

# Entropy stable schemes based on high order modal discontinuous Galerkin formulations

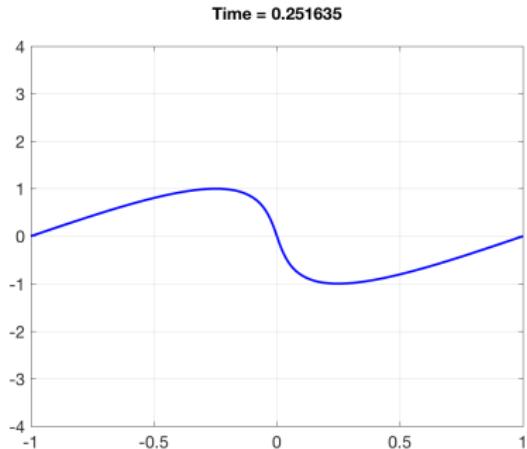
Jesse Chan

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

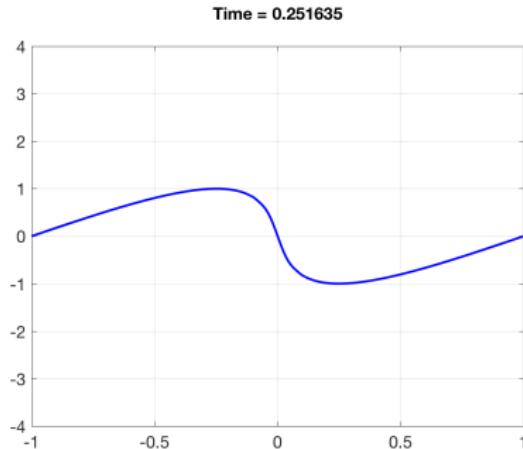
<sup>1</sup>Department of Computational and Applied Mathematics

Finite Elements in Flow, Chicago, Illinois  
April 3, 2019

# High order methods typically unstable for nonlinear PDEs



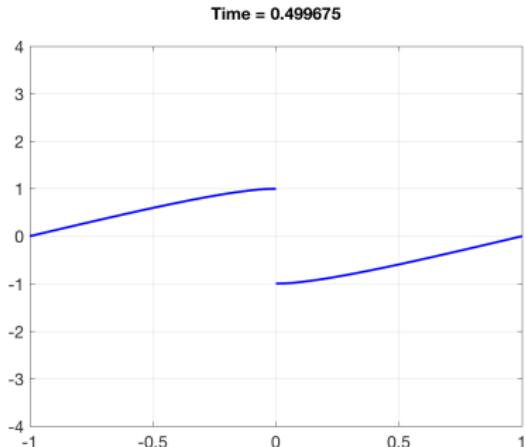
(a) Inviscid Burgers' solution



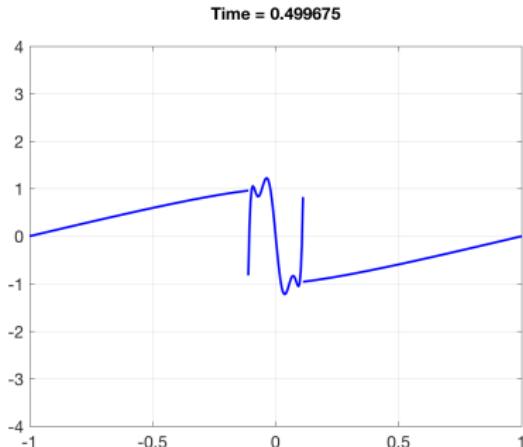
(b) 8th order DG

- 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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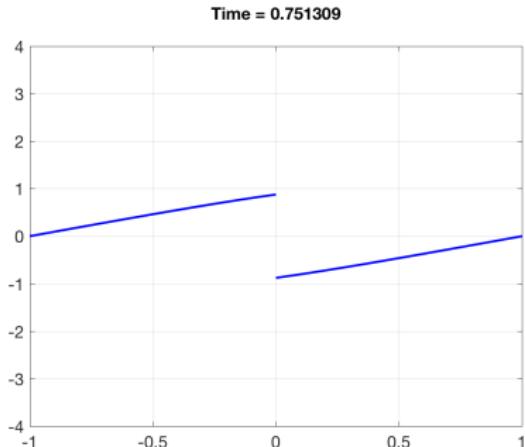
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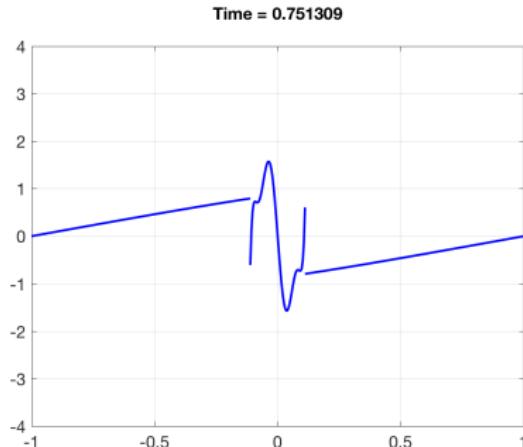
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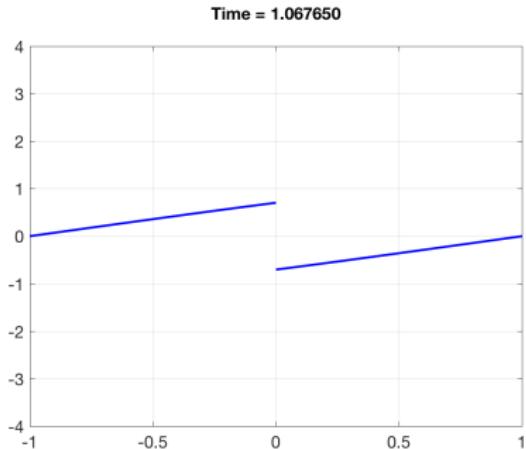
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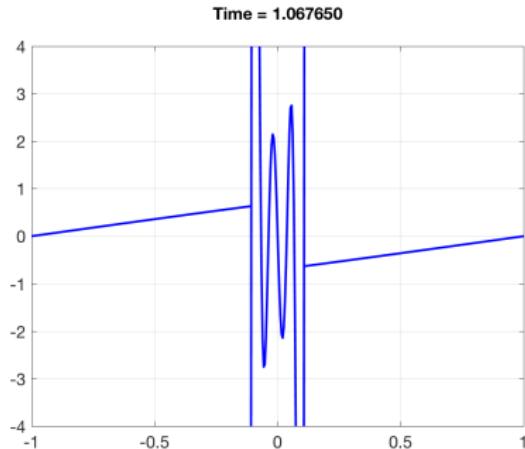
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# Entropy stability for nonlinear problems uses the chain rule

- 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”  $\psi(\mathbf{u})$ ,

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

- 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

# Talk outline

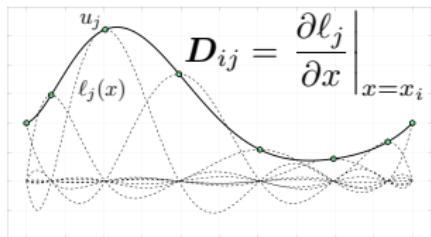
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# Nodal DG, summation-by-parts (SBP), flux differencing



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

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

$$\boxed{\mathbf{Q} = \mathbf{B} - \mathbf{Q}^T, \quad \mathbf{Q} = \mathbf{M}\mathbf{D}, \quad \mathbf{M} \text{ diagonal mass matrix.}}$$

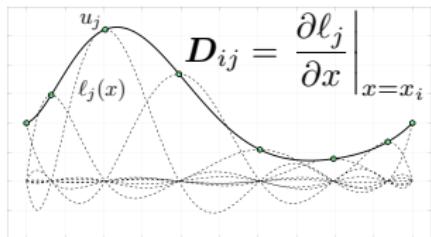
- Nodal “collocation” over a single element:

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + \mathbf{Q}\mathbf{f}(\mathbf{u}) = 0 \implies \mathbf{M}_{ii} \frac{d\mathbf{u}_i}{dt} + \sum_j \mathbf{Q}_{ij} \mathbf{f}(\mathbf{u}_j) = 0.$$

- Let  $\mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_j) = \frac{1}{2} (\mathbf{f}(\mathbf{u}_i) + \mathbf{f}(\mathbf{u}_j)) = (\mathbf{F}_S)_{ij}$ . Collocation equiv. to

$$\mathbf{M}_{ii} \frac{d\mathbf{u}_i}{dt} + \sum_j \mathbf{Q}_{ij} 2\mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_j) = 0 \implies \boxed{\mathbf{M} \frac{d\mathbf{u}}{dt} + 2(\mathbf{Q} \circ \mathbf{F}_S)\mathbf{1} = 0.}$$

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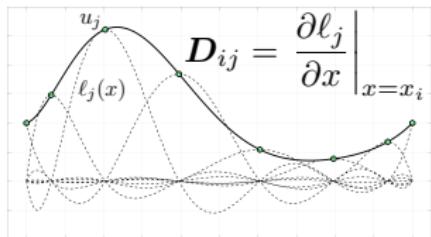
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# Entropy stable schemes: a brief derivation

- 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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- 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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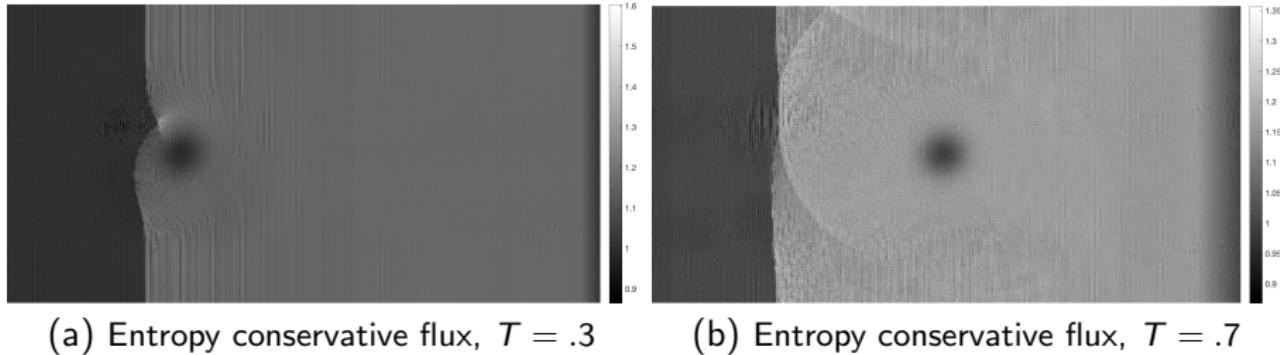


Figure: Compressible Euler shock vortex interaction:  $200 \times 100$  degree  $N = 4$  elements, 4th order **explicit** RK time-stepping, no limiters or artificial viscosity.

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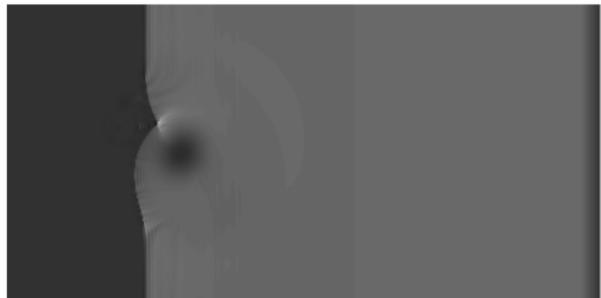
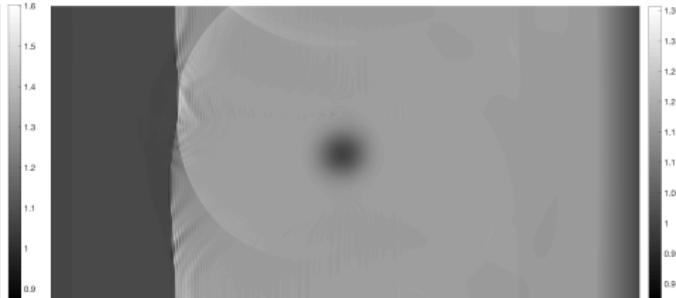
(a) Local Lax-Friedrichs flux,  $T = .3$ (b) Local Lax-Friedrichs flux,  $T = .7$ 

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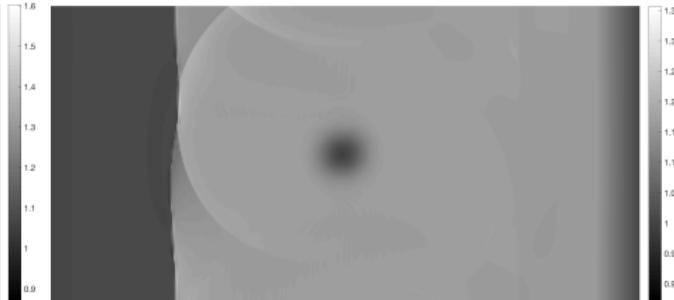
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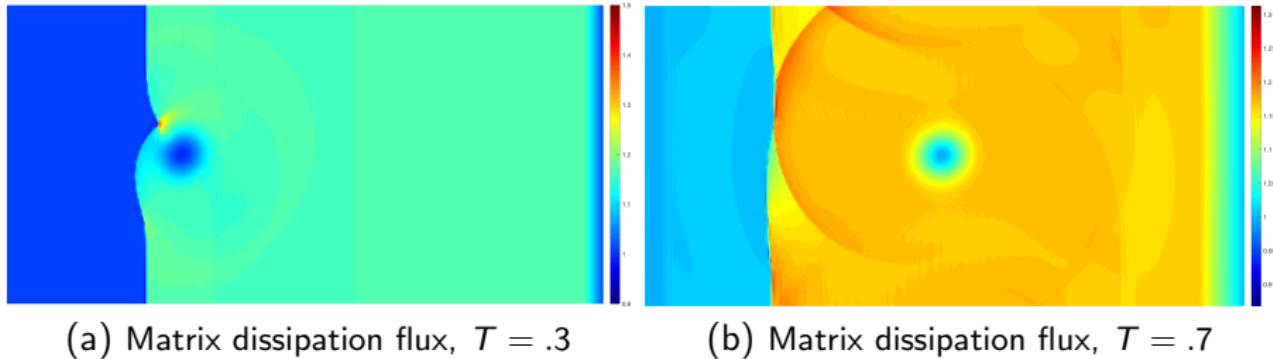


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# Talk outline

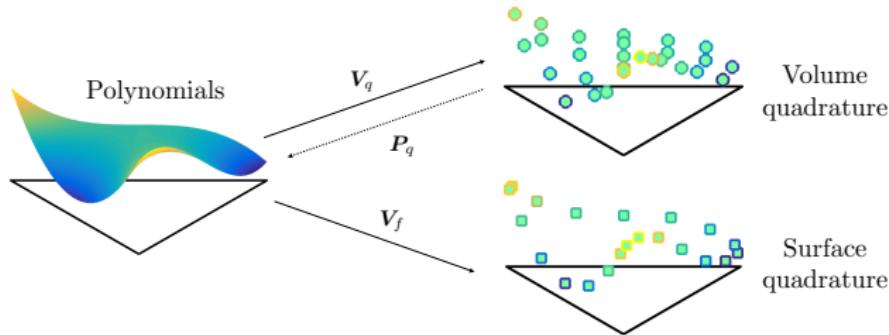
1 Entropy stable nodal DG and summation-by-parts

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# Modal formulations: general bases and quadrature



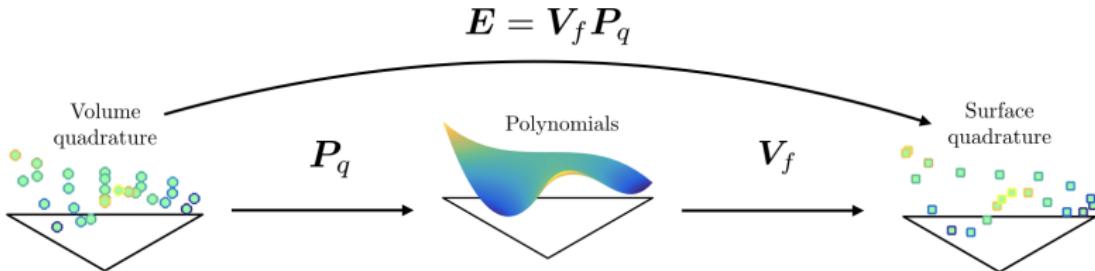
- Assume degree  $2N$  volume + surface quadratures  $(\mathbf{x}_i^q, \mathbf{w}_i^q)$ ,  $(\mathbf{x}_i^f, \mathbf{w}_i^f)$ , and basis functions  $\phi_i(\mathbf{x})$ . Define interpolation and weight matrices

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

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

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

# Quadrature-based “finite difference” matrices



- Matrix  $D_q^i$ : evaluates  $i$ th derivative of  $L^2$  projection  $P_N$  at  $x^q$ .

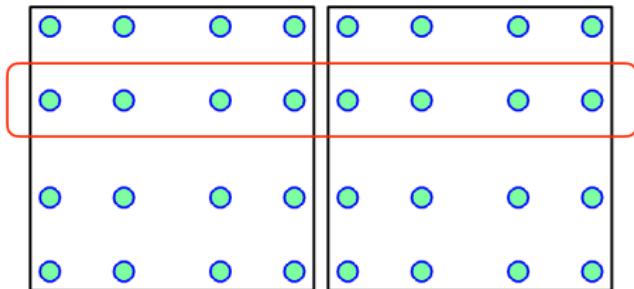
$$D_q^i = V_q D^i P_q, \quad D^i \text{ exactly differentiates polynomials.}$$

- 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



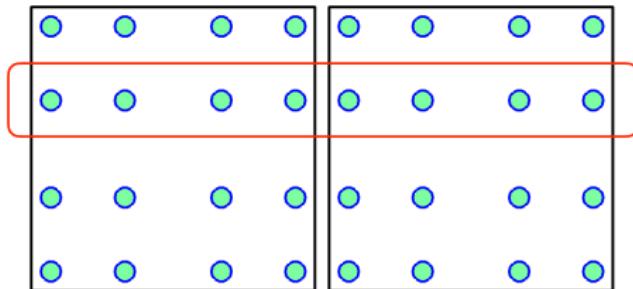
Coupling between quadrature nodes on neighboring elements.

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

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

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

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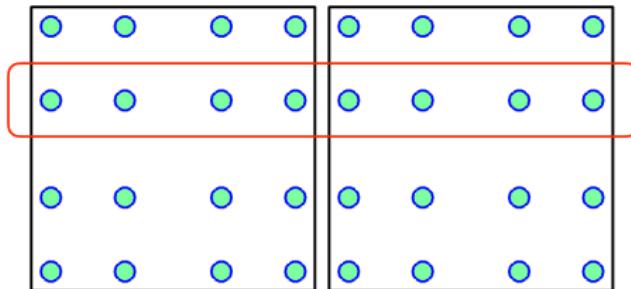
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- The presence of the interpolation matrix  $\boldsymbol{E}$  increases inter-element coupling, complicates imposition of BCs.

# 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

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

- $\mathbf{Q}_N$  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

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

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

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

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

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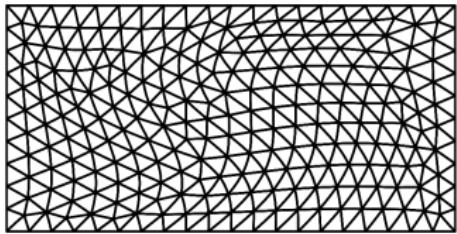
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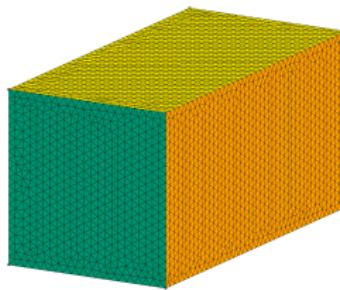
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# Smooth isentropic vortex and curved meshes in 2D/3D



(a) 2D triangular mesh



(b) 3D tetrahedral mesh

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

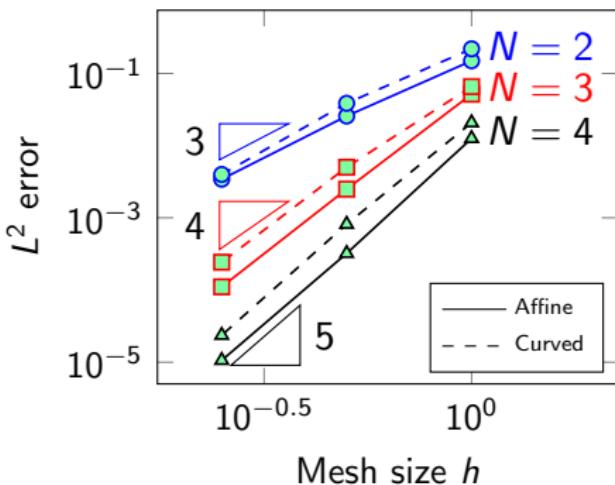
$$J \frac{\partial u}{\partial x_i} = \sum_{j=1}^d J \frac{\partial \hat{x}_j}{\partial x_i} \frac{\partial u}{\partial \hat{x}_j} = \frac{1}{2} \sum_{j=1}^d \left( J \frac{\partial \hat{x}_j}{\partial x_i} \frac{\partial u}{\partial \hat{x}_j} + \frac{\partial}{\partial \hat{x}_j} \left( J \frac{\partial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

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

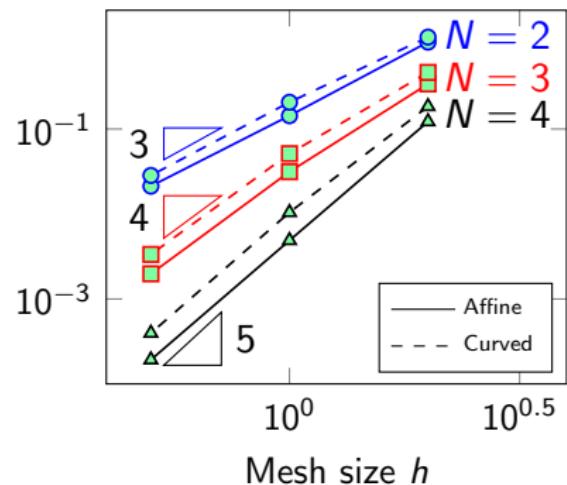
Visbal and Gaitonde (2002). On the Use of Higher-Order Finite-Difference Schemes on Curvilinear and Deforming Meshes.

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# 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.

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# Inviscid Taylor-Green vortex

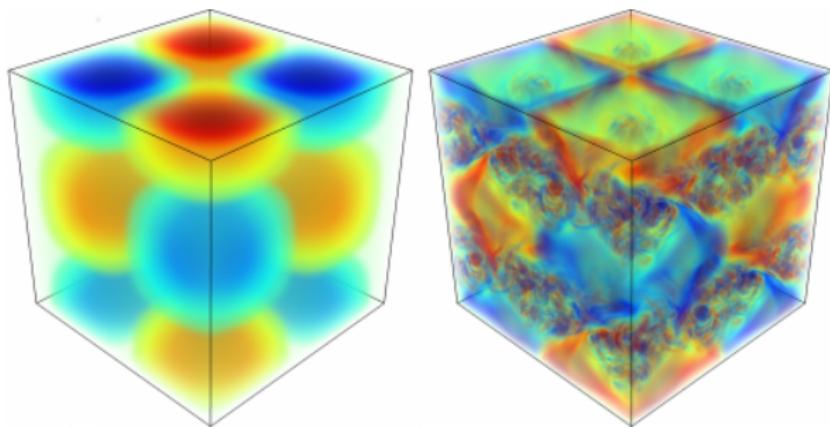
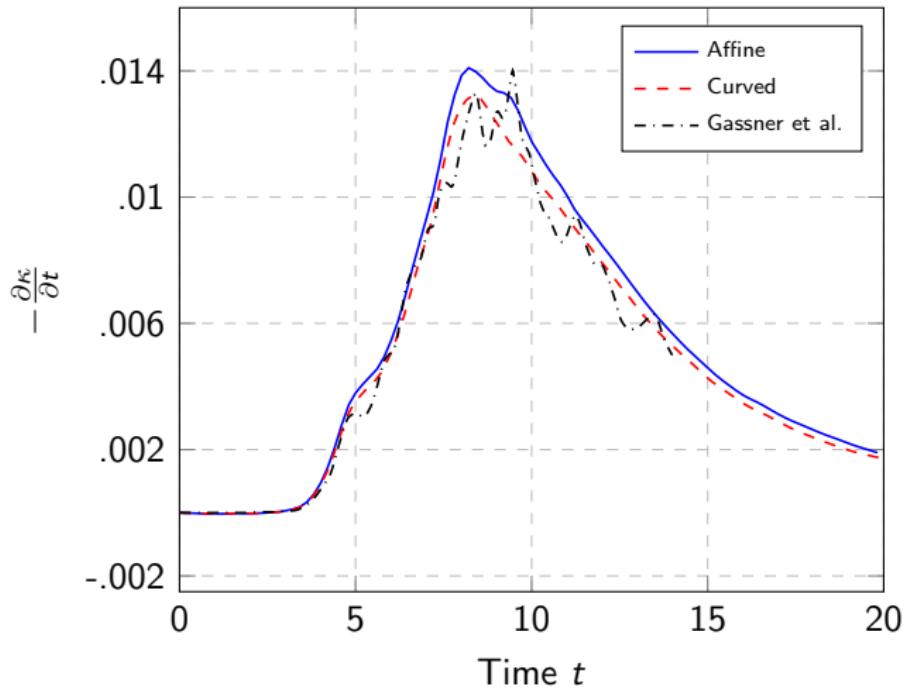


Figure: Isocontours of  $z$ -vorticity for Taylor-Green at  $t = 0, 10$  seconds.

- 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

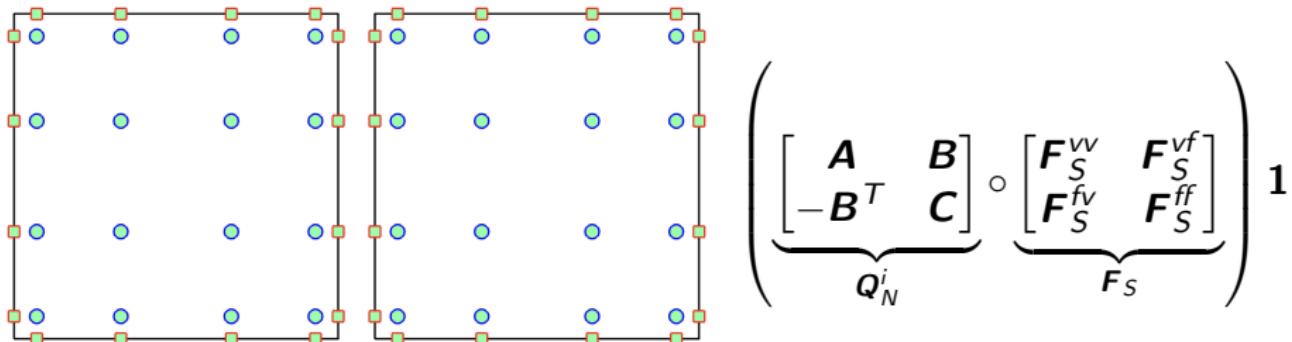


Kinetic energy dissipation rate  $-\frac{\partial\kappa}{\partial t}$  for  $N = 3, h = \pi/8, \text{CFL} = .25$  (tet meshes).

# Talk outline

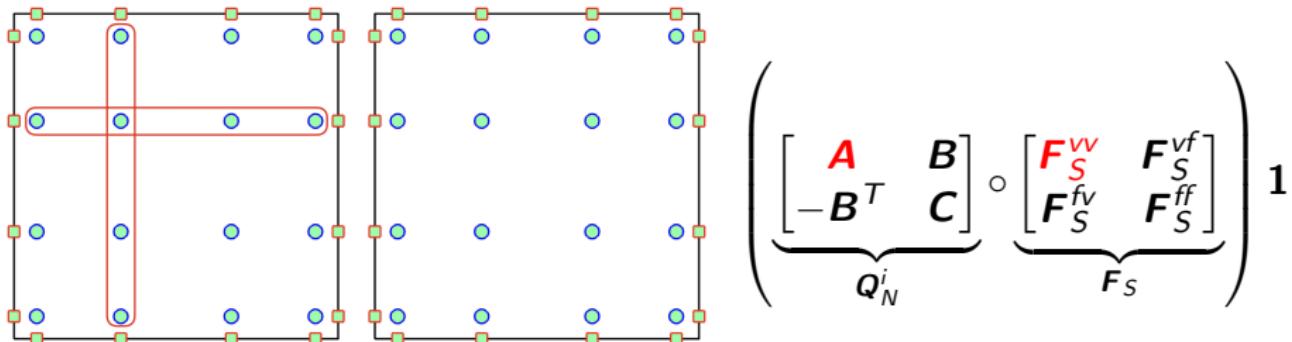
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# Entropy stable Gauss collocation: main steps



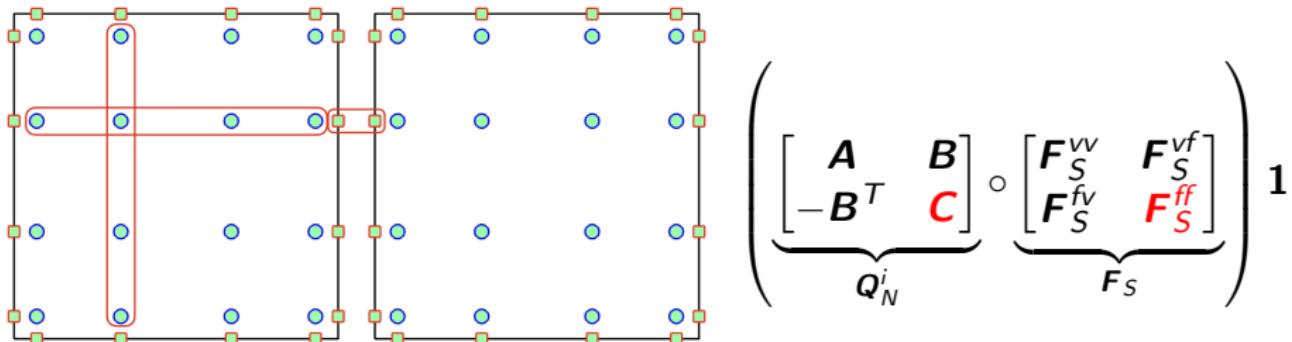
- Advantage of hexahedra vs. tetrahedra: tensor product structure.
- $(N + 1)$ -point Gauss quadrature reduces to a **collocation scheme**.
- Reduces computational costs from  $O(N^6)$  to  $O(N^4)$  in 3D.

# Entropy stable Gauss collocation: main steps



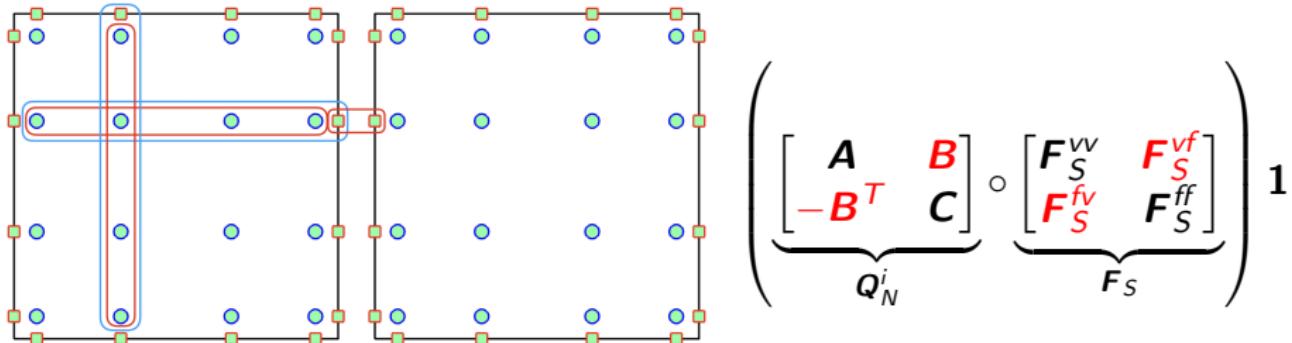
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# Gauss quadrature improves errors on curved meshes

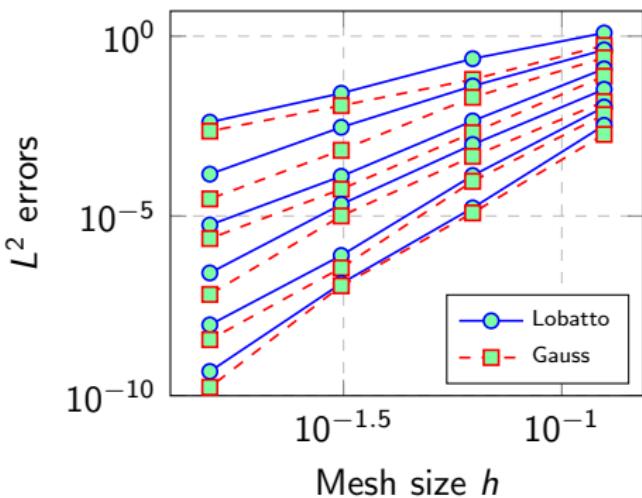
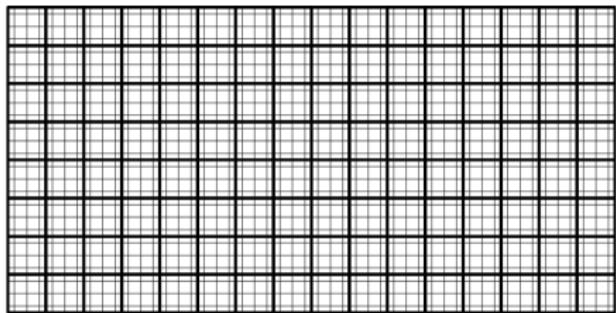


Figure:  $L^2$  errors for the 2D isentropic vortex at time  $T = 5$  for degree  $N = 2, \dots, 7$  Lobatto and Gauss collocation schemes (similar behavior in 3D).

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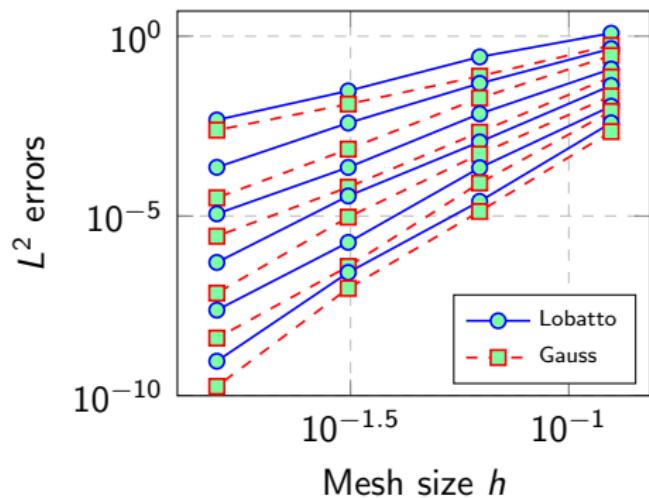
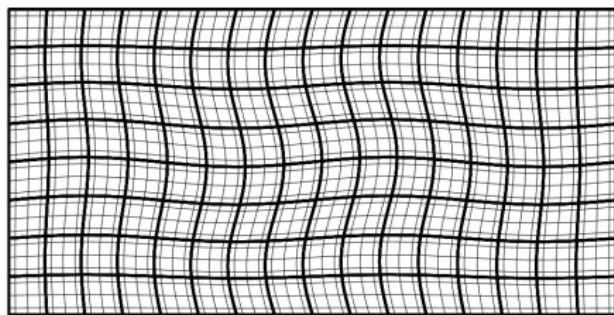


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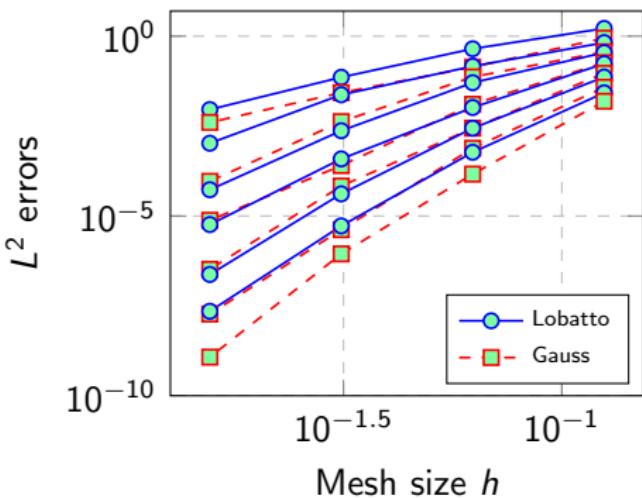
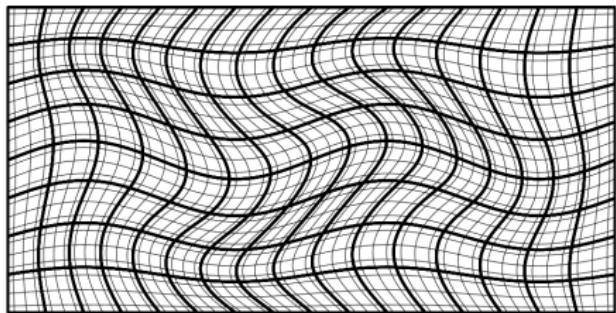


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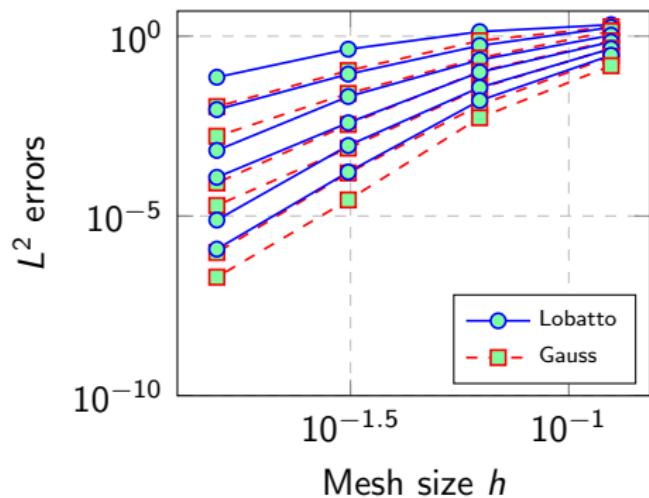
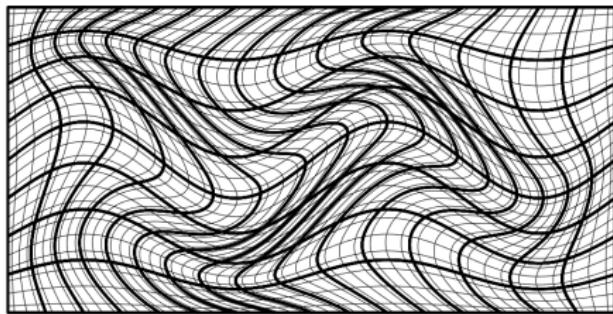
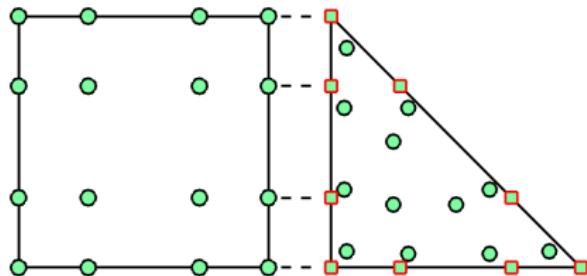


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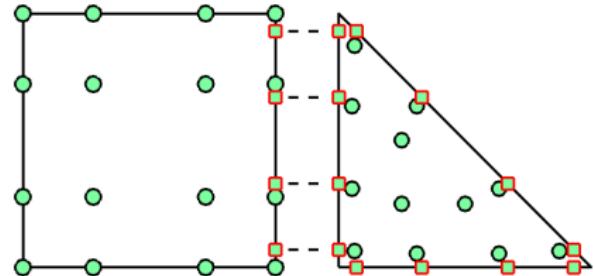
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# Mixed quadrilateral-triangle meshes



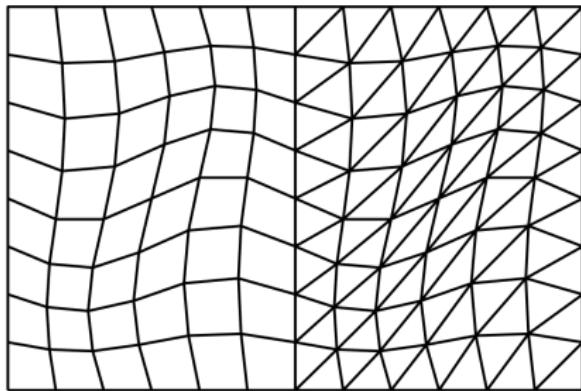
(a) No SBP (tri. under-integrated)



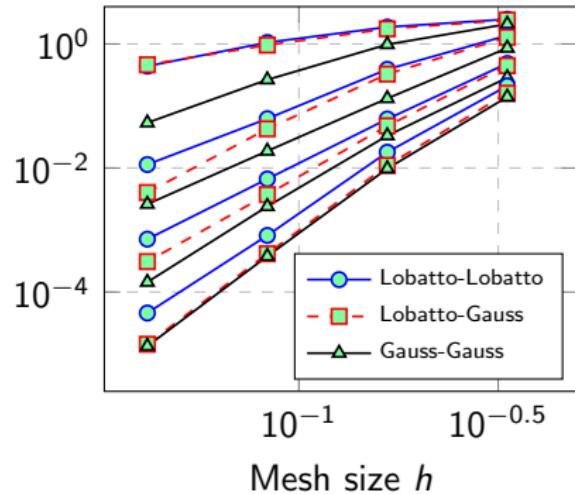
(b) No SBP (quad. under-integrated)

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

# Numerical results: mixed triangle-quadrilateral meshes

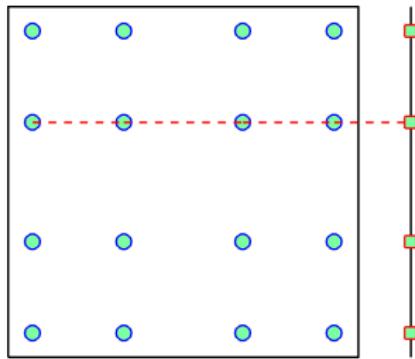


(a) Coarse hybrid mesh

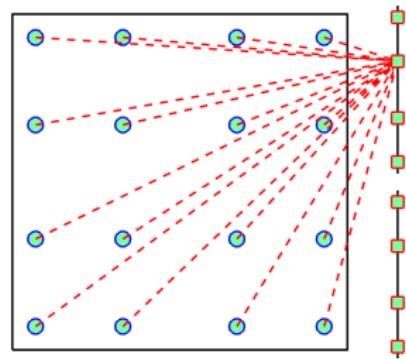
(b)  $L^2$  errors for  $N = 1, 2, 3, 4$ 

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

# Non-conforming interfaces



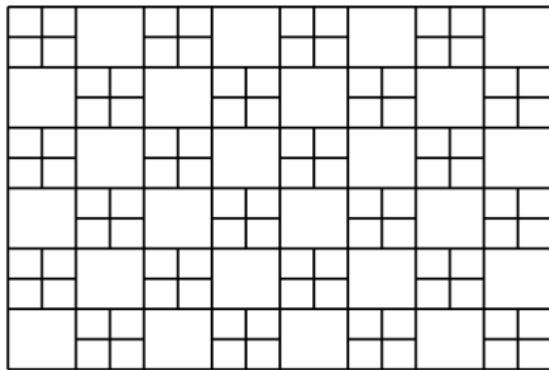
(a) Conforming surface quadrature nodes



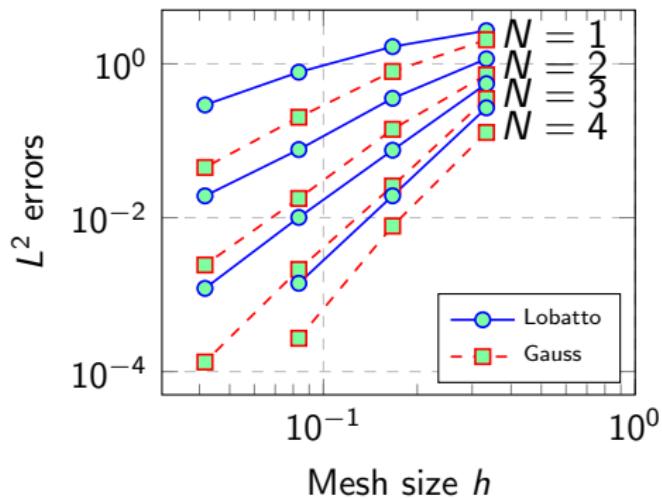
(b) Non-conforming surface nodes

- 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?



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

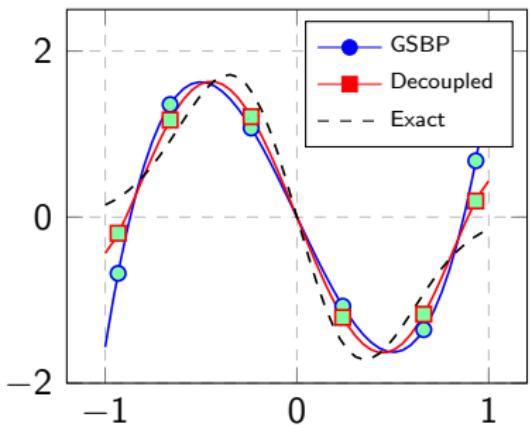
Chan, Del Rey Fernandez, Carpenter (2018). *Efficient entropy stable Gauss collocation methods*.

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

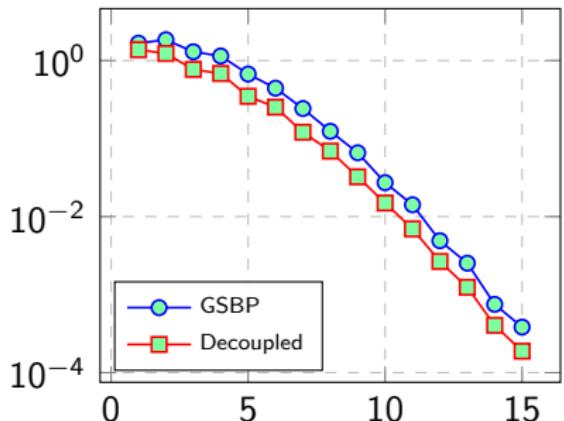
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# Additional slides

# 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  $u(\mathbf{x}) \approx f \frac{\partial g}{\partial \mathbf{x}}$ .

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

# 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

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

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

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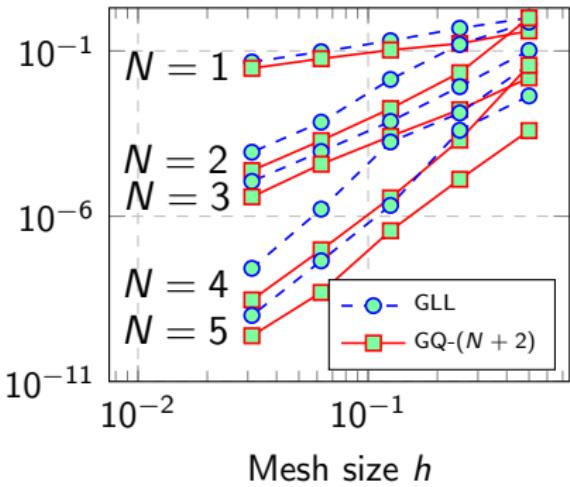
- Recovering the Burgers' split formulation

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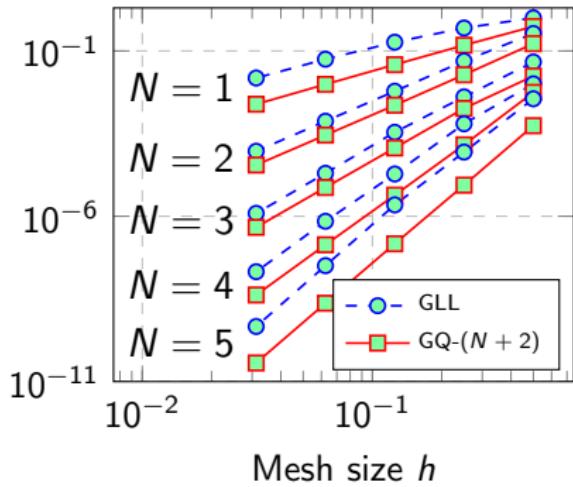
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# 1D compressible Euler equations

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



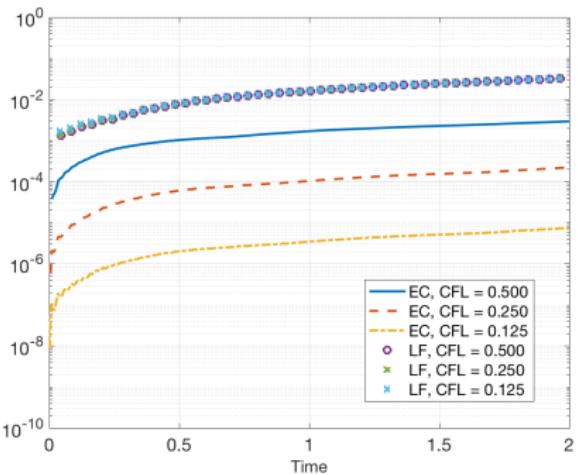
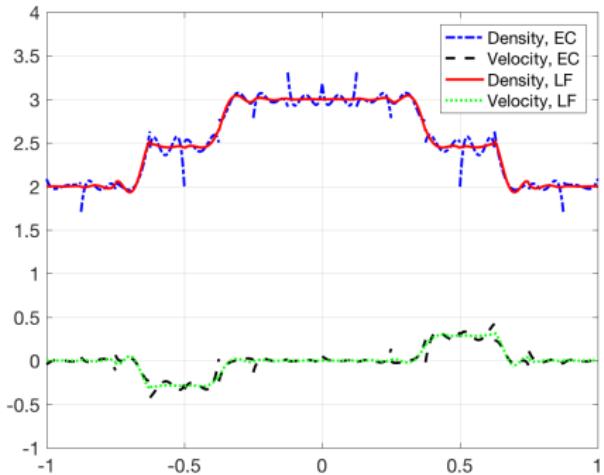
(c) Entropy conservative flux



(d) With Lax-Friedrichs penalization

# Conservation of entropy: semi-discrete vs. fully discrete

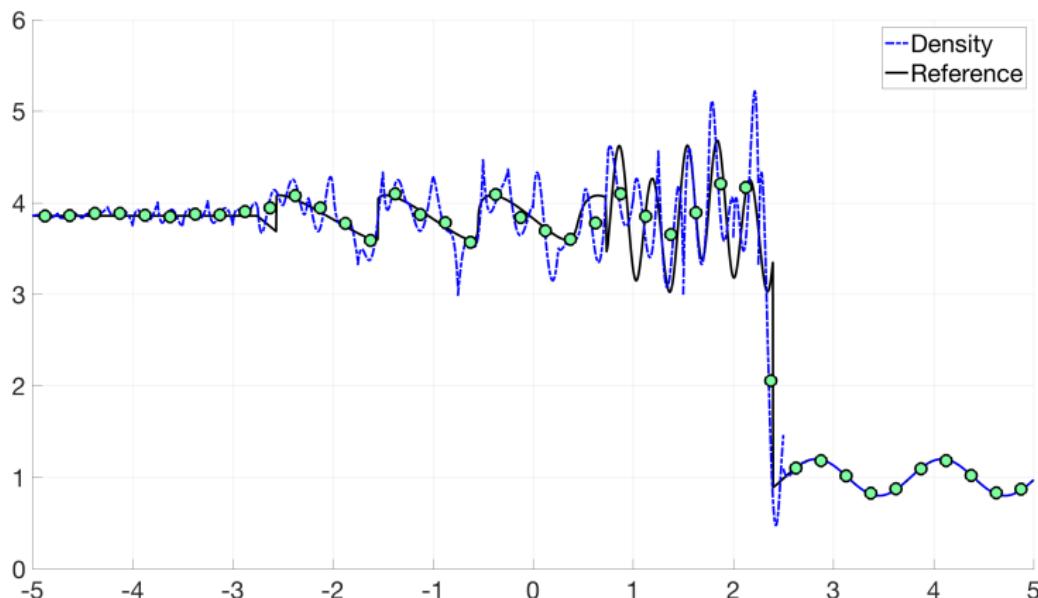
$$\Delta S(\mathbf{u}) = |S(\mathbf{u}(x, t)) - S(\mathbf{u}(x, 0))| \rightarrow 0 \text{ as } \Delta t \rightarrow 0.$$

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

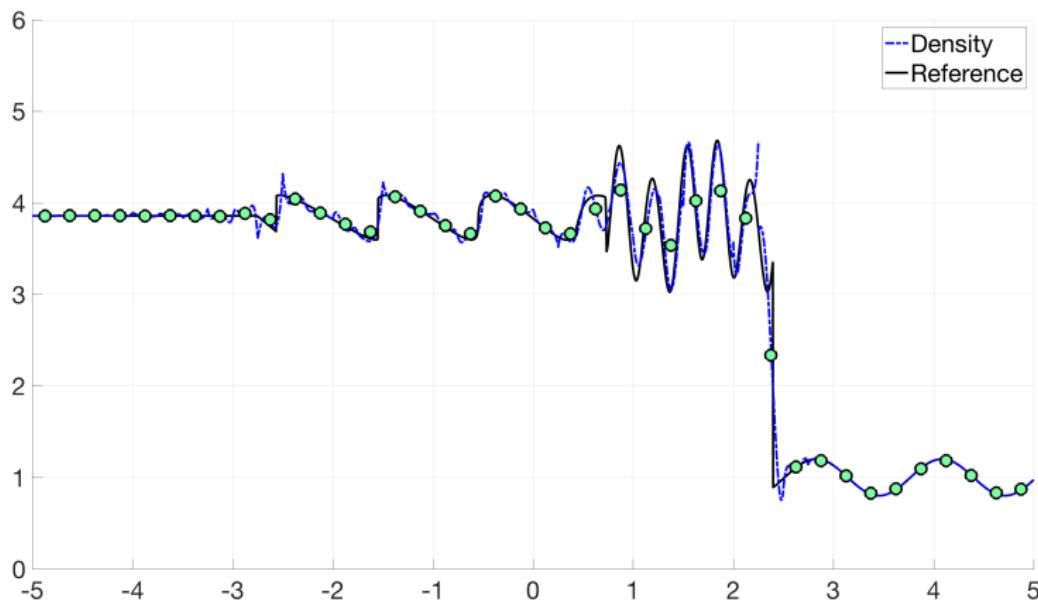
- $(N + 2)$ -point Gauss needs a smaller CFL (.05 vs .125) for stability.



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

# 1D sine-shock interaction

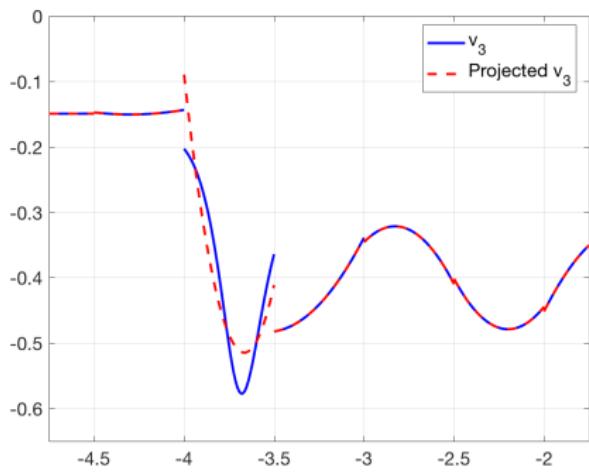
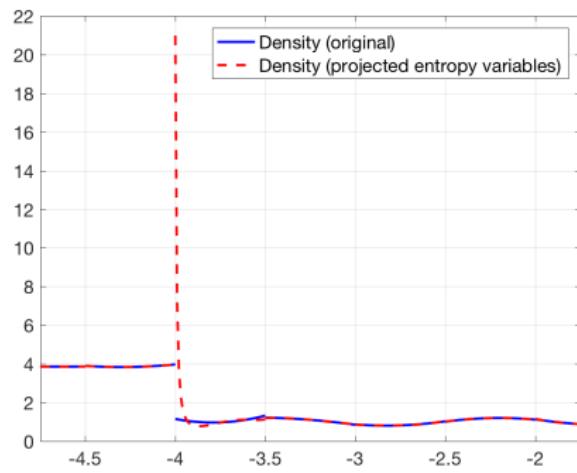
- $(N + 2)$ -point Gauss needs a smaller CFL (.05 vs .125) for stability.



$N = 4, K = 40, \text{CFL} = .05, (N + 2)$  point Gauss 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

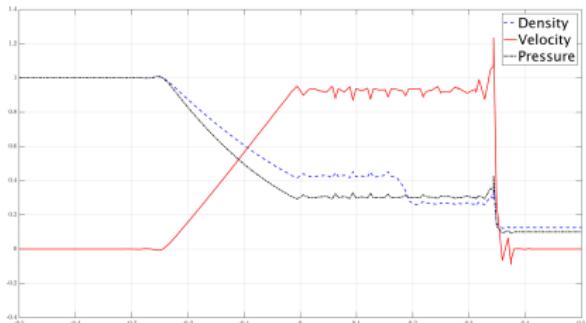
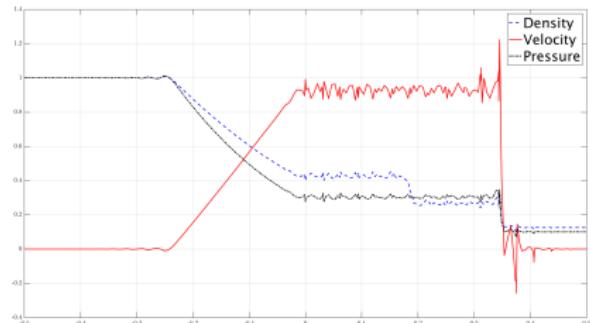
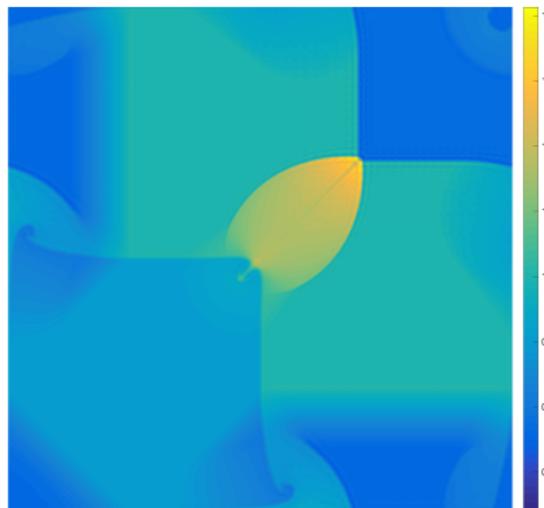
(e)  $(N + 1)$  points(f)  $(N + 4)$  points

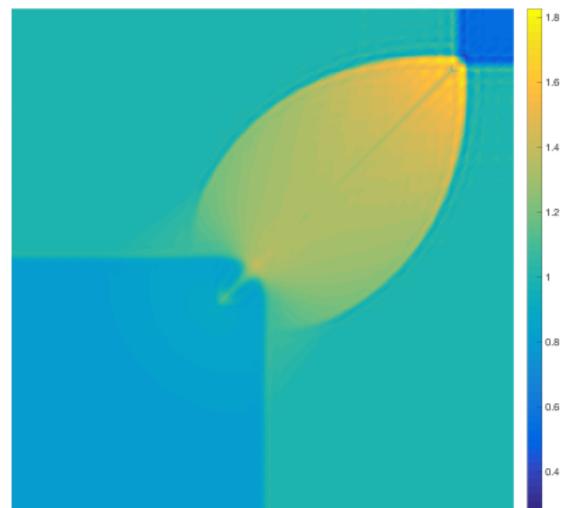
Figure: Numerical results for the Sod shock tube for  $N = 4$  and  $K = 32$  elements. Over-integrating by increasing the number of quadrature points does not improve solution quality.

# 2D Riemann problem

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

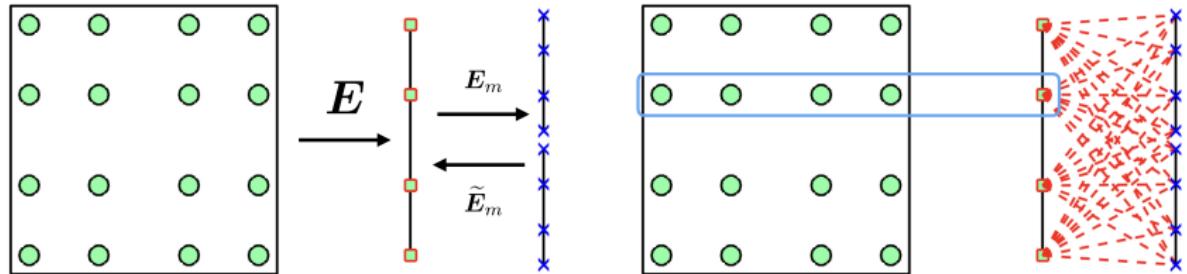


(a)  $\Omega = [-1, 1]^2$



(b)  $\Omega = [-0.5, 0.5]^2$ ,  $32 \times 32$  elements

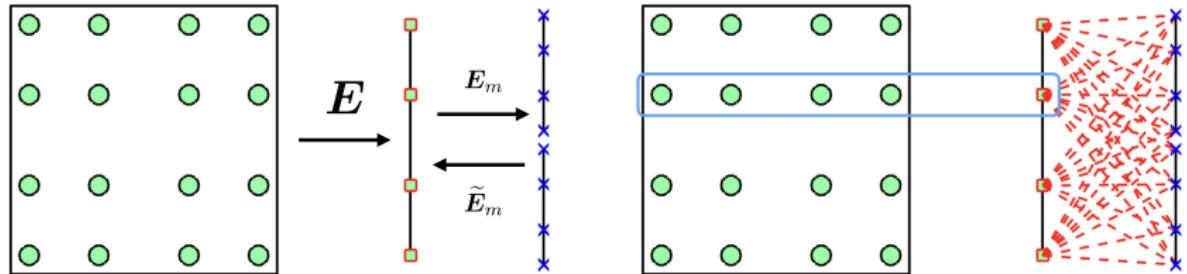
# Non-conforming interfaces and SBP mortars



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

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

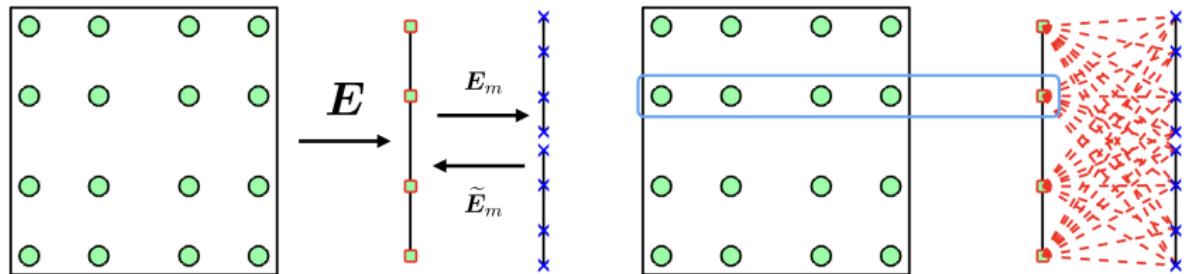
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# Non-conforming interfaces and SBP mortars



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

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