Entropy stable discontinuous Galerkin methods using arbitrary bases and quadratures

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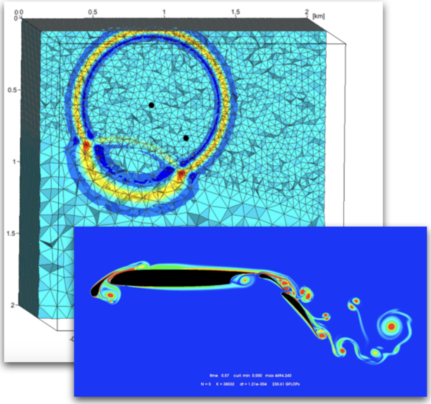
High order methods for time-dependent hyperbolic PDEs

- 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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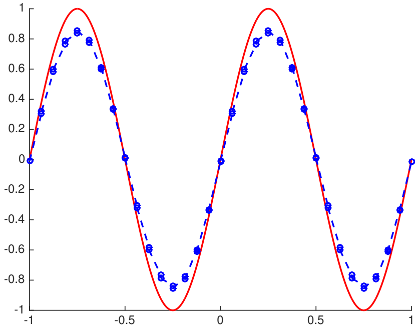

Fine linear approximation.

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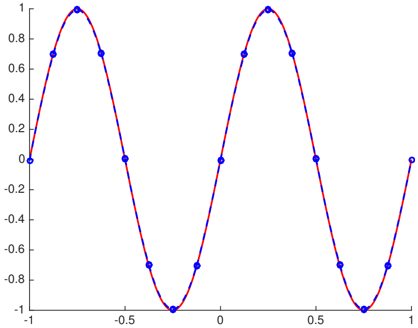

Coarse quadratic approximation.

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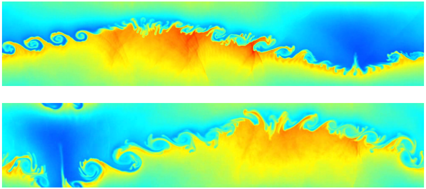

Figure from Per-Olof Persson.

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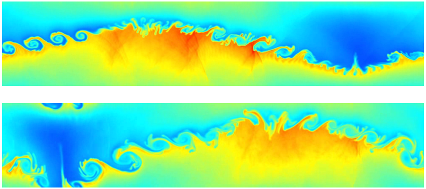

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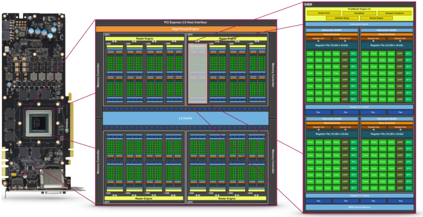

A graphics processing unit (GPU).

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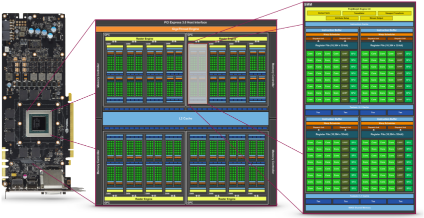

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Entropy stability for nonlinear conservation laws

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

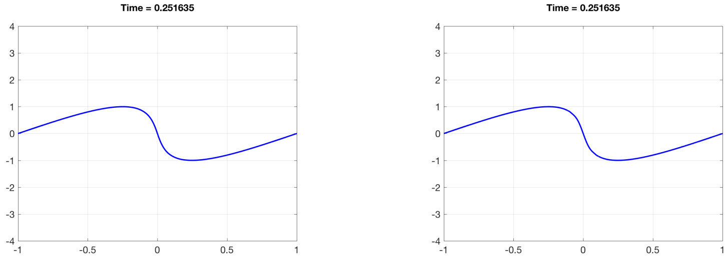
$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = 0.$$

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

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

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

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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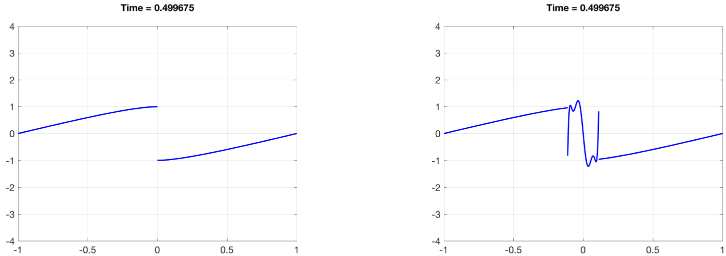

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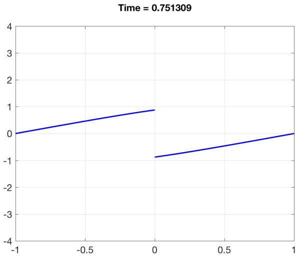

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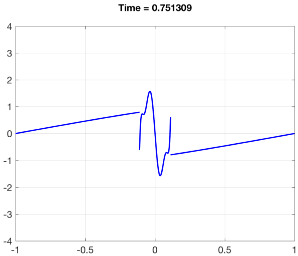

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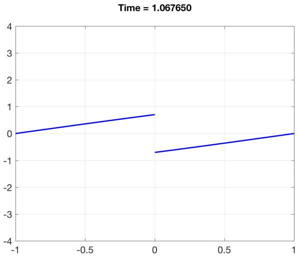

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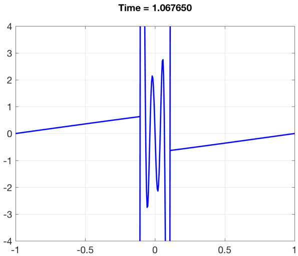

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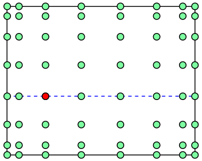
Talk outline

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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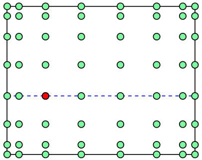

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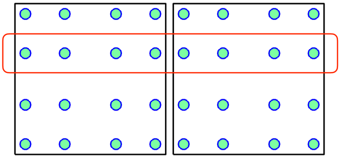

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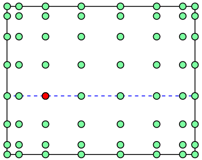

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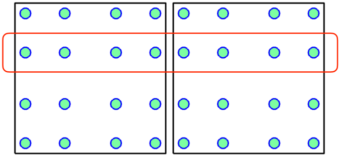

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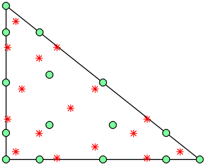

(c) Nodes vs cubature

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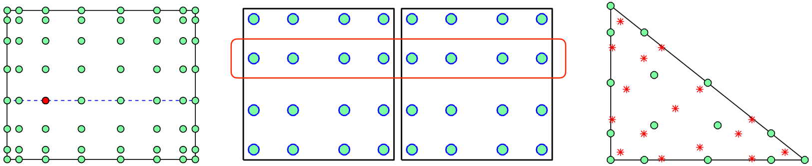

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Quadrature-based matrices for polynomial bases

- 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

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

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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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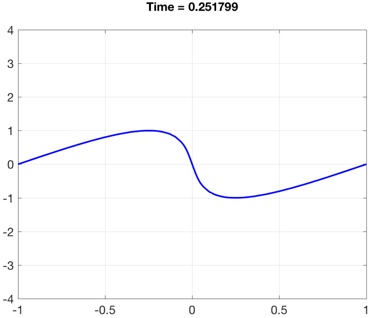
Talk outline

1 Summation by parts methods

2 Entropy stable formulations and flux differencing

3 Numerical experiments

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

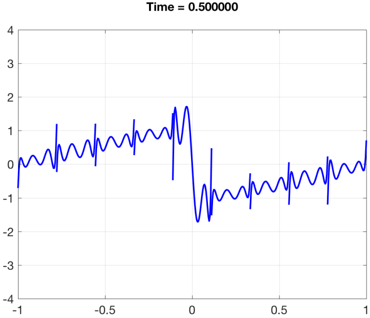


(a) Energy conservative (b) Energy stable

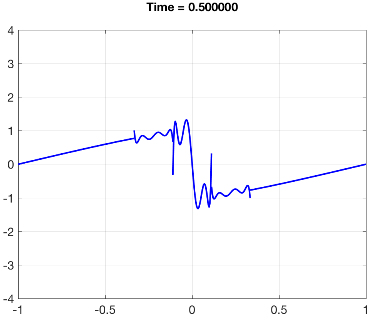
$$\boldsymbol{u} = \begin{bmatrix} \boldsymbol{V}_q \\ \boldsymbol{V}_f \end{bmatrix} \widehat{\boldsymbol{u}}, \qquad \boldsymbol{f}^* = \boldsymbol{f}^*(u^+, u) = \text{numerical flux}$$

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

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



(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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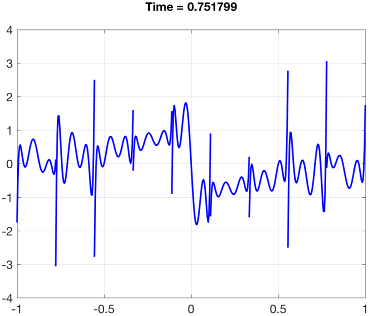

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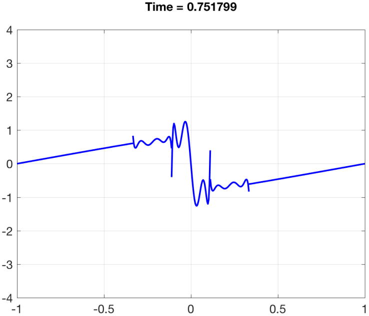

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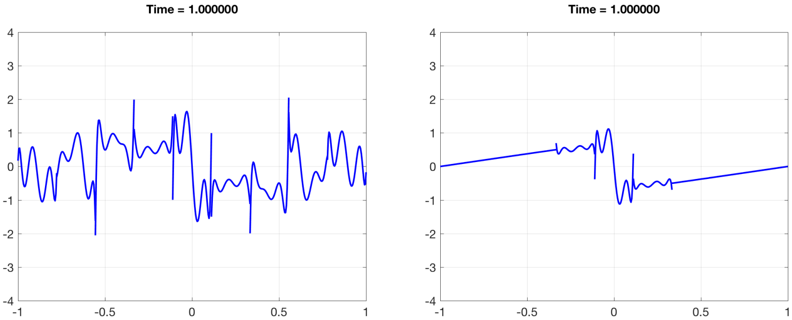

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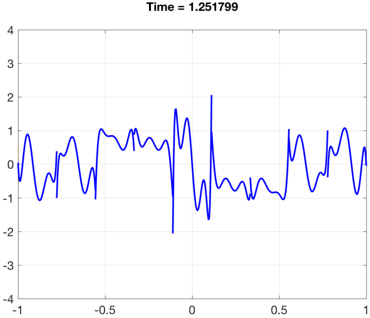

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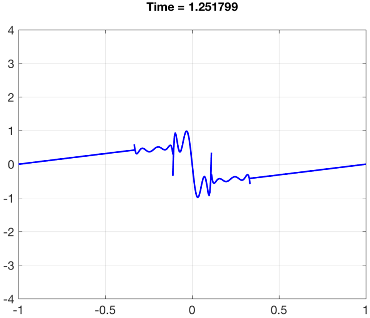

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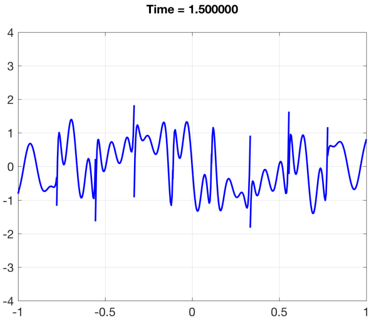

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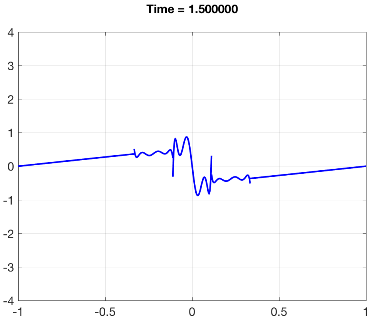

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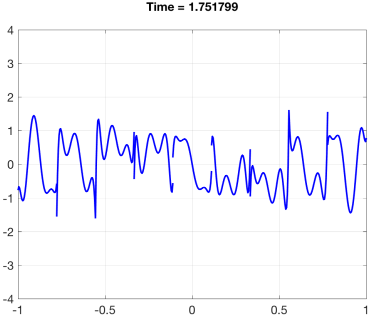

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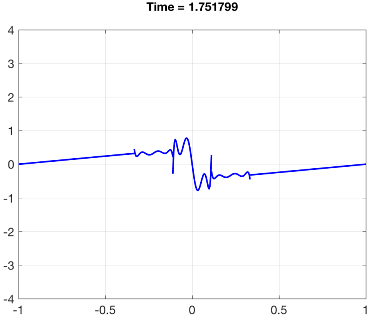

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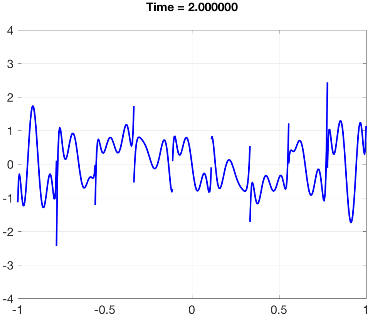

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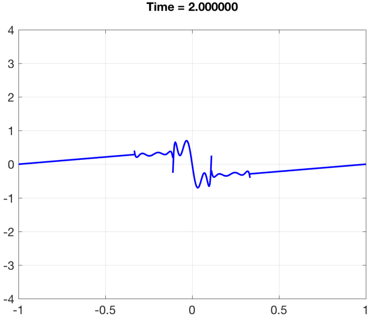

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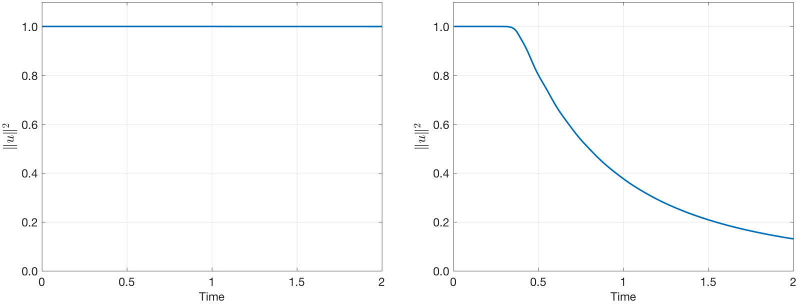

(a) Energy conservative   (b) Energy stable

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

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

- 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

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

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

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

- 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*

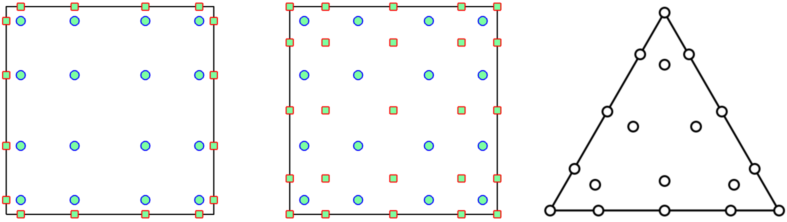
$$\int_\Omega \frac{\partial S(\boldsymbol{u}_h)}{\partial t} + \sum_{i=1}^{d} \int_{\partial\Omega} \left(\left(P_N \boldsymbol{v}\right)^T \boldsymbol{f}^i(\widetilde{\boldsymbol{u}}) - \psi_i(\widetilde{\boldsymbol{u}})\right)\boldsymbol{n}_i = 0.$$

- 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.*

Unifying (some) finite difference SBP formulations



(a) Generalized SBP (b) Staggered-grid (c) Triangular SBP

- Specific basis and quadrature: recovers several existing entropy stable schemes (DG-SEM, Gauss collocation, staggered grid, etc).
- Setting $\boldsymbol{P}_q = \boldsymbol{I}$ recovers non-basis SBP finite differences on simplices.
- Generates new inter-element coupling terms (SBP-SATs).

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.*

Talk outline

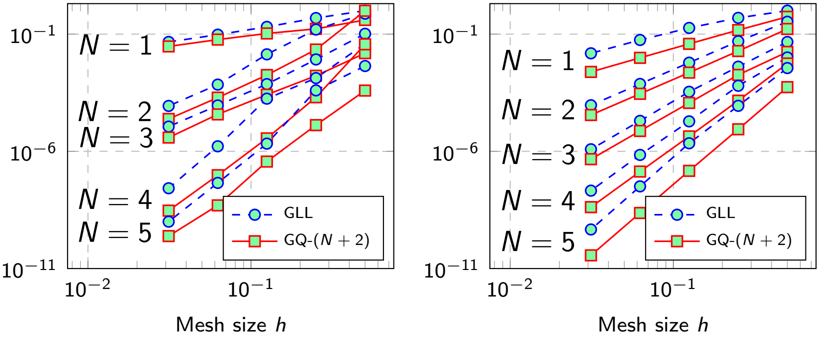
1 Summation by parts methods

2 Entropy stable formulations and flux differencing

3 Numerical experiments

1D compressible Euler equations

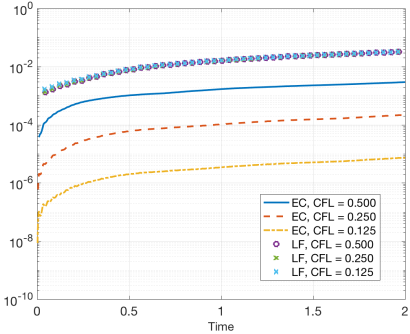
- Inexact Gauss-Legendre-Lobatto (GLL) vs Gauss (GQ) quadratures.
- Entropy conservative (EC) and Lax-Friedrichs (LF) fluxes.
- No additional stabilization, filtering, or limiting.



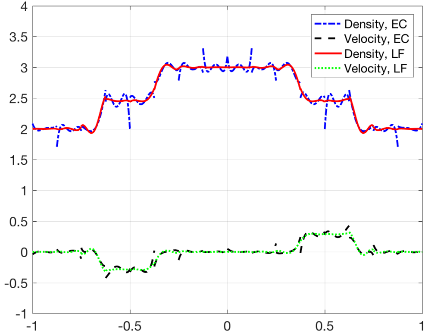
(a) Entropy conservative flux (b) With Lax-Friedrichs penalization

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

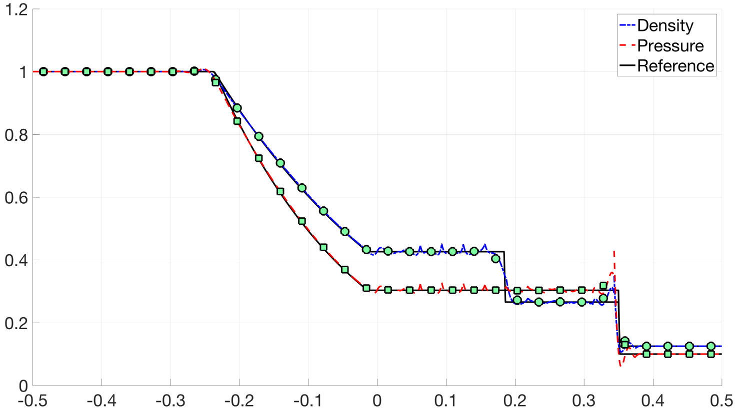


(b) $\rho(x), u(x)$ $(N = 4, K = 16)$

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.

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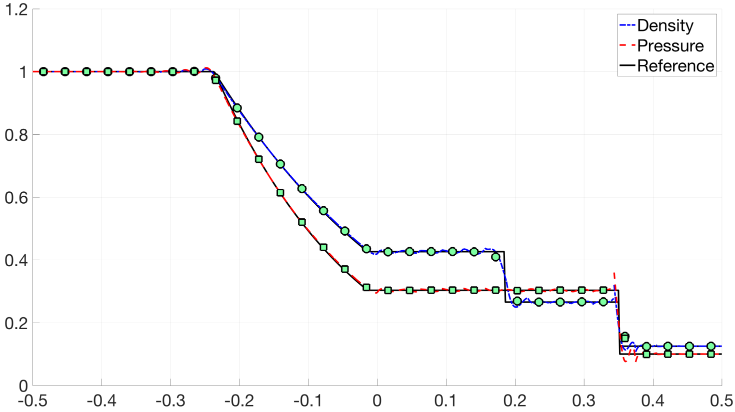
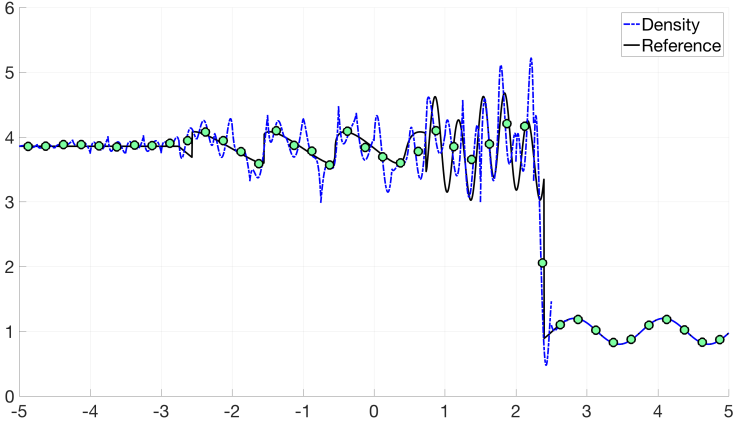


$N = 4$, $K = 32$, $(N+2)$ point Gauss quadrature.

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.

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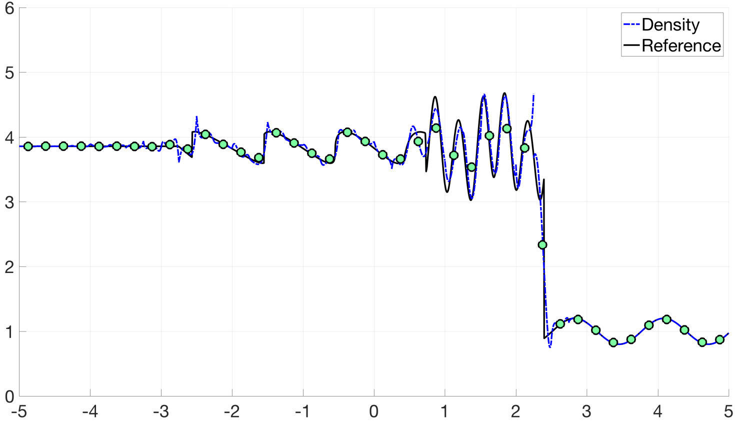
- GQ-$(N+2)$ needs smaller CFL (.05 vs .125) for stability.



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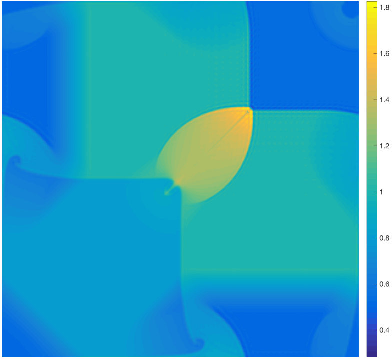
2D Riemann problem

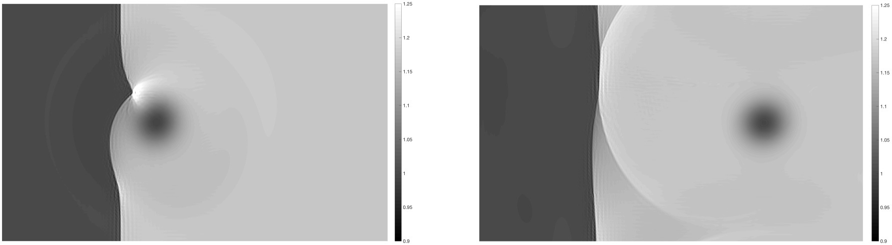


(a) $\Omega = [-1, 1]^2$

(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

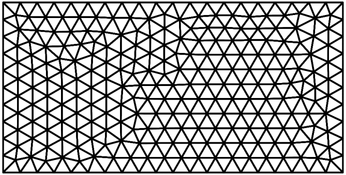


(a) $t = .3$

(b) $t = .7$

- Vortex passing through a shock on a periodic domain.
- Entropy stable wall boundary conditions for GSBP still needed.

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


(a) Affine mesh

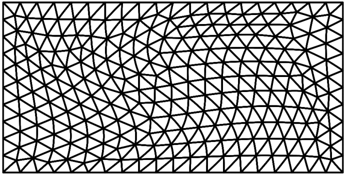
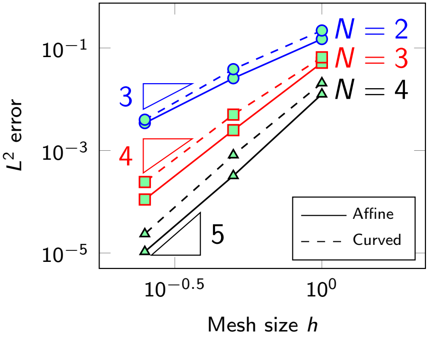

(b) Curved mesh

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

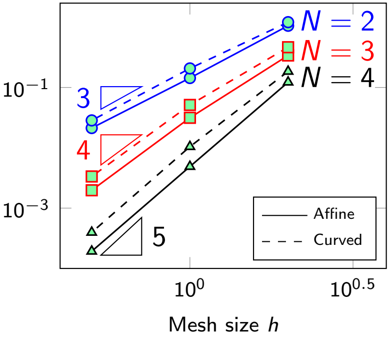
- Entropy stability: needs discrete geometric conservation law (GCL).
- Generalized mass lumping: weight-adjusted mass matrices.
- Modify $\widetilde{\boldsymbol{u}} = \boldsymbol{u}(\widetilde{\boldsymbol{v}})$, $\widetilde{\boldsymbol{v}} = \widetilde{P}_N^k \boldsymbol{v}(\boldsymbol{u}_h)$ using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

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

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



(a) 2D results

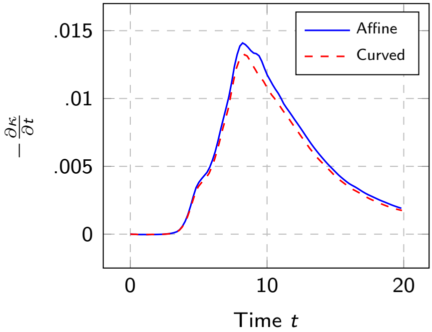


(b) 3D results

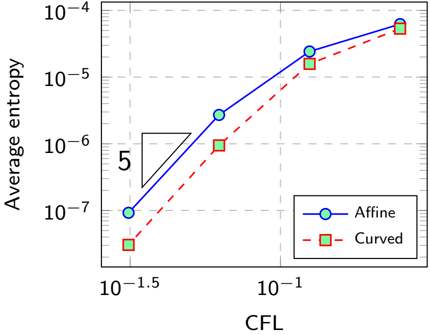
L^2 errors for 2D/3D isentropic vortex at $T = 5$ on affine, curved meshes.

Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.
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 ($N = 3$, $h = \frac{\pi}{8}$)



(b) $\int_\Omega U(\boldsymbol{u})$ for entropy cons. scheme

- 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
- Additional work required for strong shocks, positivity preservation.
- 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.

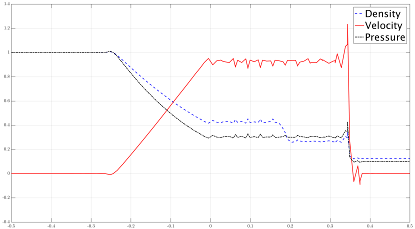
Thank you! Questions?

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

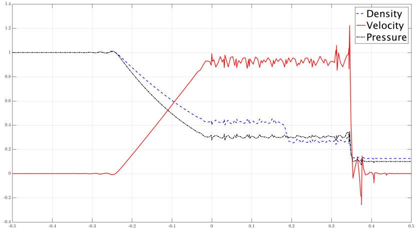
Chan (2017). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods.*

Additional slides

Over-integration is ineffective without L^2 projection



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

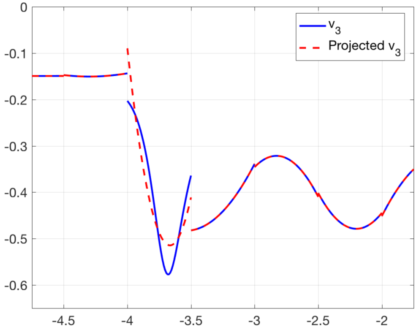


(b) Degree N GLL, $(N+4)$ points

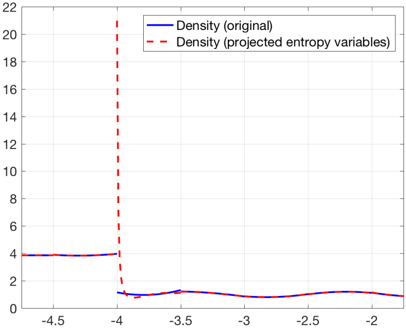
Figure: Sod shock tube for $N = 4$ and $K = 32$ elements. Over-integrating by increasing the number of quadrature points does not improve solution quality.

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!

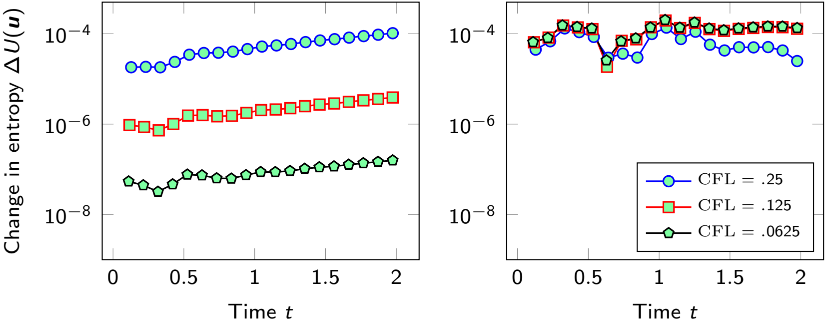


(a) $v_3(x), \left(P_N v_3\right)(x)$



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