

Entropy stable schemes based on high order modal discontinuous Galerkin formulations

Jesse Chan

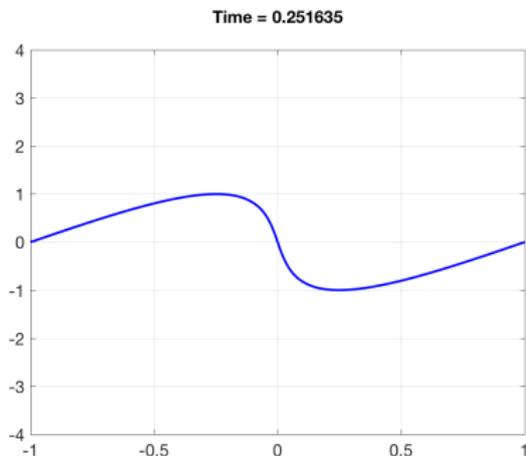
with Lucas Wilcox (NPS), DCDR Fernandez, Mark Carpenter (NASA Langley)

¹Department of Computational and Applied Mathematics

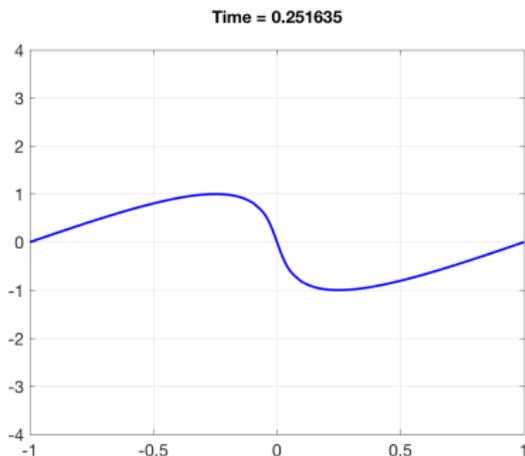
Finite Elements in Flow, Chicago, Illinois

April 3, 2019

High order methods typically unstable for nonlinear PDEs



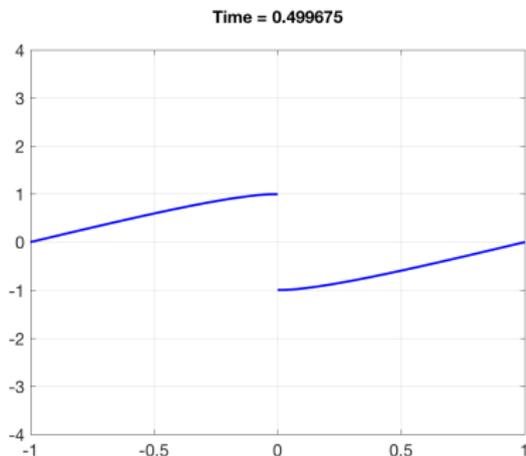
(a) Inviscid Burgers' solution



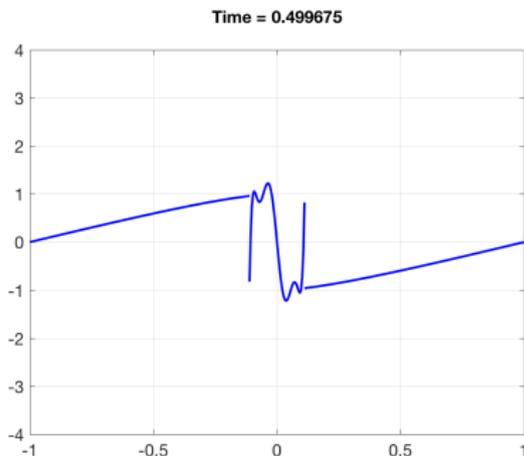
(b) 8th order DG

- High order methods tend to blow up for under-resolved solutions (shocks, turbulence), sensitive to discretization.
- Instability: **quadrature error** + loss of the discrete **chain rule** in space.

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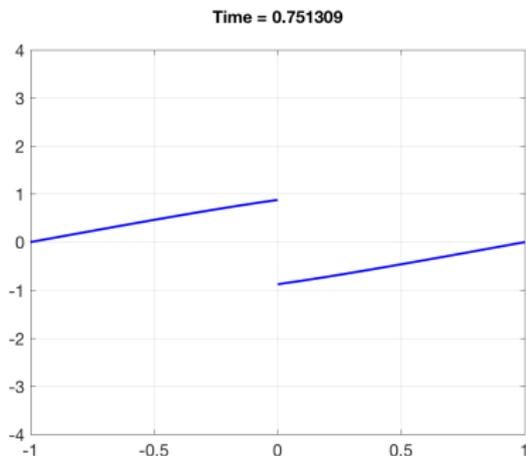
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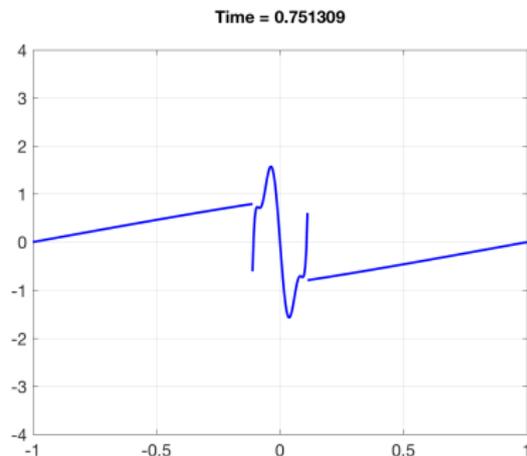
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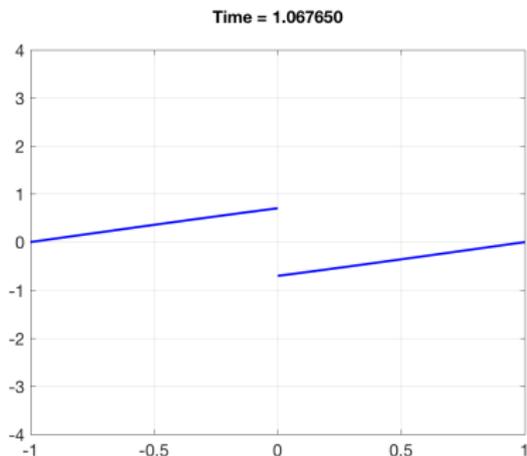
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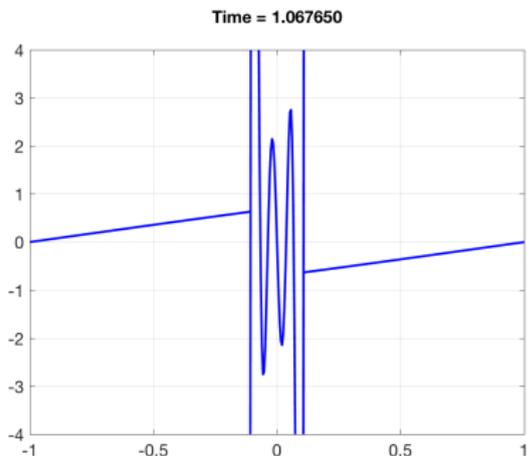
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Entropy stability for nonlinear problems uses the chain rule

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

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = 0 \quad x \in [-1, 1].$$

- Continuous entropy inequality: given a scalar convex **entropy** function $S(\mathbf{u})$ and “entropy potential” $\psi(\mathbf{u})$,

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

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

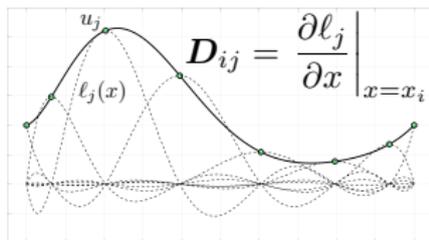
Talk outline

- 1 Entropy stable nodal DG and summation-by-parts
- 2 Entropy stable modal DG formulations
- 3 Numerical experiments
 - Triangular and tetrahedral meshes
 - Quadrilateral and hexahedral meshes
 - Hybrid and non-conforming meshes

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Nodal DG, summation-by-parts (SBP), flux differencing



$$B = \begin{bmatrix} -1 & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$

- Gauss-Lobatto nodes mimic **integration by parts** algebraically

$$Q = B - Q^T,$$

$$Q = MD,$$

M diagonal mass matrix.

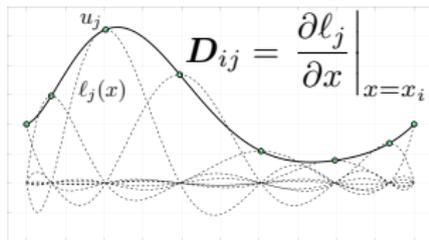
- Nodal “collocation” over a single element:

$$M \frac{du}{dt} + Qf(u) = 0 \quad \Rightarrow \quad M_{ii} \frac{du_i}{dt} + \sum_j Q_{ij} f(u_j) = 0.$$

- Let $f_S(u_i, u_j) = \frac{1}{2} (f(u_i) + f(u_j)) = (F_S)_{ij}$. Collocation equiv. to

$$M_{ii} \frac{du_i}{dt} + \sum_j Q_{ij} 2f_S(u_i, u_j) = 0 \quad \Rightarrow \quad M \frac{du}{dt} + 2(Q \circ F_S) \mathbf{1} = 0.$$

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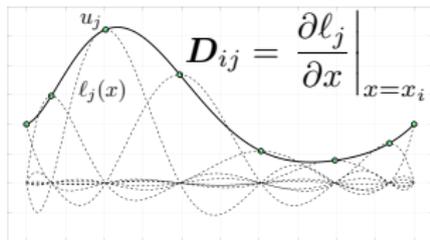
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Entropy stable schemes: a brief derivation

- DG: derive local formulation (one element) with interface flux \mathbf{f}^*

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + 2(\mathbf{Q} \circ \mathbf{F}_S) \mathbf{1} = 0$$

- Trick: use Tadmor's entropy conservative numerical flux for $\mathbf{f}_S, \mathbf{f}^*$

$$\mathbf{f}_S(\mathbf{u}, \mathbf{u}) = \mathbf{f}(\mathbf{u}), \quad (\text{consistency})$$

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$$(\mathbf{v}_L - \mathbf{v}_R)^T \mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R) = \psi_L - \psi_R, \quad (\text{conservation}).$$

- Proof of entropy conservation: multiply by \mathbf{v}^T

$$\mathbf{v}^T \mathbf{M} \frac{d\mathbf{u}}{dt} + \mathbf{v}^T \left((\mathbf{Q} - \mathbf{Q}^T) \circ \mathbf{F}_S \right) \mathbf{1} + \mathbf{v}^T \mathbf{B} \mathbf{f}^* = 0.$$

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Tadmor, Eitan (1987), Gassner, Winters, and Kopriva (2016).

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$$\mathbf{1}^T \mathbf{M} \frac{d\mathcal{S}(\mathbf{u})}{dt} + \psi^T \mathbf{Q} \mathbf{1} - \mathbf{1}^T \mathbf{Q} \psi + \mathbf{v}^T \mathbf{B}\mathbf{f}^* = 0.$$

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Benefits of entropy stability (conservation)

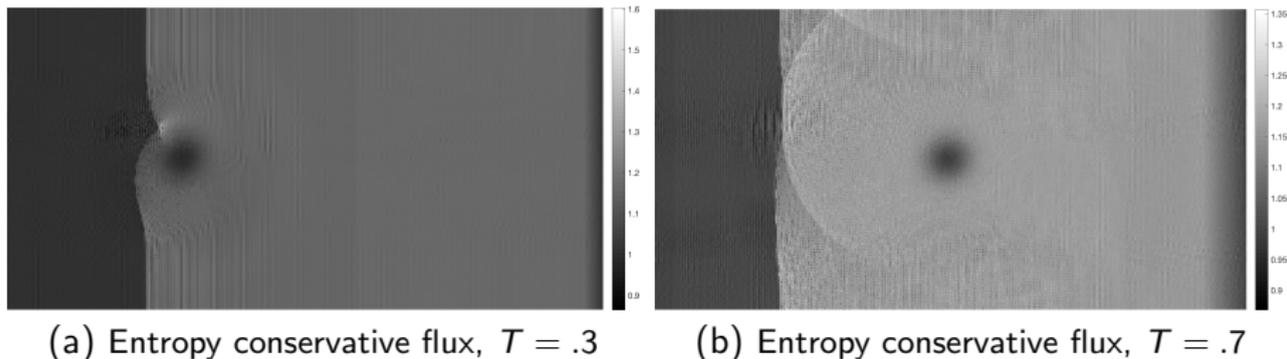


Figure: Compressible Euler shock vortex interaction: 200×100 degree $N = 4$ elements, 4th order **explicit** RK time-stepping, no limiters or artificial viscosity.

Jiang, Shu (1998). *Efficient Implementation of Weighted ENO Schemes*.

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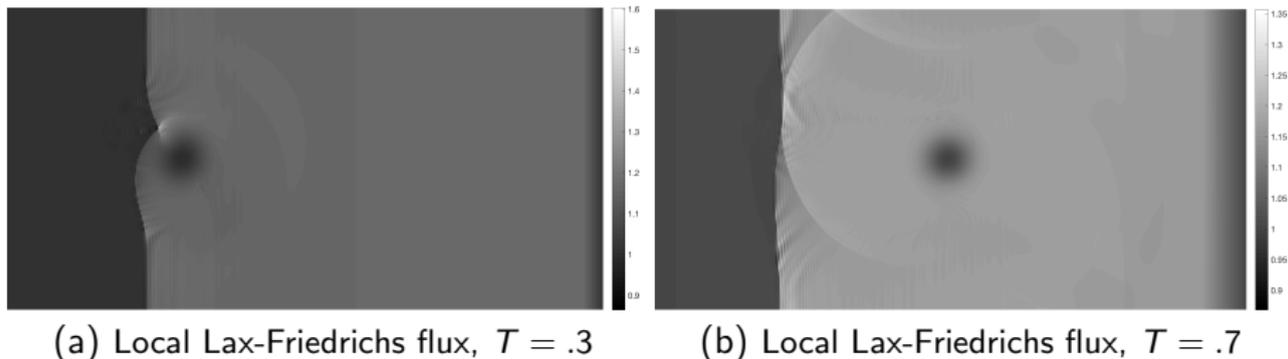


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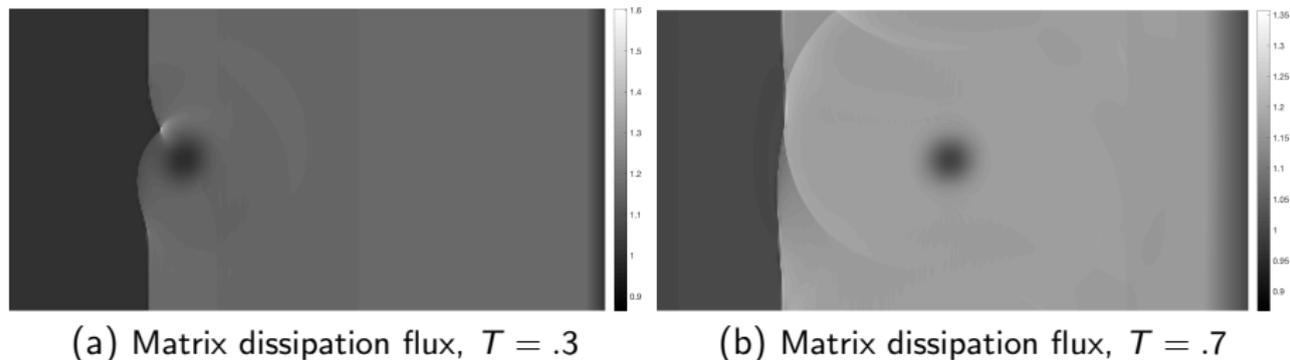


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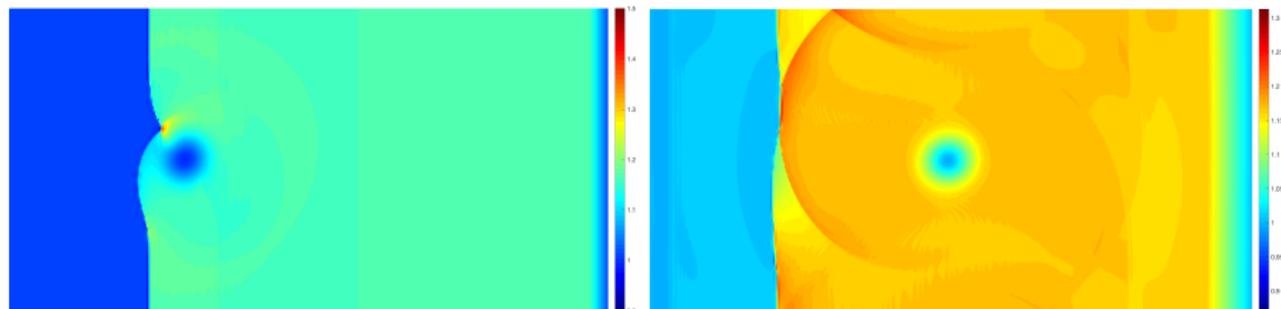
(a) Matrix dissipation flux, $T = .3$ (b) Matrix dissipation flux, $T = .7$

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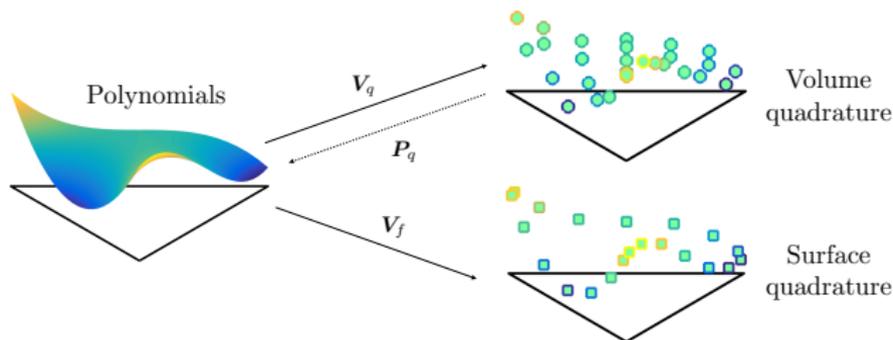
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Modal formulations: general bases and quadrature



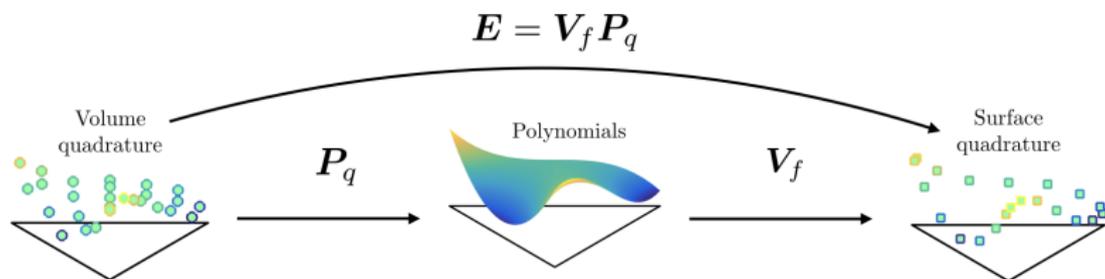
- Assume degree $2N$ volume + surface quadratures $(\mathbf{x}_i^q, \mathbf{w}_i^q)$, $(\mathbf{x}_i^f, \mathbf{w}_i^f)$, and basis functions $\phi_j(\mathbf{x})$. Define interpolation and weight matrices

$$\begin{aligned}
 (\mathbf{V}_q)_{ij} &= \phi_j(\mathbf{x}_i^q), & (\mathbf{V}_f)_{ij} &= \phi_j(\mathbf{x}_i^f), \\
 \mathbf{W} &= \text{diag}(\mathbf{w}^q), & \mathbf{W}_f &= \text{diag}(\mathbf{w}^f).
 \end{aligned}$$

- Discretize $P_N : L^2 \rightarrow P^N$, yields a quadrature-based **projection** matrix

$$(P_N u, v) = (u, v) \quad \forall v \in P^N \quad \implies \quad P_q = \mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W}.$$

Quadrature-based “finite difference” matrices



- Matrix D_q^i : evaluates i th derivative of L^2 projection P_N at \mathbf{x}^q .

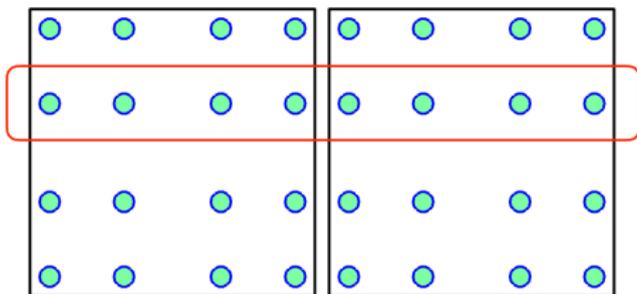
$$D_q^i = V_q D^i P_q, \quad D^i \text{ exactly differentiates polynomials.}$$

- Generalized summation-by-parts: let $Q_i = W D_q^i$ and $E = V_f P_q$

$$Q_i + Q_i^T = E^T B_i E, \quad B_i = W_f \text{diag}(\mathbf{n}_i)$$

$$\Rightarrow \int_{\hat{D}} \frac{\partial P_N u}{\partial x_i} v + \int_{\hat{D}} u \frac{\partial P_N v}{\partial x_i} = \int_{\partial \hat{D}} (P_N u) (P_N v) \hat{n}_i.$$

Problems with generalized SBP on multiple elements



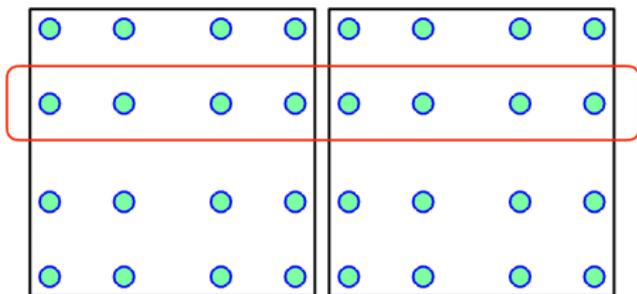
Coupling between quadrature nodes on neighboring elements.

- Re-deriving the local DG formulation with GSBP operators:

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + 2(\mathbf{Q} \circ \mathbf{F}_S) \mathbf{1} = 0.$$

- The presence of the interpolation matrix \mathbf{E} increases inter-element coupling, complicates imposition of BCs.

Problems with generalized SBP on multiple elements



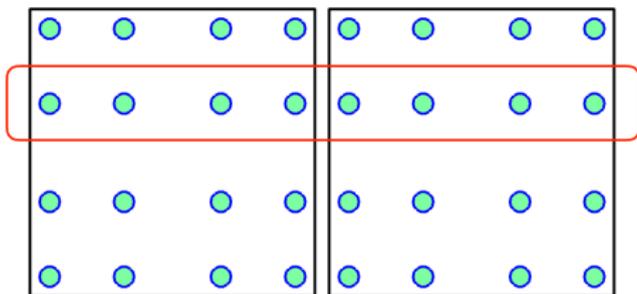
Coupling between quadrature nodes on neighboring elements.

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- The presence of the interpolation matrix \mathbf{E} increases inter-element coupling, complicates imposition of BCs.

A “decoupled” SBP operator

- Goal: SBP property without \mathbf{E} in the boundary terms

$$\mathbf{Q}_N = \begin{bmatrix} \mathbf{Q} - \frac{1}{2}\mathbf{E}^T\mathbf{B}\mathbf{E} & \frac{1}{2}\mathbf{E}^T\mathbf{B} \\ -\frac{1}{2}\mathbf{B}\mathbf{E} & \frac{1}{2}\mathbf{B} \end{bmatrix},$$

- If $\mathbf{Q} + \mathbf{Q}^T = \mathbf{E}^T\mathbf{B}\mathbf{E}$, then the block matrix \mathbf{Q}_N satisfies

$$\boxed{\mathbf{Q}_N + \mathbf{Q}_N^T = \begin{bmatrix} \mathbf{0} & \\ & \mathbf{B} \end{bmatrix}} \sim \boxed{\int_{-1}^1 \frac{\partial P_N u}{\partial x} v + u \frac{\partial P_N v}{\partial x} = uv|_{-1}^1.}$$

- \mathbf{Q}_N approximates $f \frac{\partial g}{\partial x}$ by \mathbf{u} using data at $\mathbf{x} = [\mathbf{x}_{\text{vol}}, \mathbf{x}_{\text{face}}]$

$$\mathbf{M}\mathbf{u} = \begin{bmatrix} \mathbf{V}_q \\ \mathbf{V}_f \end{bmatrix}^T \text{diag}(\mathbf{f}) \mathbf{Q}_N \mathbf{g}, \quad \mathbf{f}_i, \mathbf{g}_i = f(\mathbf{x}_i), g(\mathbf{x}_i).$$

- Reduces to traditional SBP operator under appropriate quadrature.

Entropy stable schemes using decoupled SBP operators

- Replace SBP operator with decoupled SBP operator

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + \left((\mathbf{Q} - \mathbf{Q}^T) \circ \mathbf{F}_S \right) \mathbf{1} + \mathbf{B}\mathbf{f}^* = 0.$$

- \mathbf{F}_S is the matrix of flux evaluations between solution values at *both* volume and face nodes using **entropy projection**:

$$(\mathbf{F}_S)_{ij} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j), \quad \tilde{\mathbf{u}} = \text{evaluate } \mathbf{u}(P_N \mathbf{v}(\mathbf{u})).$$

- Semi-discrete scheme is verifiably entropy conservative for inexact quadrature! Add appropriate interface dissipation (e.g. Lax-Friedrichs, HLLC) for entropy stability.

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

Parsani et al. (2016), *Entropy Stable Staggered Grid Discontinuous Spectral Collocation Methods*

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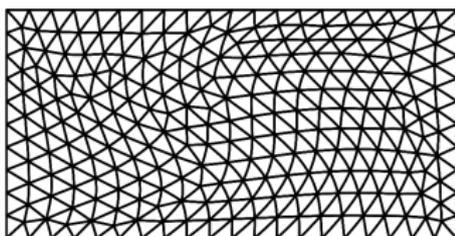
Talk outline

- 1 Entropy stable nodal DG and summation-by-parts
- 2 Entropy stable modal DG formulations
- 3 Numerical experiments
 - Triangular and tetrahedral meshes
 - Quadrilateral and hexahedral meshes
 - Hybrid and non-conforming meshes

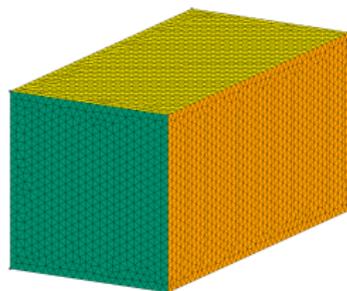
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Smooth isentropic vortex and curved meshes in 2D/3D



(a) 2D triangular mesh



(b) 3D tetrahedral mesh

- “Split” form of derivatives on curved elements for entropy stability.

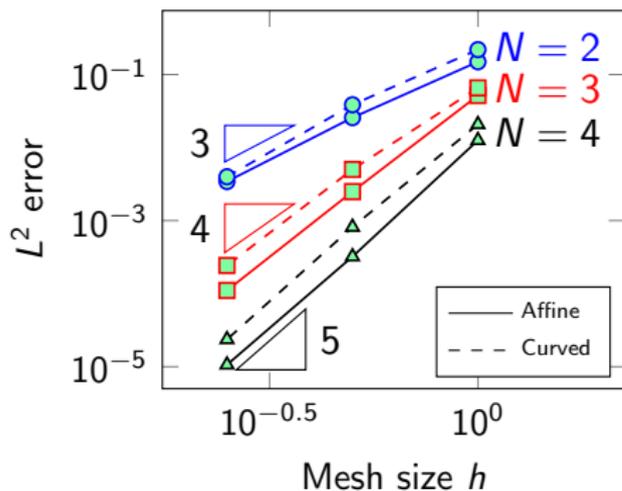
$$J \frac{\partial u}{\partial x_i} = \sum_{j=1}^d J \frac{\partial \hat{x}_j}{\partial x_i} \frac{\partial u}{\partial \hat{x}_j} = \frac{1}{2} \sum_{j=1}^d \left(J \frac{\partial \hat{x}_j}{\partial x_i} \frac{\partial u}{\partial \hat{x}_j} + \frac{\partial}{\partial \hat{x}_j} \left(J \frac{\partial \hat{x}_j}{\partial x_i} u \right) \right).$$

- Discrete geometric conservation law (GCL) now a **necessary** condition.

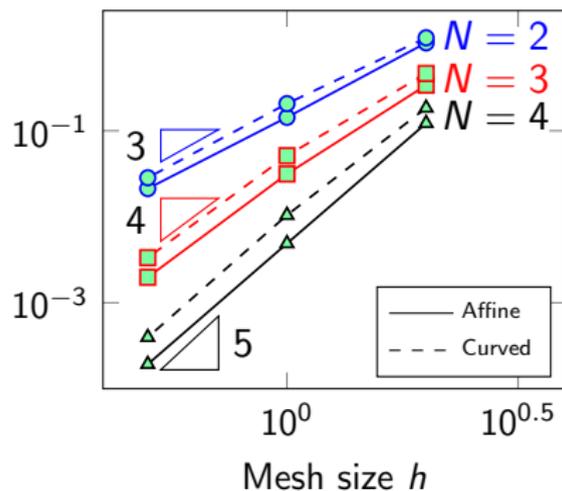
Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.

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

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



(c) 2D results



(d) 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.

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Inviscid Taylor-Green vortex

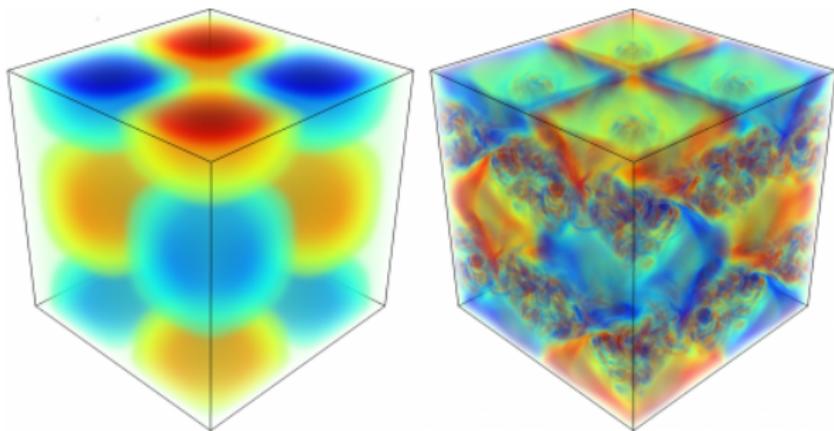
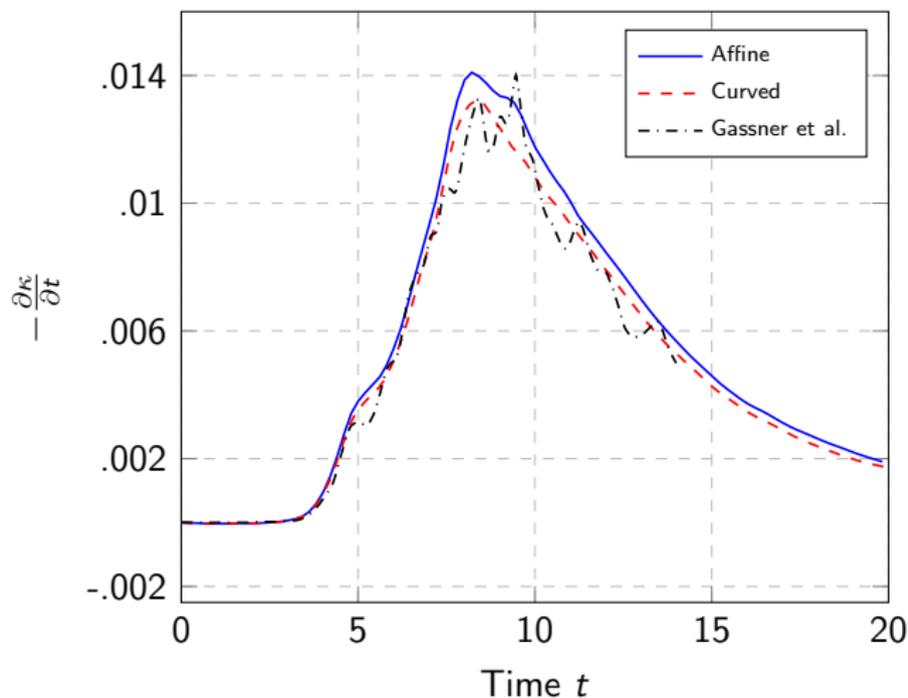


Figure: Isocontours of z-vorticity for Taylor-Green at $t = 0, 10$ seconds.

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

Inviscid Taylor-Green vortex: robust w.r.t. under-resolution

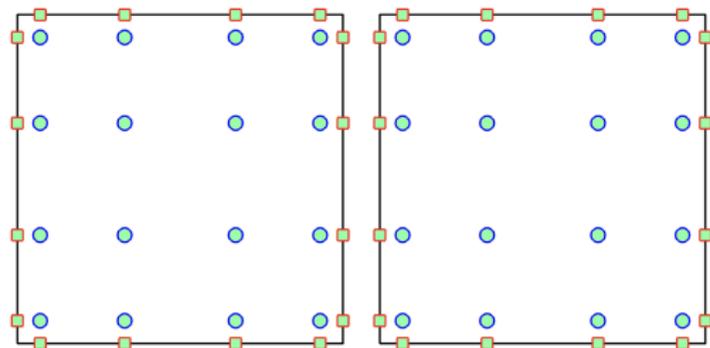


Kinetic energy dissipation rate $-\frac{\partial \kappa}{\partial t}$ for $N = 3$, $h = \pi/8$, CFL = .25 (tet meshes).

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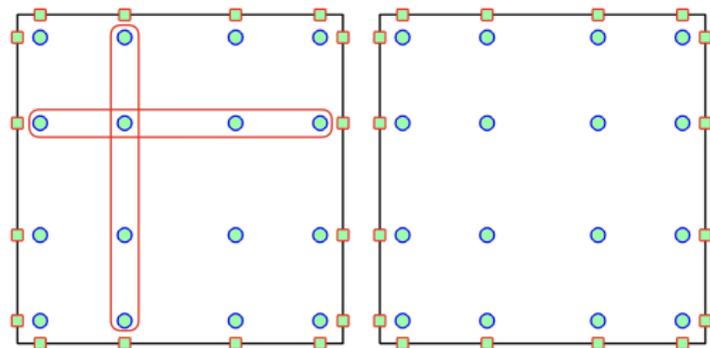
Entropy stable Gauss collocation: main steps



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

- Advantage of hexahedra vs. tetrahedra: tensor product structure.
- $(N + 1)$ -point Gauss quadrature reduces to a **collocation scheme**.
- Reduces computational costs from $O(N^6)$ to $O(N^4)$ in 3D.

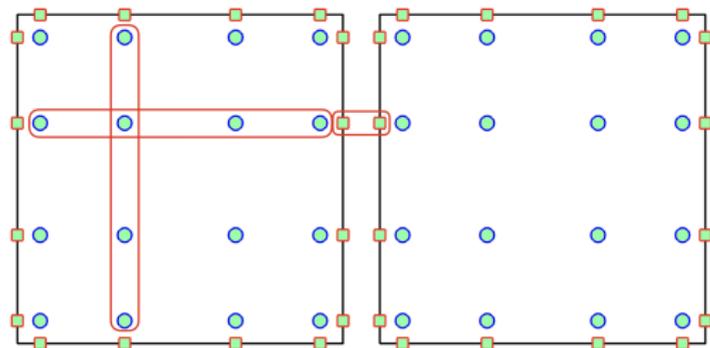
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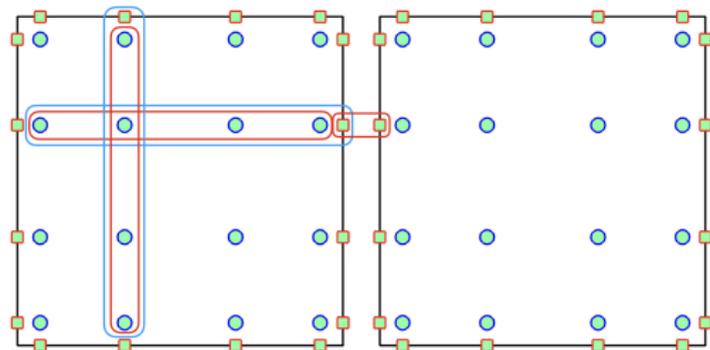
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Gauss quadrature improves errors on curved meshes

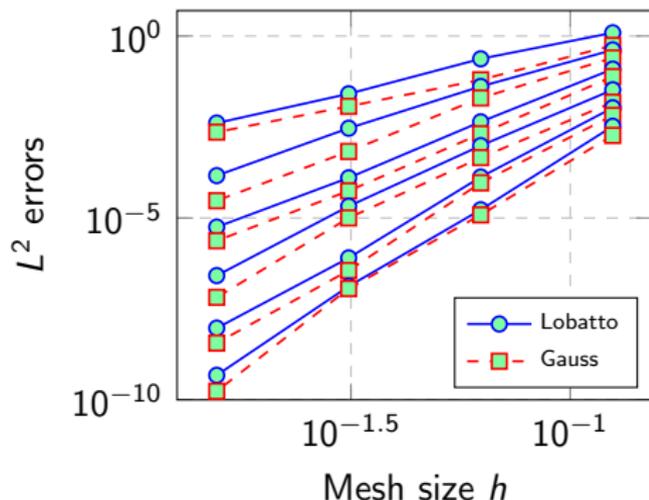
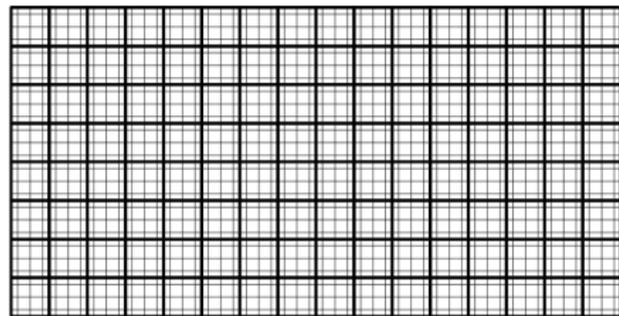


Figure: L^2 errors for the 2D isentropic vortex at time $T = 5$ for degree $N = 2, \dots, 7$ Lobatto and Gauss collocation schemes (similar behavior in 3D).

Gauss quadrature improves errors on curved meshes

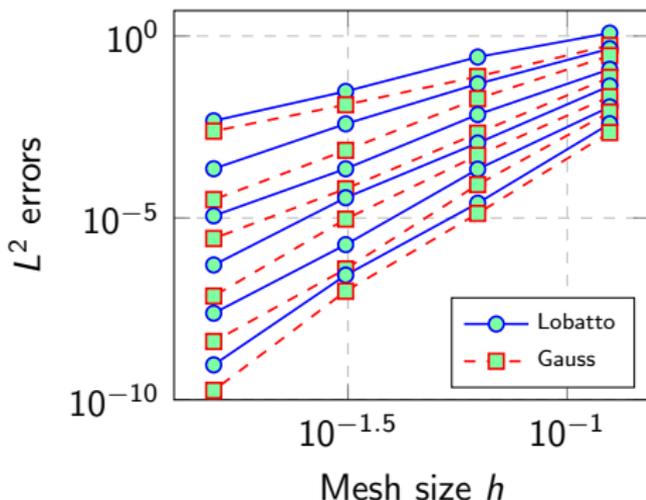
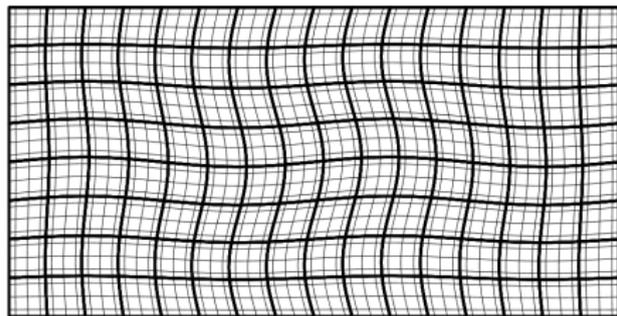


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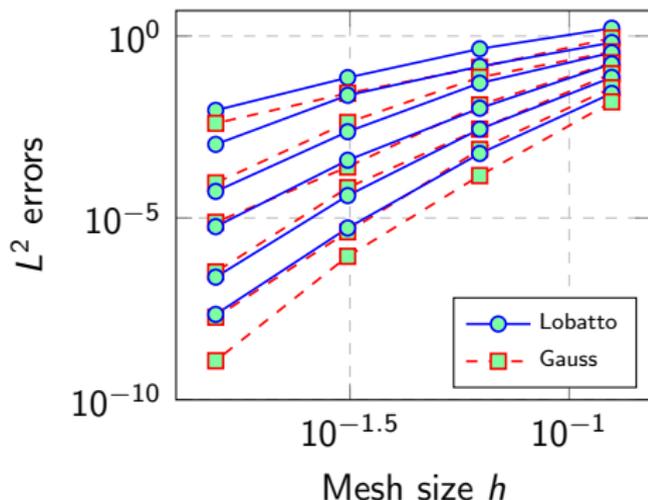
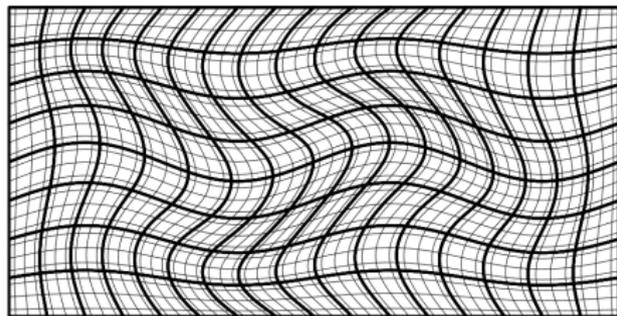


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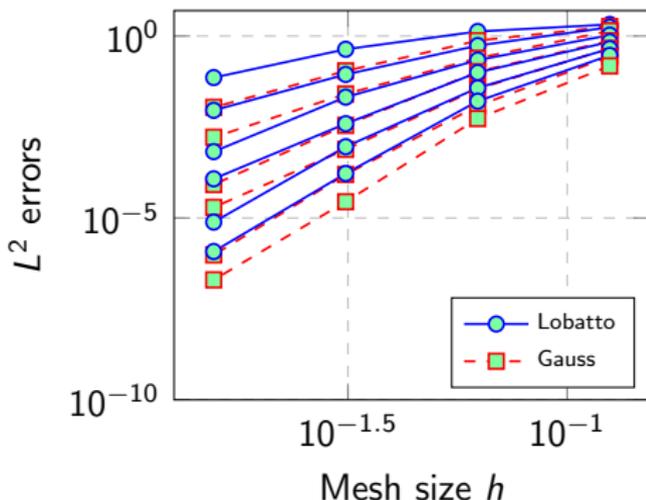
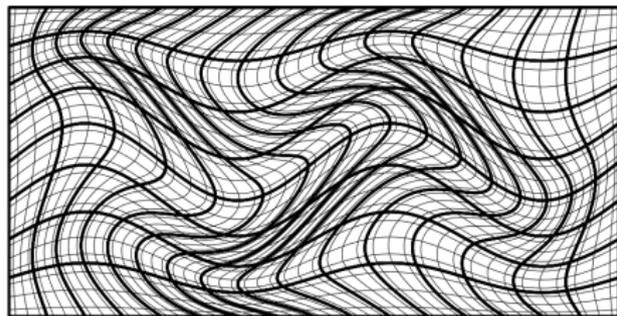
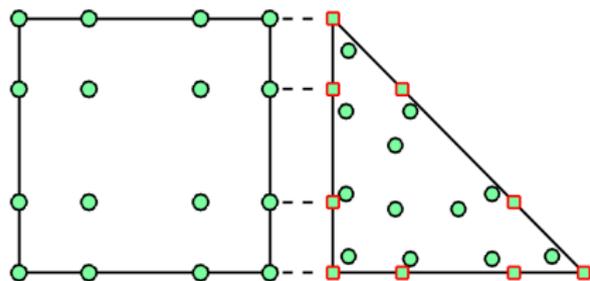


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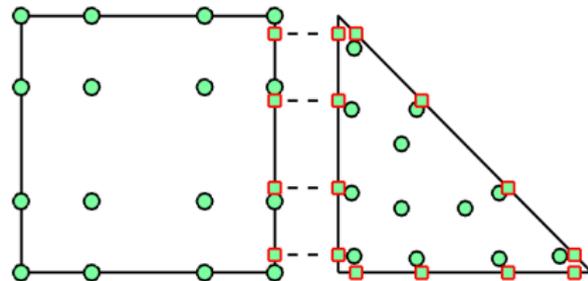
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Mixed quadrilateral-triangle meshes



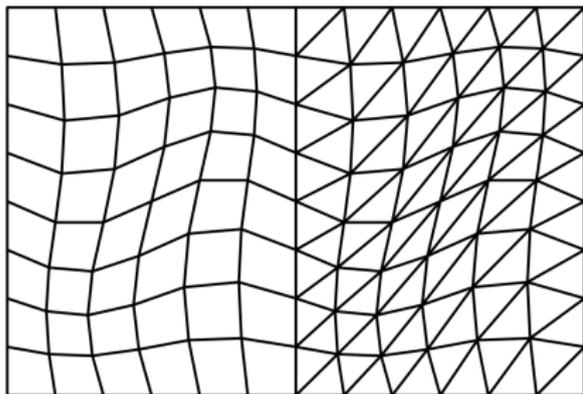
(a) No SBP (tri. under-integrated)



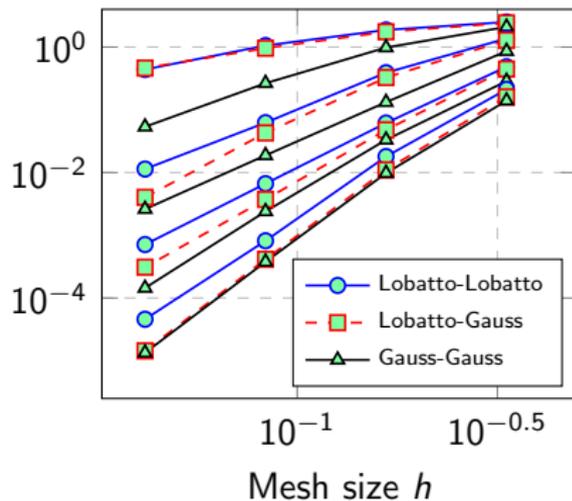
(b) No SBP (quad. under-integrated)

- GSBP property lost if surface quadrature insufficiently accurate.
- Skew-symmetric formulation remains entropy stable under “weak” GSBP property, relaxed requirements on quadrature accuracy.

Numerical results: mixed triangle-quadrilateral meshes



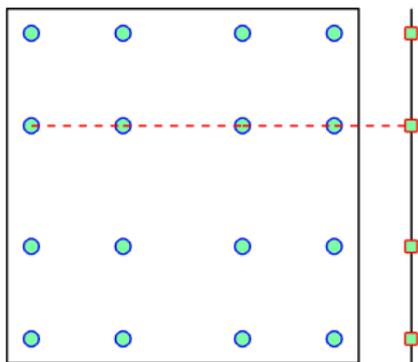
(a) Coarse hybrid mesh



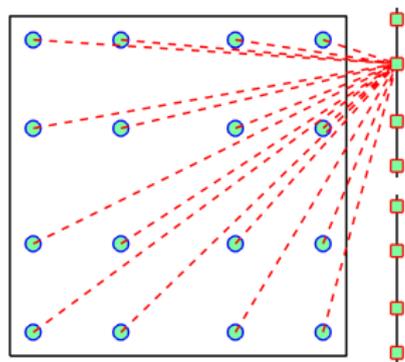
(b) L^2 errors for $N = 1, 2, 3, 4$

The skew-symmetric formulation guarantees entropy stability for all combinations of Lobatto and Gauss volume and surface quadratures.

Non-conforming interfaces



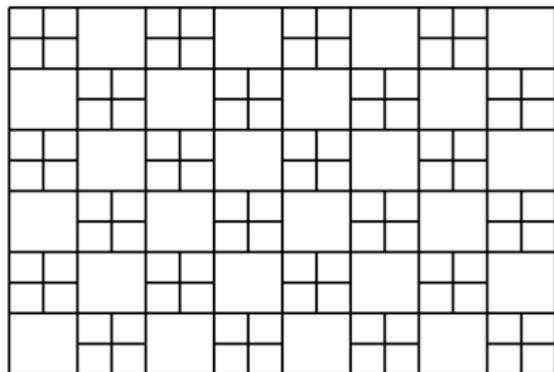
(a) Conforming surface quadrature nodes



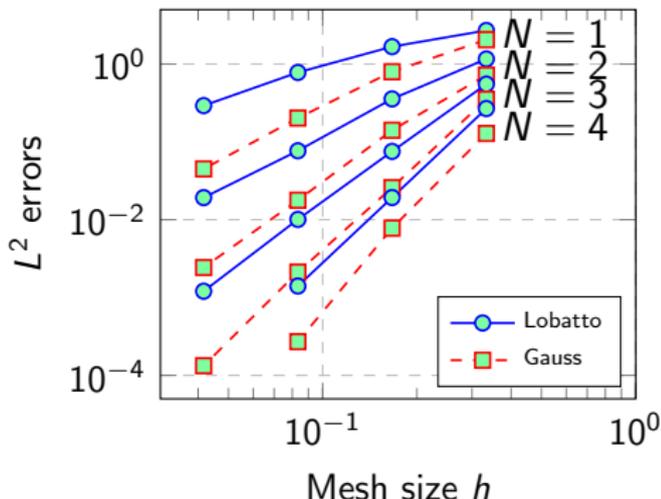
(b) Non-conforming surface nodes

- Volume/surface nodes interact through $f_S(\mathbf{u}_i, \mathbf{u}_j)$ and **interpolation**.
- Fix: weakly couple conforming+non-conforming faces using a mortar.

Numerical results: non-conforming meshes



(a) Coarse non-conforming mesh



(b) Sub-optimal rates if under-integrated

The skew-symmetric formulation guarantees entropy stability for both Lobatto and Gauss quadratures, but Gauss is more accurate.

Summary and future work

- Entropy stable high order “modal” DG: flexibility in choosing basis and quadrature, improved accuracy on curved meshes.
- Current work: ROMs, strong shocks, positivity preservation.
- This work is supported by DMS-1719818 and DMS-1712639.

Thank you! Questions?



Chan (2019). *Skew-symmetric entropy stable modal discontinuous Galerkin formulations.*

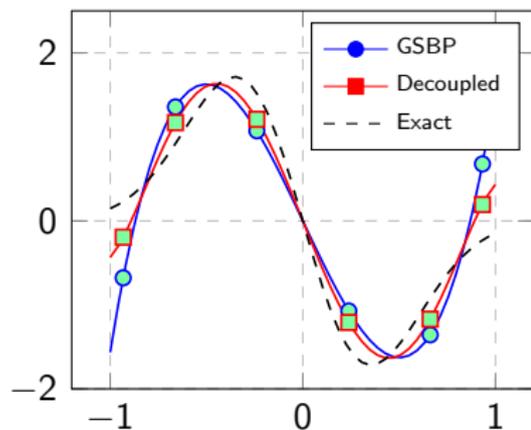
Chan, Del Rey Fernandez, Carpenter (2018). *Efficient entropy stable Gauss collocation methods.*

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

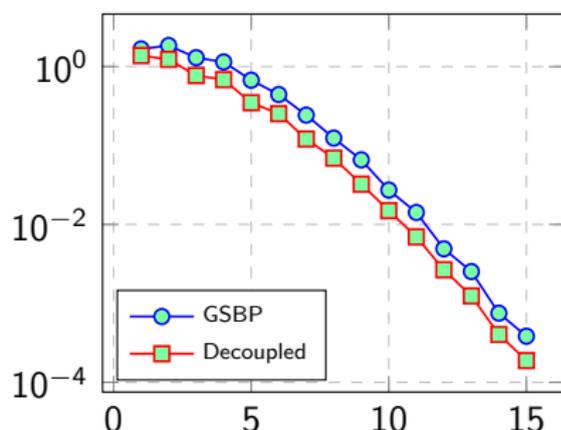
Chan (2018). *On discretely entropy conservative and entropy stable discontinuous Galerkin methods.*

Additional slides

Decoupled SBP operators add boundary corrections



(a) Derivative approximations

(b) L^2 error w.r.t. degree N

- Equivalent to a variational problem for a polynomial $u(\mathbf{x}) \approx f \frac{\partial g}{\partial \mathbf{x}}$.

$$\int_{-1}^1 u(\mathbf{x})v(\mathbf{x}) = \int_{-1}^1 f \frac{\partial P_N g}{\partial \mathbf{x}} v + (g - P_N g) \frac{(fv + P_N(fv))}{2} \Big|_{-1}^1.$$

Flux differencing: recovering split formulations

- Entropy conservative flux for Burgers' equation

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

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

$$\frac{\partial f(u)}{\partial x} \implies 2 \frac{\partial f_S(u(x), u(y))}{\partial x} \Big|_{y=x}$$

- Recovering the Burgers' split formulation

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

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

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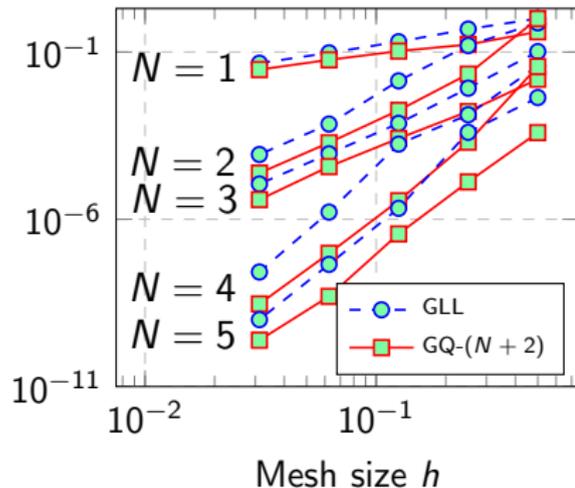
- Recovering the Burgers' split formulation

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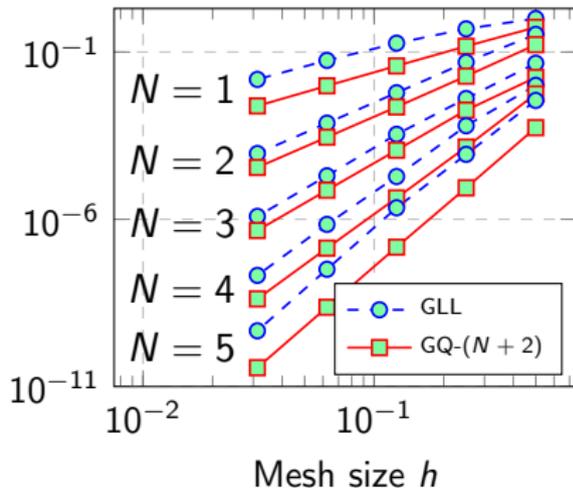
$$2 \frac{\partial f_S(u(x), u(y))}{\partial x} \Big|_{y=x} = \frac{1}{3} \frac{\partial u^2}{\partial x} + \frac{1}{3} u \frac{\partial u}{\partial x} + \frac{1}{3} \cancel{u^2 \frac{\partial u}{\partial x}}.$$

1D compressible Euler equations

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



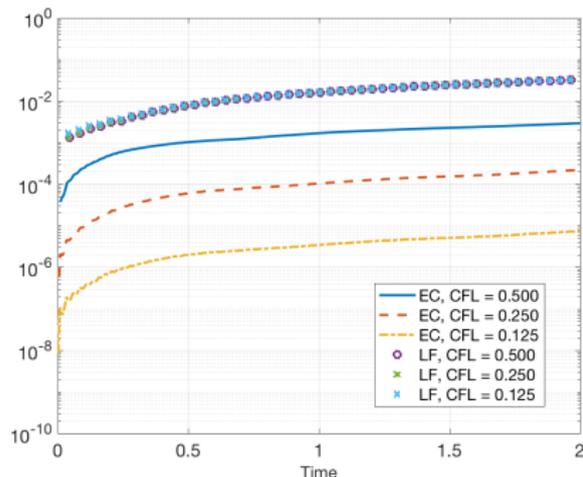
(c) Entropy conservative flux



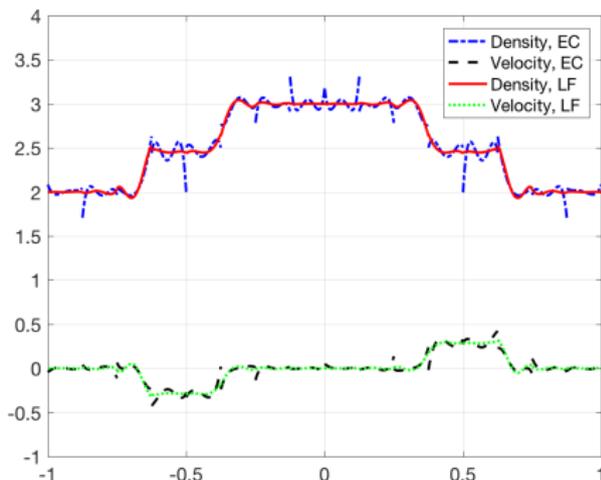
(d) With Lax-Friedrichs penalization

Conservation of entropy: semi-discrete vs. fully discrete

$$\Delta S(\mathbf{u}) = |S(\mathbf{u}(x, t)) - S(\mathbf{u}(x, 0))| \rightarrow 0 \text{ as } \Delta t \rightarrow 0.$$



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

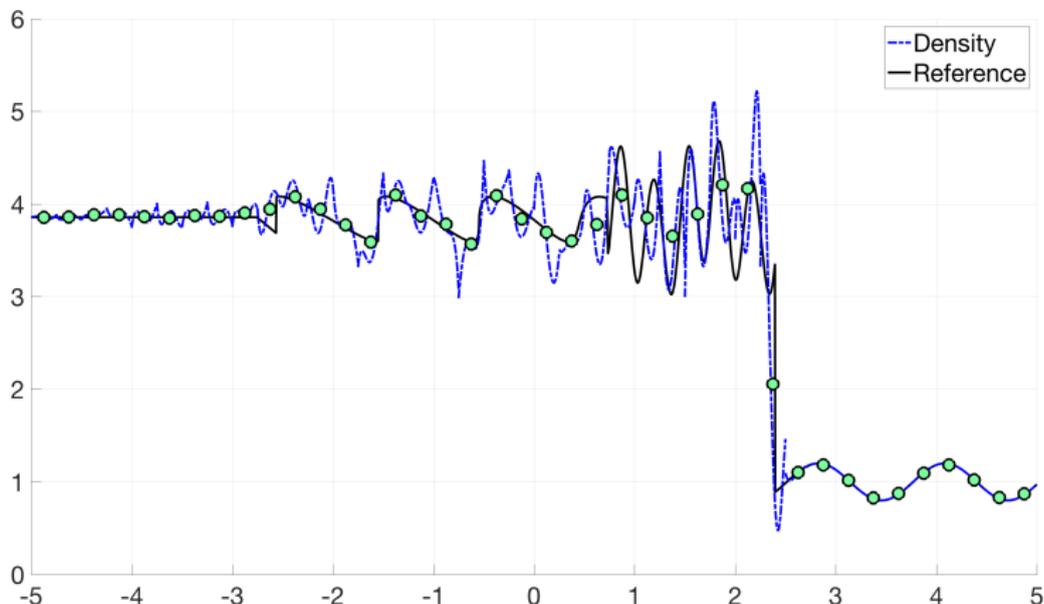


(b) $\rho(x), u(x)$ ($N = 4, K = 16$)

Solution and change in entropy $\Delta S(\mathbf{u})$ for entropy conservative (EC) and Lax-Friedrichs (LF) fluxes (using GQ- $(N + 2)$ quadrature).

1D sine-shock interaction

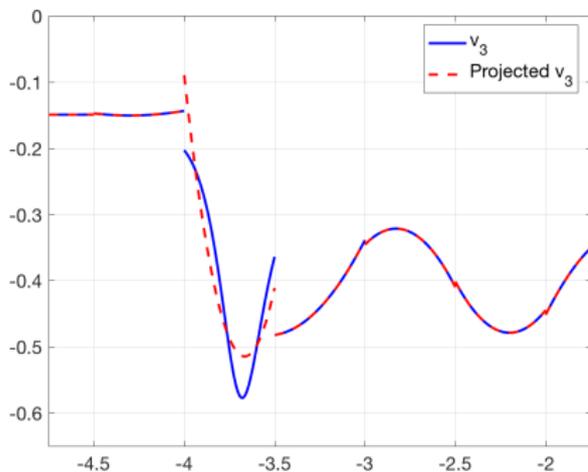
- $(N + 2)$ -point Gauss needs a smaller CFL (.05 vs .125) for stability.



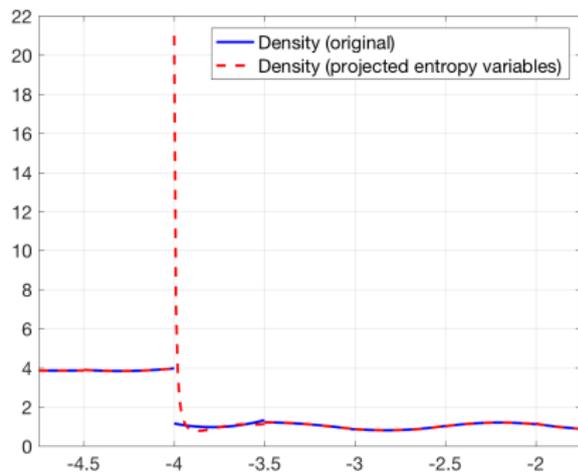
$N = 4, K = 40, CFL = .05, (N + 1)$ point Lobatto quadrature.

Loss of control with the entropy projection

- For $(N + 1)$ -Lobatto quadrature, $\tilde{\mathbf{u}} = \mathbf{u}(P_N \mathbf{v}) = \mathbf{u}$ at nodal points.
- For $(N + 2)$ -Gauss, discrepancy between $\mathbf{v}(\mathbf{u})$ and L^2 projection.
- Still need **positivity** of thermodynamic quantities for stability!

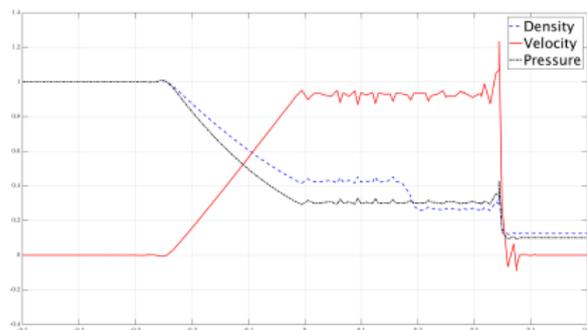


(c) $v_3(x), (P_N v_3)(x)$

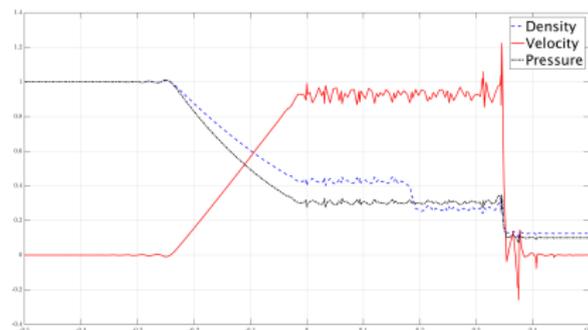


(d) $\rho(x), \rho((P_N \mathbf{v})(x))$

Over-integration is ineffective without L^2 projection



(e) ($N + 1$) points

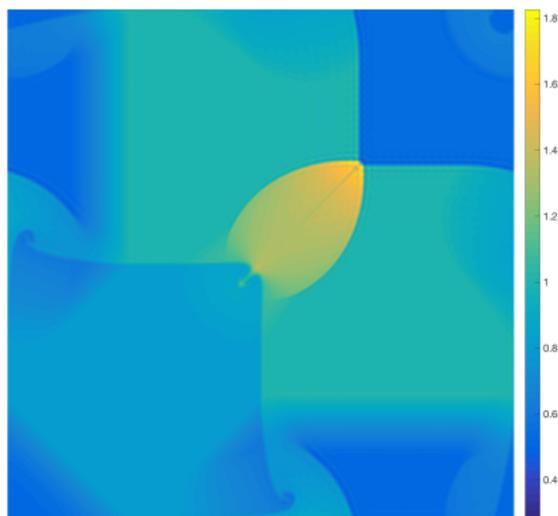


(f) ($N + 4$) points

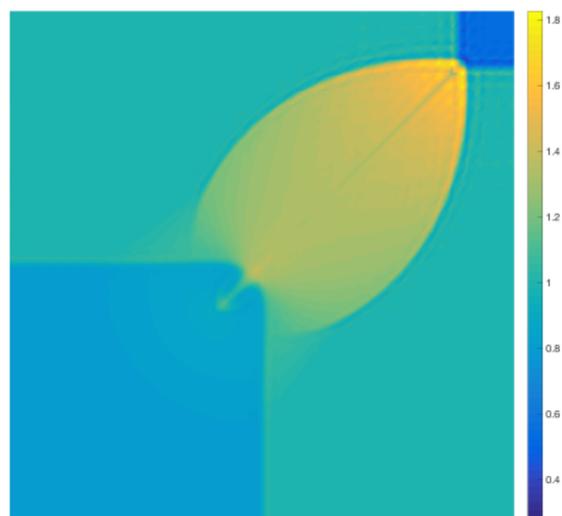
Figure: Numerical results for the Sod shock tube for $N = 4$ and $K = 32$ elements. Over-integrating by increasing the number of quadrature points does not improve solution quality.

2D Riemann problem

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

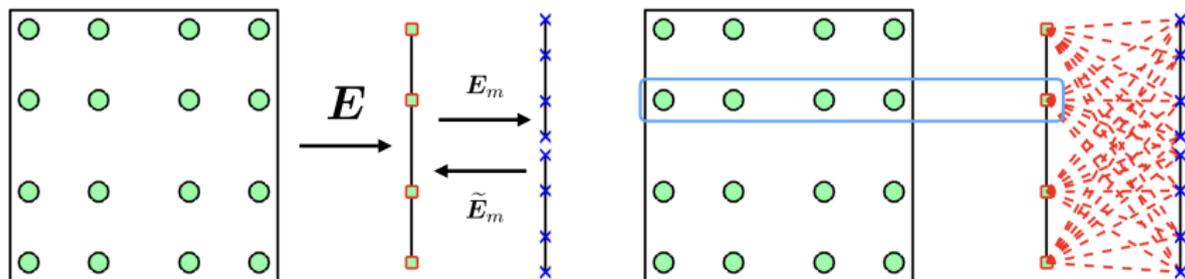


(a) $\Omega = [-1, 1]^2$



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

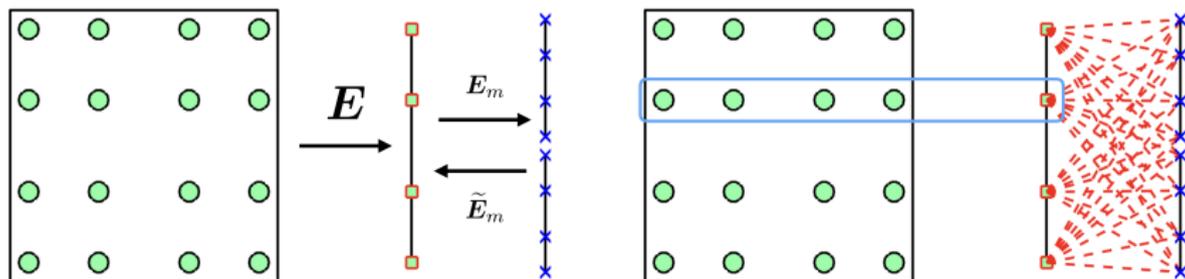
Non-conforming interfaces and SBP mortars



- Define appropriate interpolation operators $\mathbf{E}_m, \tilde{\mathbf{E}}_m$ between conforming and non-conforming (mortar) nodes.
- Modify the skew-symmetric formulation as follows:

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + \sum_{i=1}^d \begin{bmatrix} \mathbf{V}_q \\ \mathbf{V}_f \end{bmatrix}^T \begin{bmatrix} \mathbf{Q}_i - \mathbf{Q}_i^T & \mathbf{E}^T \mathbf{B}_i \\ -\mathbf{B}_i \mathbf{E} & \end{bmatrix} + \mathbf{E}^T \mathbf{B}_i \mathbf{f}_i^* = 0.$$

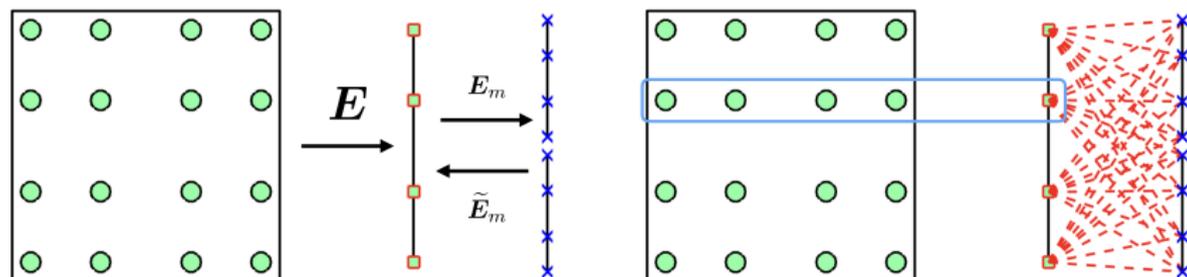
Non-conforming interfaces and SBP mortars



- Define appropriate interpolation operators $\mathbf{E}_m, \tilde{\mathbf{E}}_m$ between conforming and non-conforming (mortar) nodes.
- Modify the skew-symmetric formulation as follows:

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + \sum_{i=1}^d \begin{bmatrix} \mathbf{V}_q \\ \mathbf{V}_f \\ \mathbf{V}_m \end{bmatrix}^T \begin{bmatrix} \mathbf{Q}_i - \mathbf{Q}_i^T & \mathbf{E}^T \mathbf{B}_i \\ -\mathbf{B}_i \mathbf{E} & \mathbf{B}_i \tilde{\mathbf{E}}_m \\ & -\tilde{\mathbf{B}}_i \mathbf{E}_m \end{bmatrix} + \mathbf{V}_m^T \tilde{\mathbf{B}}_i \mathbf{f}_i^* = 0.$$

Non-conforming interfaces and SBP mortars



- Define appropriate interpolation operators $\mathbf{E}_m, \tilde{\mathbf{E}}_m$ between conforming and non-conforming (mortar) nodes.
- Rewrite as modification of numerical flux.

$$\tilde{\mathbf{f}}_i^* = \tilde{\mathbf{E}}_m \mathbf{f}_i^* + \left(\tilde{\mathbf{E}}_m \circ \mathbf{F}_S^{sm} \right) \mathbf{1} - \tilde{\mathbf{E}}_m \left(\mathbf{E}_m \circ \mathbf{F}_S^{ms} \right) \mathbf{1}$$