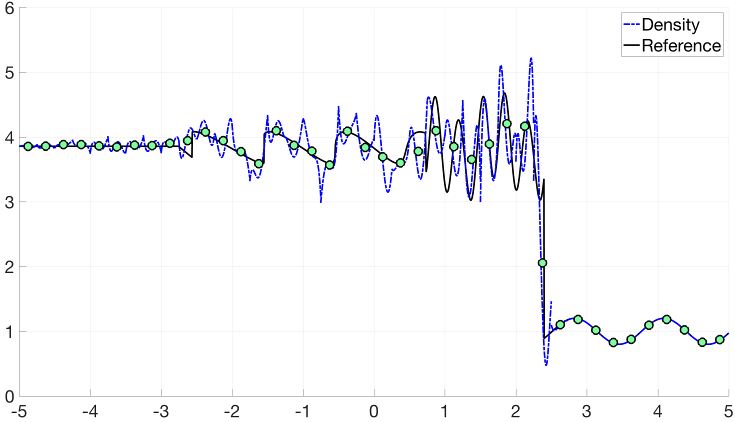


$N = 4, K = 32$, $(N+2)$ point Gauss quadrature.

1D sine-shock interaction

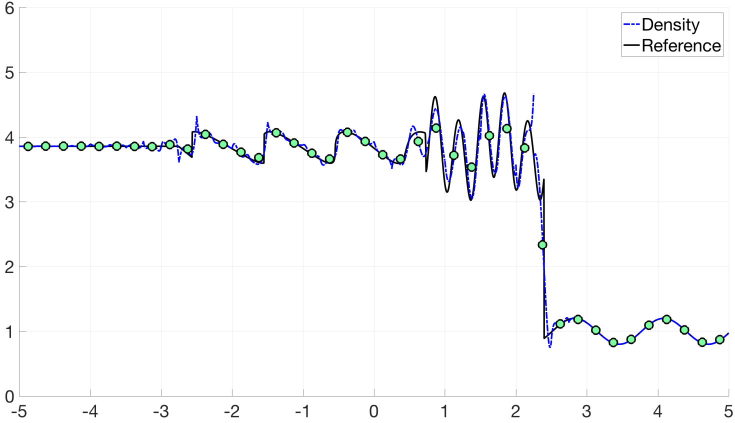
- GQ-($N+2$) needs smaller CFL (.05 vs .125) for stability.



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

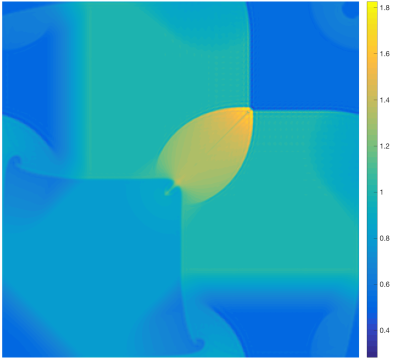
1D sine-shock interaction

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



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

2D Riemann problem

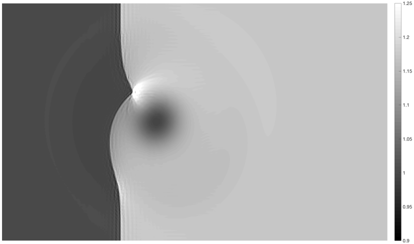


(a) $\Omega = [-1, 1]^2$

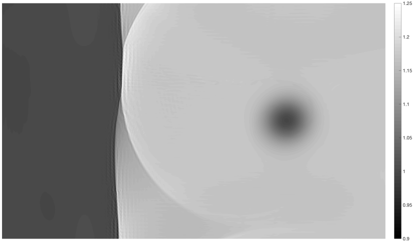
(b) $\Omega = [-.5, .5]^2$, 32×32 elements

- 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).

2D shock-vortex interaction



(a) $t = .3$

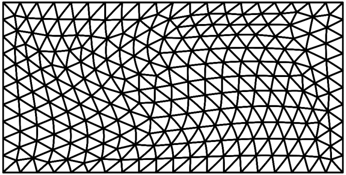


(b) $t = .7$

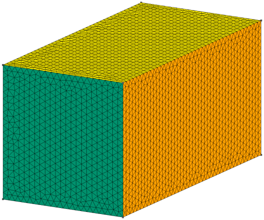
- Vortex passing through a shock on a periodic domain (matrix dissipation, degree $N = 3$ approximation, mesh size $h = 1/128$).
- Entropy stable wall boundary conditions for GSBP still needed.

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

2D and 3D isentropic vortex: affine and curved meshes



(a) 2D triangular mesh



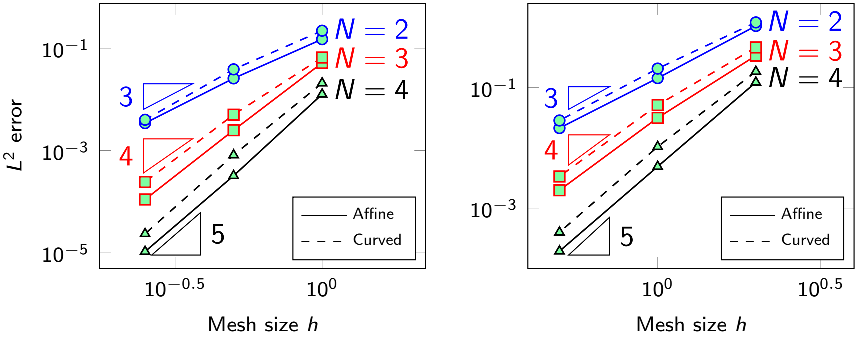
(b) 3D tetrahedral mesh

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

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

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.*

2D and 3D isentropic vortex: affine and curved meshes



(a) 2D results (b) 3D results

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

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

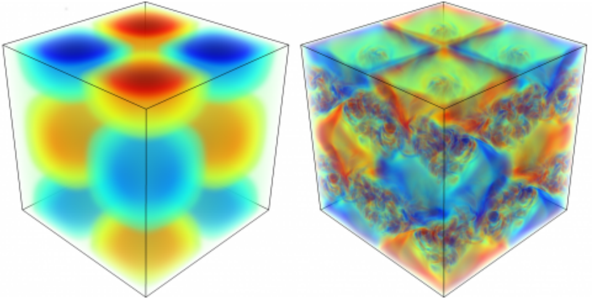
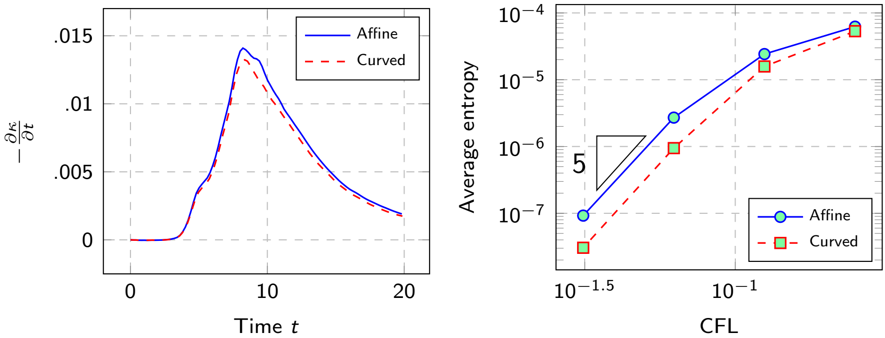


Figure: Isocontours of z-vorticity for Taylor-Green at $t = 0, 10$ seconds.

- 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.

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

- More general class of high order DG methods which satisfy a semi-discrete entropy inequality.
- Challenges: BCs, positivity, strong shocks, 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.

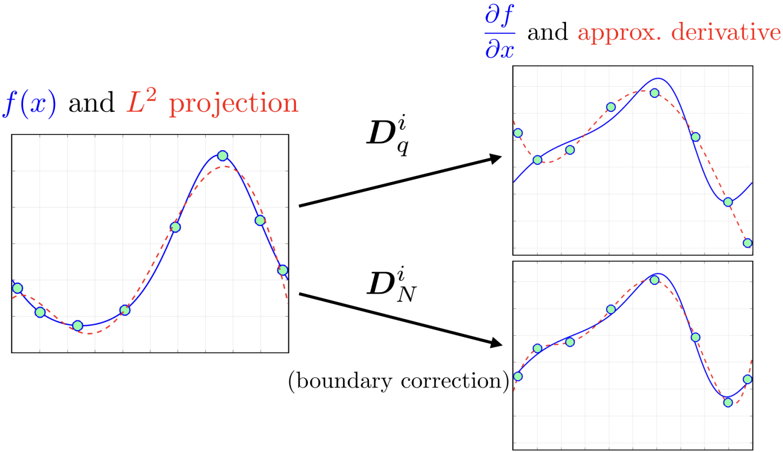
Thank you! Questions?

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

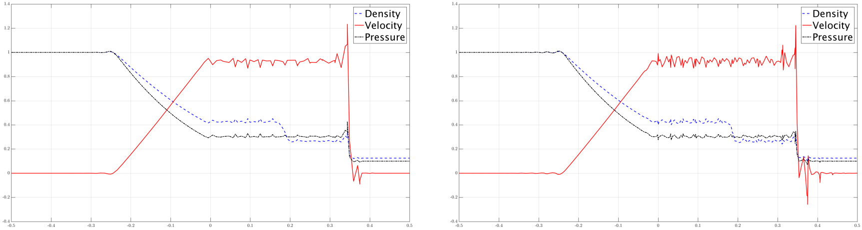
Chan (2017). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods.*

Additional slides

Accuracy of D_N^i



Over-integration is ineffective without L^2 projection

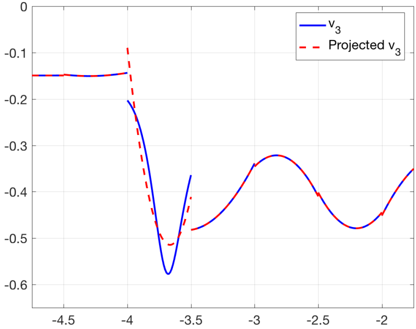


(a) Degree N GLL, $(N+1)$ points (b) Degree N GLL, $(N+4)$ points

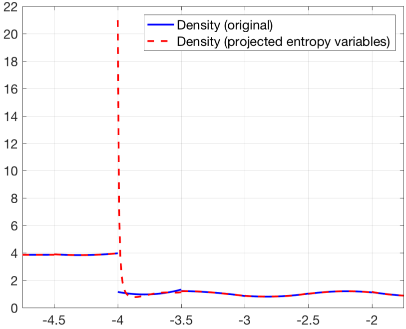
Figure: Sod shock tube for $N = 4$ and $K = 32$ elements. Over-integrating by increasing the number of quadrature points does not improve solution quality.

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!

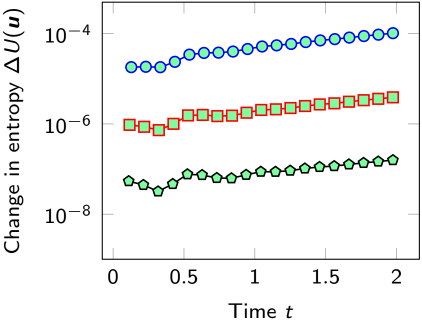


(a) $v_3(x), \left(P_N v_3\right)(x)$

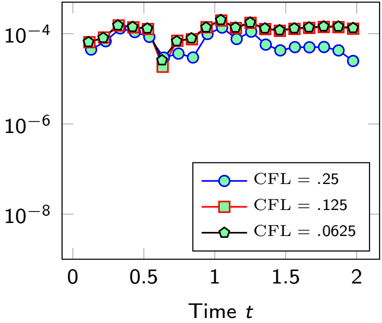


(b) $\rho(x), \rho\left(\left(P_N \boldsymbol{v}\right)(x)\right)$

2D curved meshes: conservation of entropy



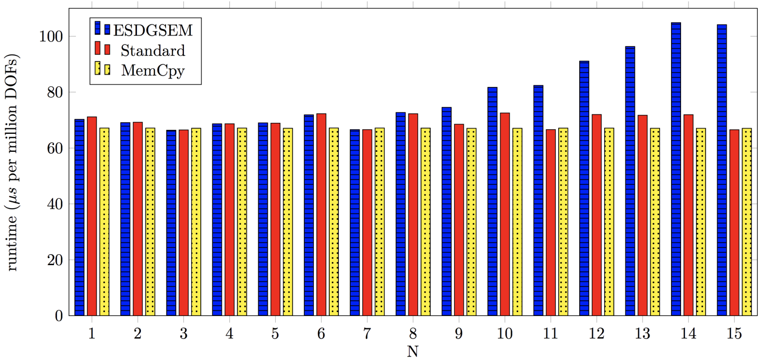
(c) With weight-adjusted projection



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

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.*