Entropy stable discontinuous Galerkin methods with arbitrary bases and quadratures

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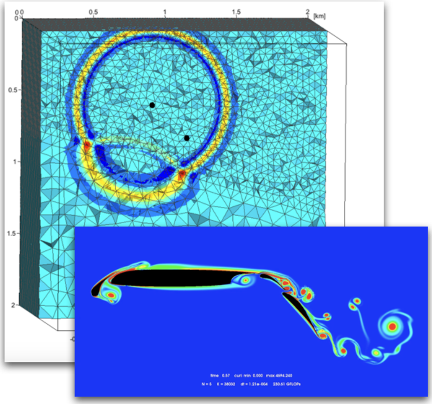
High order methods for time-dependent hyperbolic PDEs

- 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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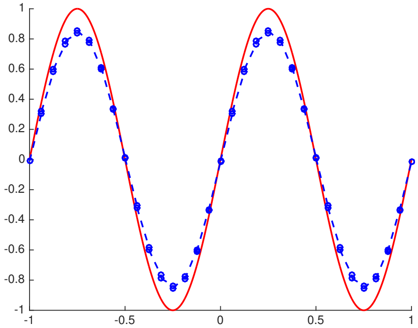

Fine linear approximation.

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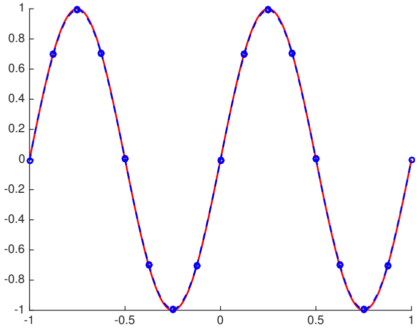

Coarse quadratic approximation.

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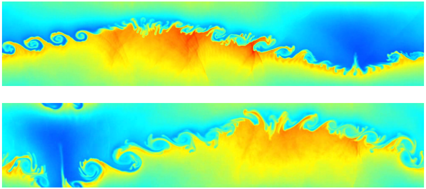

Figure from Per-Olof Persson.

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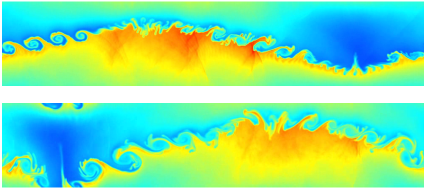

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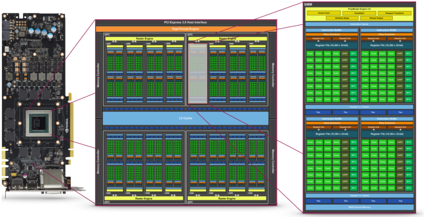

A graphics processing unit (GPU).

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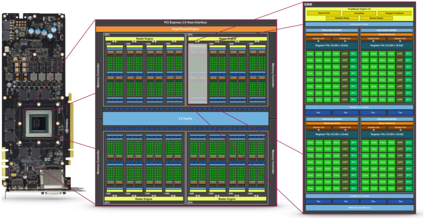

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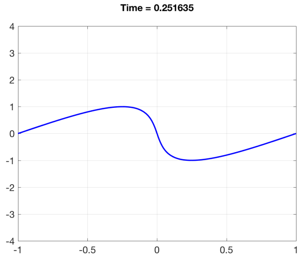
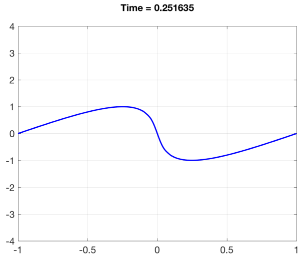
Why are high order methods for nonlinear PDEs unstable?



(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.

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

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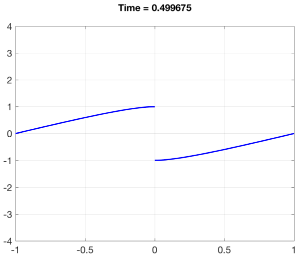

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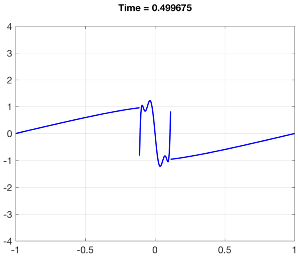

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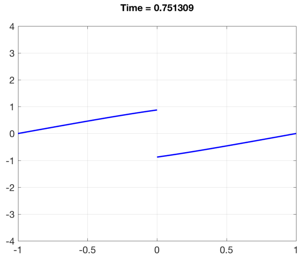

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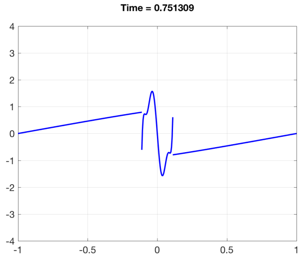

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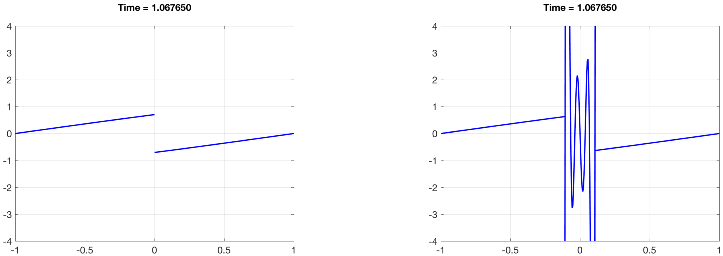

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Entropy stability for nonlinear conservation laws

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

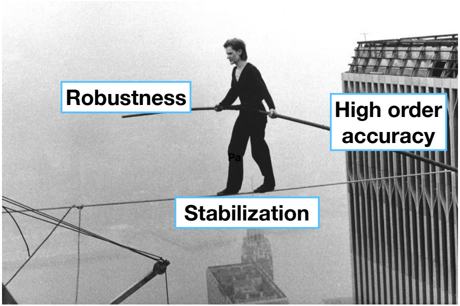
$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = 0.$$

- 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 integration by parts, chain rule.

Why discretely entropy stable (ES) schemes?



- Existing discrete stability theory: regularization, viscosity, TVD, etc.
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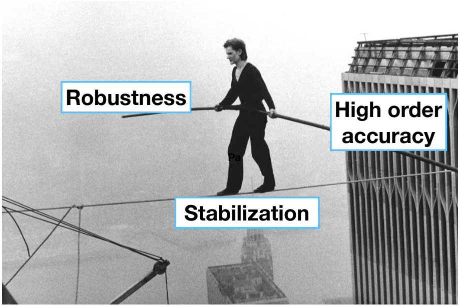

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Talk outline

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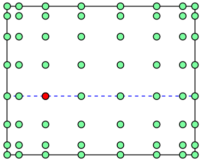
Overview of entropy stable high order SBP schemes



(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, prisms, pyramids, etc (over-integration, dense norms)?

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

Fisher, Carpenter, Nordström, Yamaleev, Swanson (2013), Fisher, Carpenter (2013), Gassner, Winters, and Kopriva (2016), Wintermeyer et al. (2017), Chen and Shu (2017), Crean, Hicken, DCDR Fernandez, et al. (2018), and more ...

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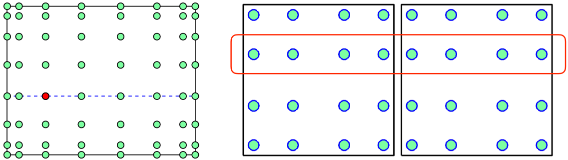

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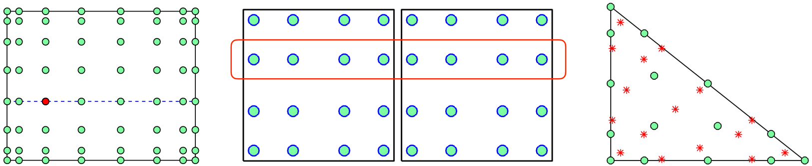

(a) GLL collocation (b) Gauss nodes coupling (c) Nodes vs cubature

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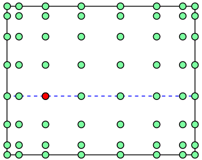

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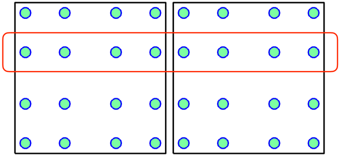

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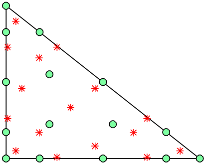

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Quadrature-based matrices for polynomial bases

- Volume and surface quadratures $(\boldsymbol{x}_i^q, \boldsymbol{w}_i^q)$, $(\boldsymbol{x}_i^f, \boldsymbol{w}_i^f)$, exact for degree $2N$ 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 the interpolation matrices $\boldsymbol{V}_q, \boldsymbol{V}_f$

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

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

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

- These matrices map to and from modal and quadrature spaces.

Quadrature-based differentiation matrices

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

$$\boldsymbol{D}_q^i = \boldsymbol{V}_q \boldsymbol{D}^i \boldsymbol{P}_q, \qquad \boldsymbol{D}^i = \text{ modal differentiation matrix.}$$

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

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

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

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

- Recovers GSBP, but entropy stable interface terms are expensive.

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 ith derivative (block matrix operating on volume + surface values).

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

- $\boldsymbol{D}_N^i$ satisfies a summation-by-parts (SBP) property + $\boldsymbol{D}_N^i\boldsymbol{1} = 0$

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

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

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

Differentiation using decoupled SBP operators

- Note: $\boldsymbol{D}_N^i$ is not a differentiation matrix on its own.
- $\boldsymbol{P}_q, \boldsymbol{L}_f$, and $\boldsymbol{D}_N^i$ produce a high order polynomial approximation of $f\frac{\partial g}{\partial x}$ given data at quadrature points $\boldsymbol{x} = [\boldsymbol{x}^q, \boldsymbol{x}^f]$.

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

- 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).

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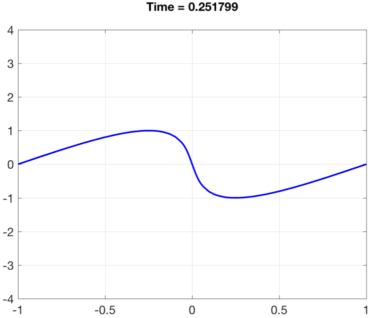
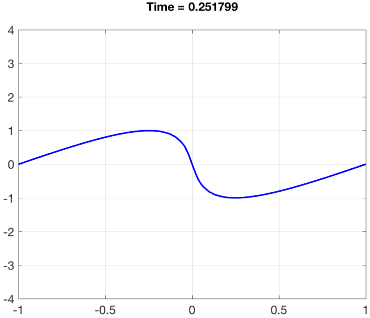
Split form of Burgers': $\frac{\partial u}{\partial t} + \frac{1}{3}\left(\frac{\partial u^2}{\partial x} + u\frac{\partial u}{\partial x}\right) = 0$



(a) Energy conservative



(b) Energy stable

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

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

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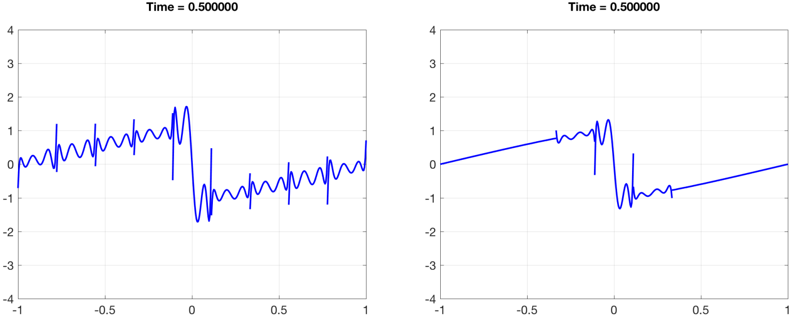

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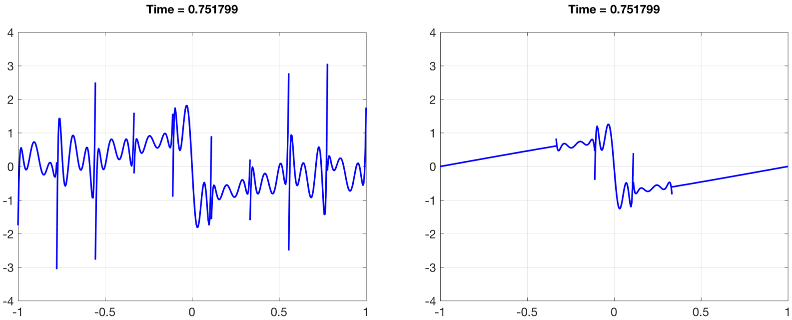

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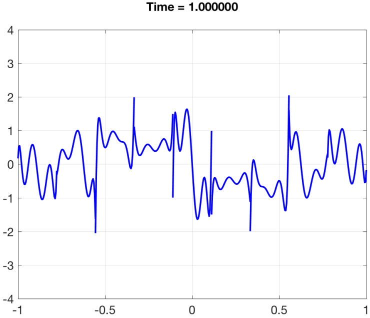

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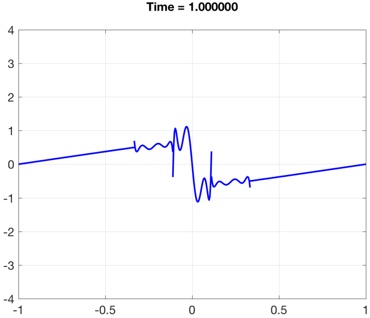

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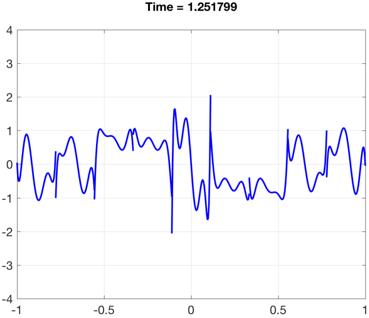
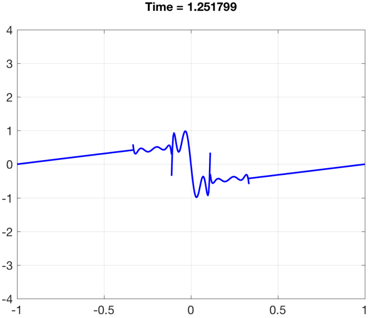
$$\frac{\mathrm{d}\widehat{\boldsymbol{u}}}{\mathrm{d}t} + \frac{1}{3}\begin{bmatrix} \boldsymbol{P}_q & \boldsymbol{L}_f \end{bmatrix}\left(\boldsymbol{D}_N\left(\boldsymbol{u}^2\right) + \operatorname{diag}\left(\boldsymbol{u}\right)\boldsymbol{D}_N\boldsymbol{u}\right) + \boldsymbol{L}_f\left(\boldsymbol{f}^*(u^+,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

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



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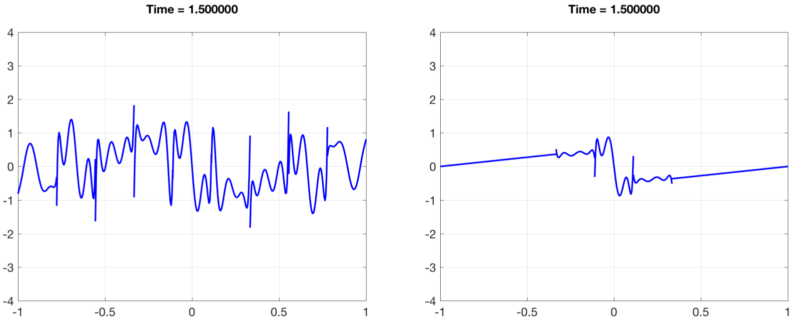

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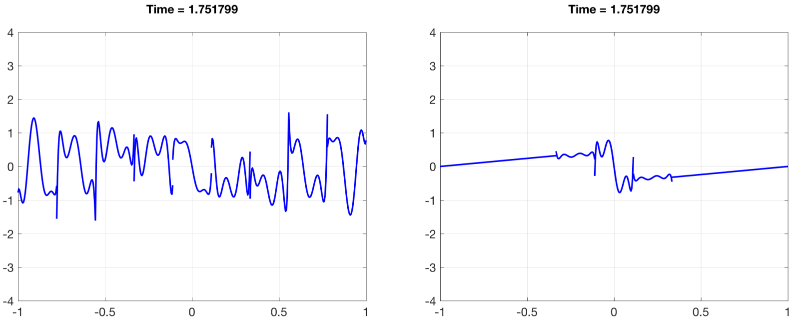

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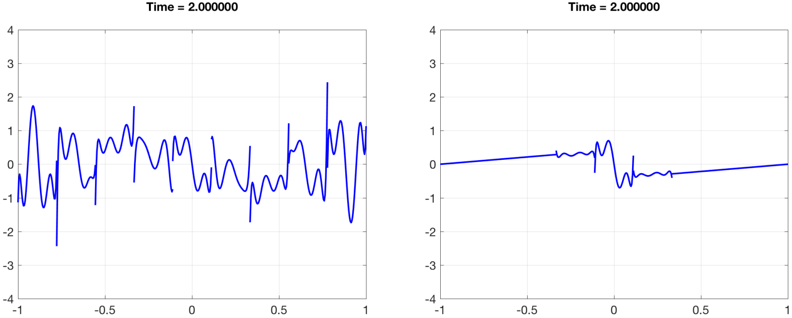

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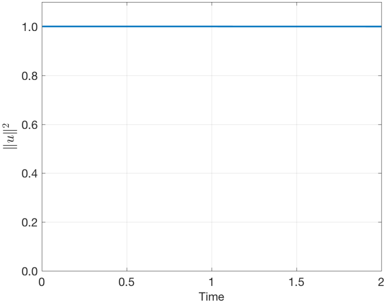

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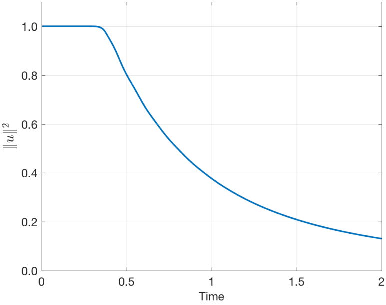

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Flux differencing: entropy conservative finite volume fluxes

- 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

$$f_S^{\rho}(\boldsymbol{u}_L,\boldsymbol{u}_R) = \{\{\rho\}\}^{\log}\{\{u\}\}, \qquad \{\{\rho\}\}^{\log} = \frac{\rho_L - \rho_R}{\log\rho_L - \log\rho_R}.$$

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Flux differencing: implementational details

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

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

- 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 $\boldsymbol{F}_S$)

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

Flux differencing: avoiding the chain rule

- Test $(2\boldsymbol{Q}_N \circ \boldsymbol{F}_S)\,\mathbf{1}$ with entropy variables $\widetilde{\boldsymbol{v}}$, integrate, use SBP:

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

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

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

- Applying Tadmor shuffle condition 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.

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

Hughes, Franca, and Mallet (1986). *A new finite element formulation for computational fluid dynamics: I. Symmetric forms of the compressible Euler and Navier-Stokes equations and the second law of thermodynamics.*

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

A discretely entropy conservative DG method

Theorem (Chan 2018)

Let $\boldsymbol{u}_h(\boldsymbol{x},t) = \sum_j \widehat{\boldsymbol{u}}_j(t)\phi_j(\boldsymbol{x})$ *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*

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

- Add interface dissipation (e.g. Lax-Friedrichs) for entropy inequality.

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

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

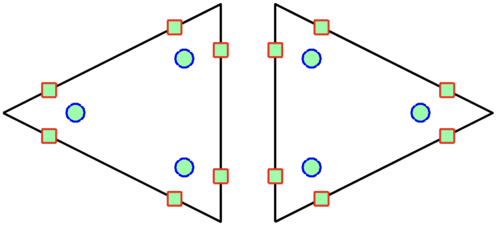
$$\int_\Omega \frac{\partial S(\boldsymbol{u}_h)}{\partial t} + \sum_{i=1}^{d}\int_{\partial\Omega}\left((P_N\boldsymbol{v})^T\boldsymbol{f}^i(\widetilde{\boldsymbol{u}}) - \psi_i(\widetilde{\boldsymbol{u}})\right)\boldsymbol{n}_i = 0.$$

- 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.*

Illustration of main steps of ESDG



$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^T & \boldsymbol{C} \end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf} \\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff} \end{bmatrix}\right)\mathbf{1}$$

- Interpolate projected entropy variables $P_N \boldsymbol{v}(\boldsymbol{u})$ to all nodes.
- Perform flux differencing at volume quadrature nodes.
- Compute $\boldsymbol{f}_S(\boldsymbol{u}_L, \boldsymbol{u}_R)$ for surface nodes of neighboring elements.
- Compute $\boldsymbol{f}_S(\boldsymbol{u}_L, \boldsymbol{u}_R)$ between volume/surface nodes, apply flux differencing with interp. matrix + transpose for volume/surface nodes.

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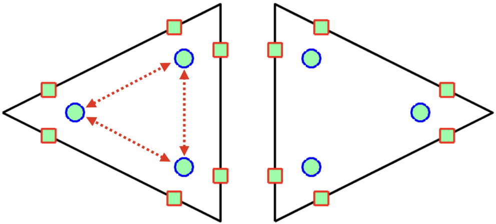

$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^T & \boldsymbol{C} \end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf} \\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff} \end{bmatrix}\right) \mathbf{1}$$

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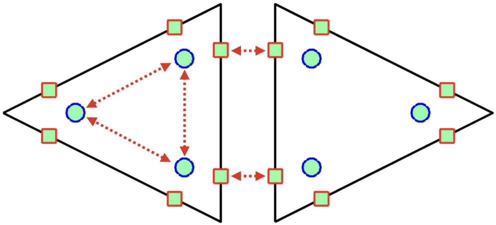

$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^T & \boldsymbol{C} \end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf} \\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff} \end{bmatrix}\right)\mathbf{1}$$

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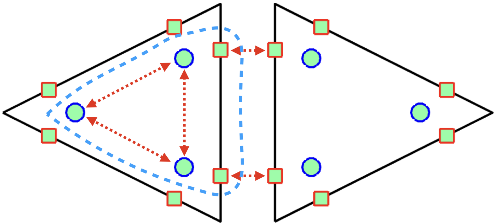
Illustration of main steps of ESDG



$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^T & \boldsymbol{C} \end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf} \\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff} \end{bmatrix} \right) \mathbf{1}$$

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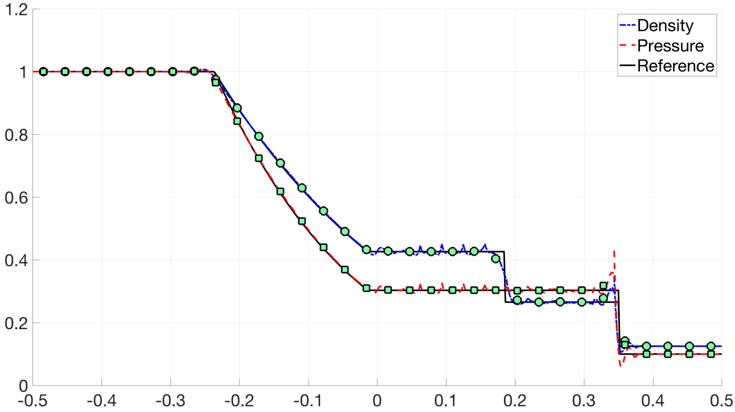
1D Sod shock tube

- 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

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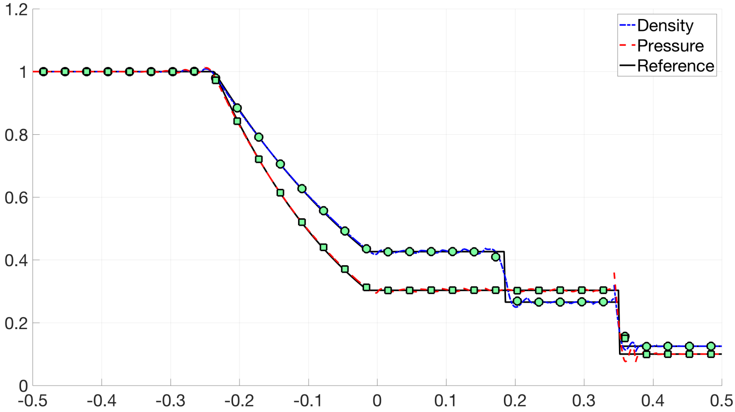
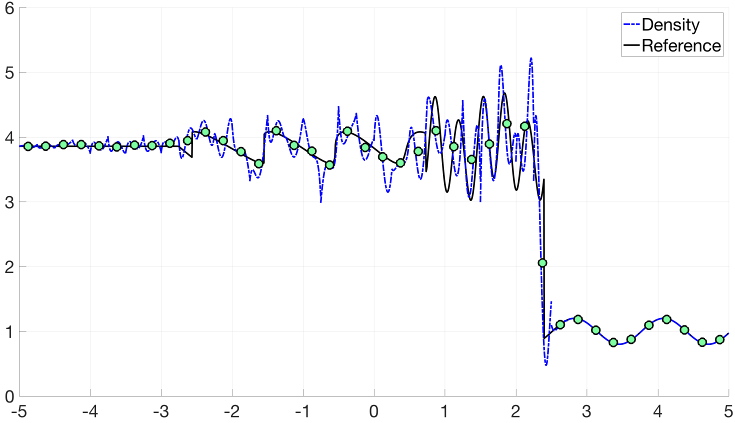
- CFL of .125 used for both GLL-$(N+1)$and GQ-$(N+2)$.



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

1D sine-shock interaction

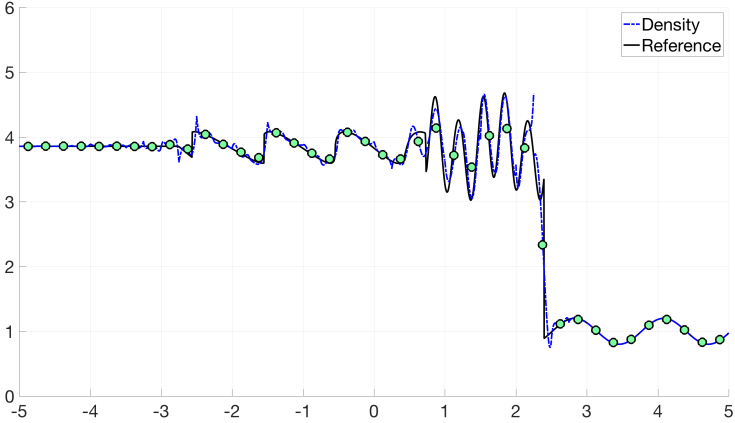
- GQ-$(N+2)$ needs smaller CFL (.05 vs .125) for stability.



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

1D sine-shock interaction

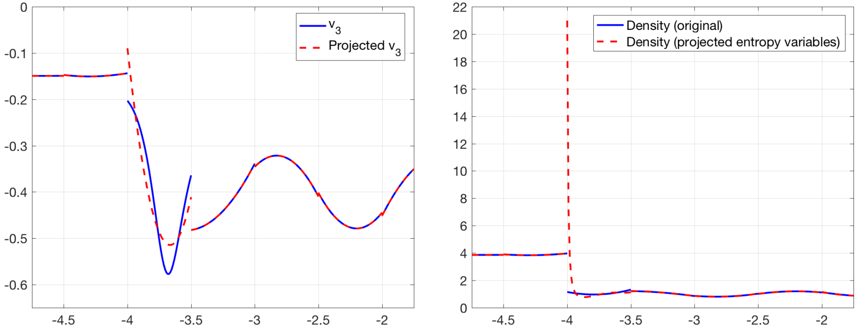
- GQ-$(N+2)$ needs smaller CFL (.05 vs .125) for stability.



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

On CFL restrictions

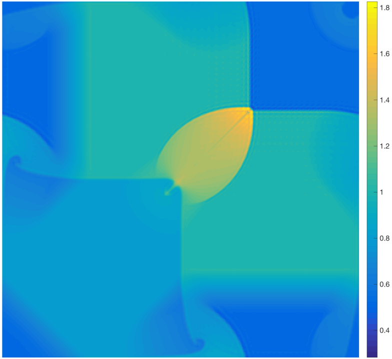
- For GLL-$(N+1)$ quadrature, $\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(P_N \boldsymbol{v}\right) = \boldsymbol{u}$ at GLL points.
- For GQ-$(N+2)$, discrepancy between L^2 projection and interpolation.
- Still need positivity of thermodynamic quantities for stability!



(a) $v_3(x), \left(P_N v_3\right)(x)$ (b) $\rho(x), \rho\left(\left(P_N \boldsymbol{v}\right)(x)\right)$

Talk outline

2D Riemann problem

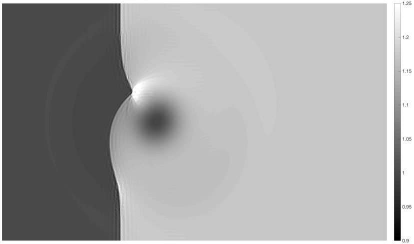


(a) $\Omega = [-1,1]^2$

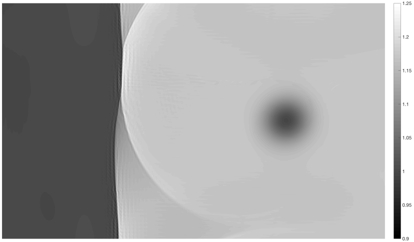
(b) $\Omega = [-.5,.5]^2$, 32×32 elements

- Degree N polynomials, degree $2N$ volume and surface quadratures.
- Uniform 64×64 triangle mesh: $N = 3$, CFL .125, Lax-Friedrichs flux.
- Periodic on larger domain ("natural" boundary conditions unstable).

2D shock-vortex interaction



(a) $t = .3$

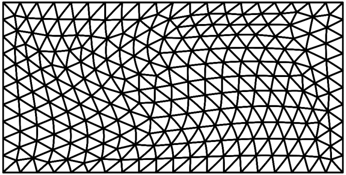


(b) $t = .7$

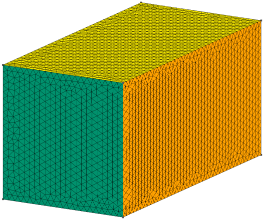
- Vortex passing through a shock on a periodic domain (matrix dissipation, degree $N = 3$ approximation, mesh size $h = 1/128$).
- Can also impose existing entropy stable wall boundary conditions for compressible Euler with decoupled SBP.

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) 2D triangular mesh



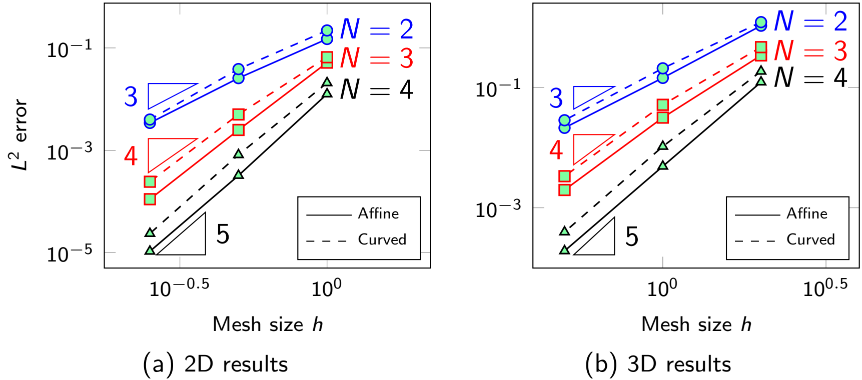
(b) 3D tetrahedral mesh

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

- Entropy stability: needs discrete geometric conservation law (GCL).
- Generalized mass lumping for curved: 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



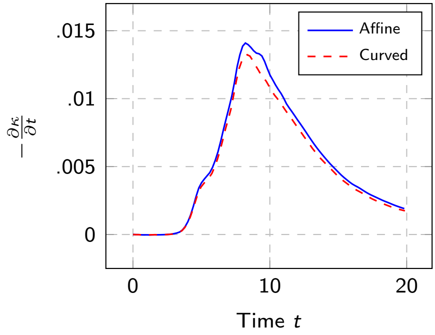
L^2 errors for 2D/3D isentropic vortex at $T = 5$ on affine, curved meshes.

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

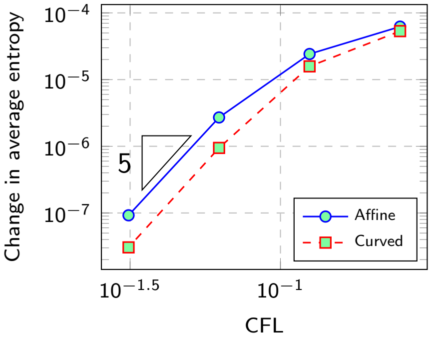
Kopriva (2006). Metric identities and the discontinuous spectral element method on curvilinear meshes.

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

3D inviscid Taylor-Green vortex: KE dissipation rate



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

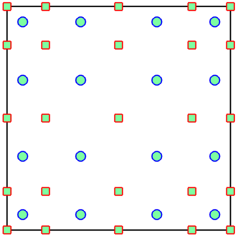


(b) Change in $\int_\Omega U(\boldsymbol{u})$ (EC scheme)

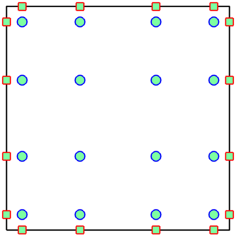
- Kinetic energy dissipation rate: good agreement with literature.
- Change in $\int_\Omega U(\boldsymbol{u}) \to 0$ as $\mathrm{CFL} \to 0$ for entropy conservative scheme.

Talk outline

ES Gauss collocation (w/M. Carpenter, DCDR Fernandez)



(a) Staggered-grid

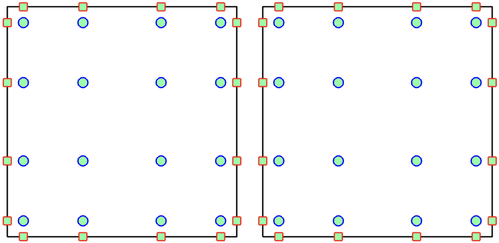


(b) Generalized SBP

- Gauss vs GLL quadrature: exact for degree $(2N+1)$ vs $(2N-1)$.
- Inter-element coupling for Gauss is expensive. Staggered grid collocation is an alternative, but requires degree $(N+1)$ GLL nodes.
- ES Gauss scheme from decoupled SBP (collocation: $\boldsymbol{V}_q = \boldsymbol{P}_q = \boldsymbol{I}$).

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

Entropy stable Gauss collocation: main steps



$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^T & \boldsymbol{C} \end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf} \\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff} \end{bmatrix} \right) \mathbf{1}$$

- Collocate $\boldsymbol{u}$, interpolate entropy variables $\boldsymbol{v}(\boldsymbol{u})$ to surface nodes.
- Perform flux differencing at Gauss nodes.
- Compute $\boldsymbol{f}_S(\boldsymbol{u}_L, \boldsymbol{u}_R)$ for surface nodes of neighboring elements.
- Compute $\boldsymbol{f}_S(\boldsymbol{u}_L, \boldsymbol{u}_R)$ between volume/surface nodes, apply flux differencing with interp. matrix + transpose for volume/surface nodes.

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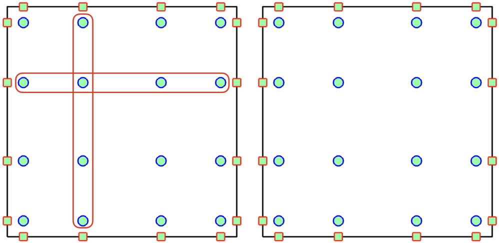

$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B}\\ -\boldsymbol{B}^T & \boldsymbol{C}\end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf}\\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff}\end{bmatrix}\right)\mathbf{1}$$

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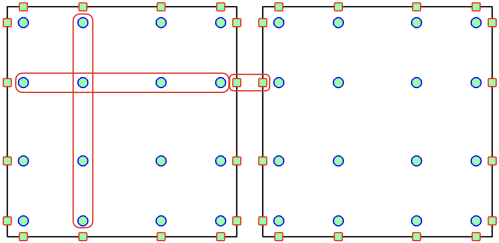

$$\left(\underbrace{\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^T & \boldsymbol{C} \end{bmatrix}}_{\boldsymbol{Q}_N^i} \circ \begin{bmatrix} \boldsymbol{F}_S^{vv} & \boldsymbol{F}_S^{vf} \\ \boldsymbol{F}_S^{fv} & \boldsymbol{F}_S^{ff} \end{bmatrix} \right) \mathbf{1}$$

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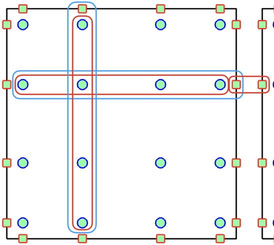

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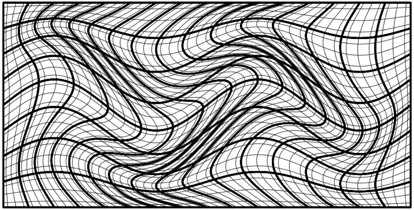
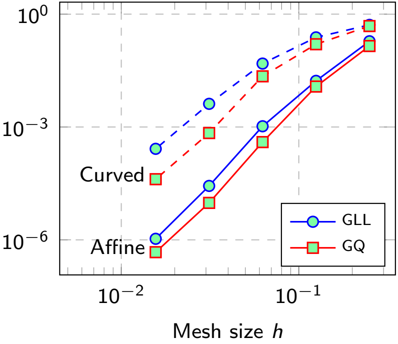
Numerical results: 2D/3D isentropic vortex



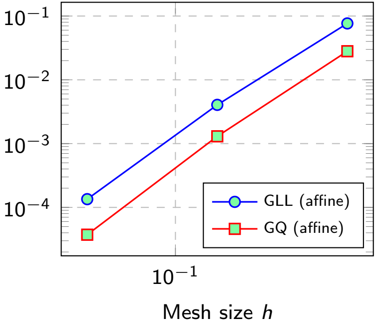
(a) Warped curvilinear mesh



(b) 2D L^2 errors ($N = 4$)

Entropy stability for Gauss collocation on curved meshes: compute geometric terms at GLL points, interpolate to volume and face points.

Numerical results: 2D/3D isentropic vortex



(a) 3D L^2 errors ($N = 4$)

Curvilinear results: in progress!

Summary and future work

- Discrete semi-discrete entropy stability for (almost) arbitrary choices of basis, quadrature. Usual challenges (positivity, Gibbs, BCs) apply.
- DG-SEM: volume/surface cross terms cancel out!
- Current work: Gauss collocation (with DCDR Fernandez, M. Carpenter), adaptivity + hybrid meshes, multi-GPU.
- 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

Sketch of proof of entropy conservation (one element)

- Multiply by mass matrix on both sides, rewrite as

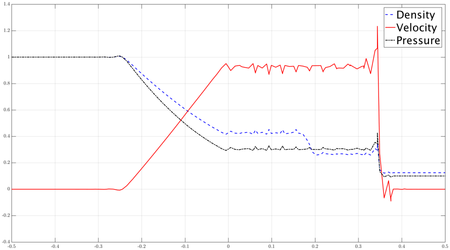
$$\boldsymbol{M}\frac{\mathrm{d}\widehat{\boldsymbol{u}}}{\mathrm{d}t} + \begin{bmatrix}\boldsymbol{V}_q\\ \boldsymbol{V}_f\end{bmatrix}^T \left(\boldsymbol{Q}_N \circ \boldsymbol{f}_S\left(\begin{bmatrix}\boldsymbol{V}_q\\ \boldsymbol{V}_f\end{bmatrix}\boldsymbol{P}_q\boldsymbol{v}_q\right)\right)\mathbf{1} = 0.$$

- Test with L^2 projection of entropy variables $\boldsymbol{P}_q\boldsymbol{v}_q = \boldsymbol{M}^{-1}\boldsymbol{V}_q^T\boldsymbol{W}\boldsymbol{v}_q$.

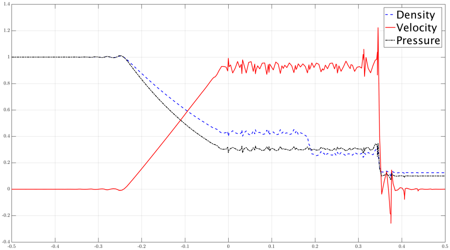
$$\begin{aligned}(\boldsymbol{P}_q\boldsymbol{v}_q)^T\boldsymbol{M}\frac{\mathrm{d}\widehat{\boldsymbol{u}}}{\mathrm{d}t} &= \boldsymbol{v}_q^T\boldsymbol{W}\boldsymbol{V}_q\boldsymbol{M}^{-1}\boldsymbol{M}\boldsymbol{V}_q\frac{\mathrm{d}\widehat{\boldsymbol{u}}}{\mathrm{d}t}\\ &= \boldsymbol{v}_q^T\boldsymbol{W}\frac{\mathrm{d}(\boldsymbol{V}_q\widehat{\boldsymbol{u}})}{\mathrm{d}t} = \mathbf{1}^T\boldsymbol{W}\left(\frac{\mathrm{d}S(\boldsymbol{u}_q)}{\mathrm{d}\boldsymbol{u}}\frac{\mathrm{d}\boldsymbol{u}_q}{\mathrm{d}t}\right) = \frac{\mathrm{d}S(\boldsymbol{u}_q)}{\mathrm{d}t}.\end{aligned}$$

- Spatial term vanishes using SBP, skew-symmetry, and properties of $\boldsymbol{f}_S$.

1D Sod: over-integration ineffective w/out L^2 projection



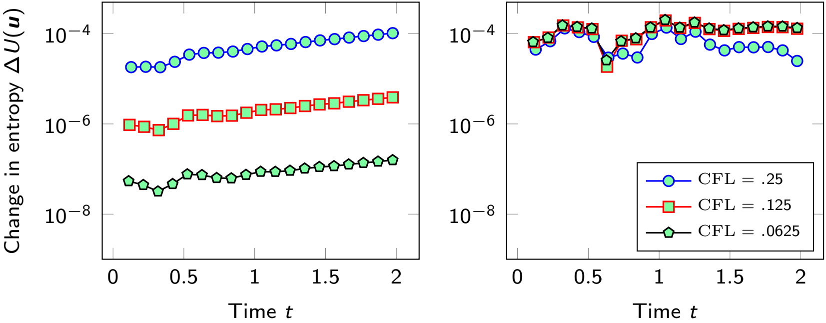
(a) Degree N GLL, $(N+1)$ points



(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.

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