

Entropy stable schemes for nonlinear conservation laws: high order discontinuous Galerkin methods and reduced order modeling

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Collaborators



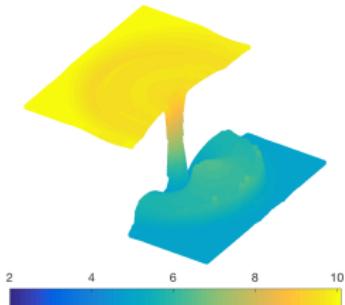
Lucas Wilcox
(NPS)



DCDR Fernandez
(NASA Langley)



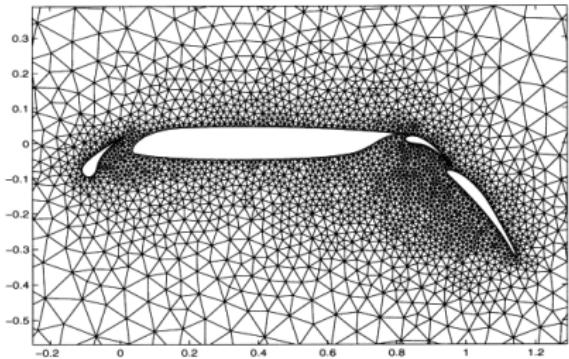
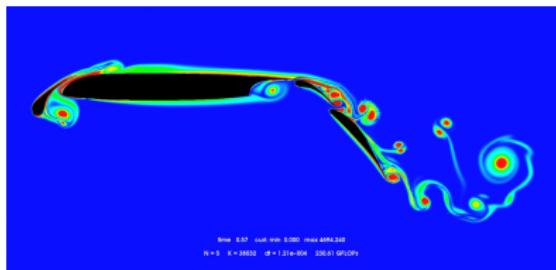
Mark Carpenter
(NASA Langley)



Philip Wu (PhD, shallow water + GPU)

High order finite element methods for hyperbolic PDEs

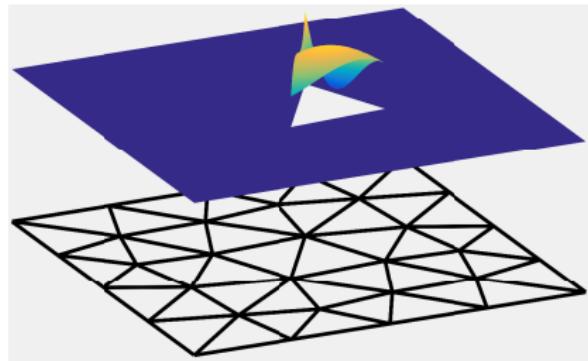
- Aerodynamics applications:
acoustics, vorticular flows,
turbulence, shocks.
- Goal: **accurate** simulations on
unstructured meshes.
- Discontinuous Galerkin (DG)
methods: geometric flexibility,
high order accuracy.



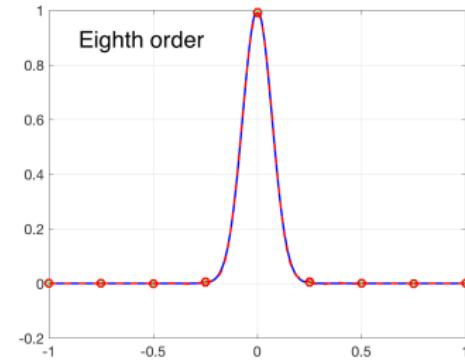
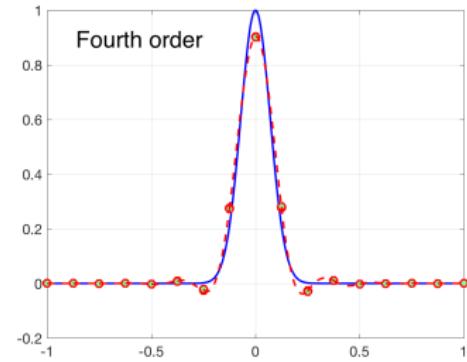
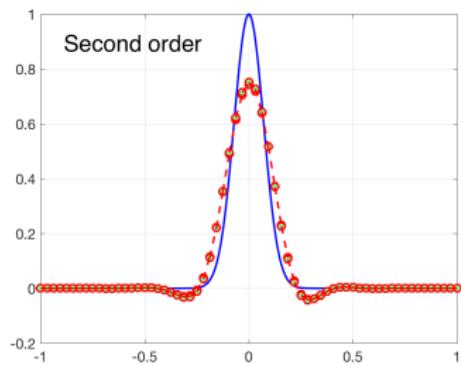
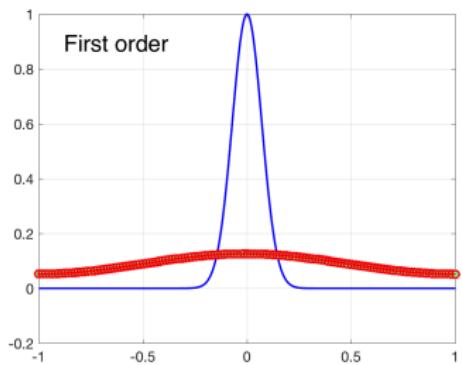
Mesh from Slawig 2001.

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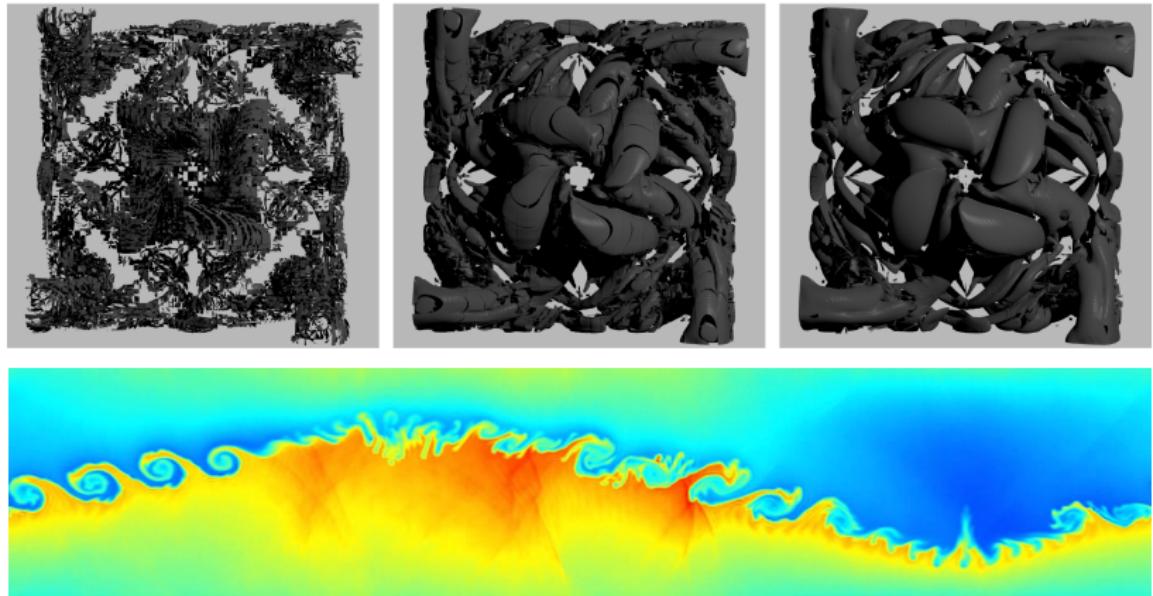


Why high order accuracy?



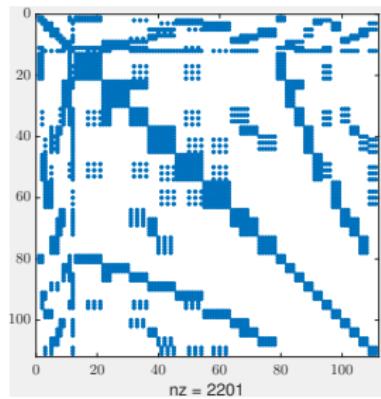
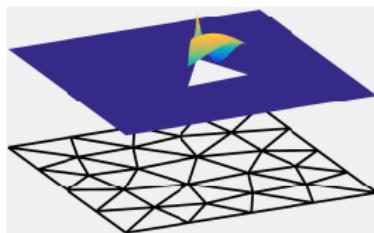
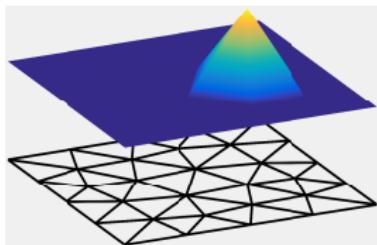
High order accurate resolution of propagating vortices and waves.

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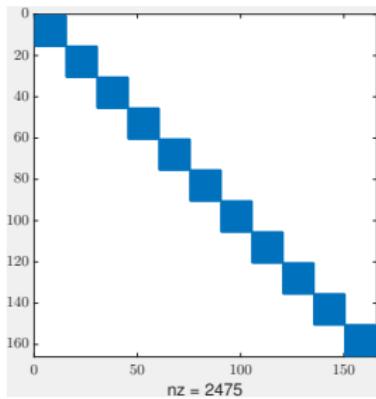


2nd, 4th, and 16th order Taylor-Green (top), 8th order Kelvin-Helmholtz (bottom). Vorticicular structures and acoustic waves are both sensitive to numerical dissipation. Results from Beck and Gassner (2013) and Per-Olof Persson's website.

Why discontinuous Galerkin methods?



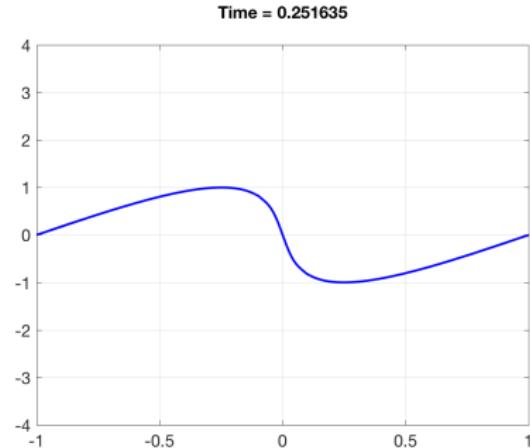
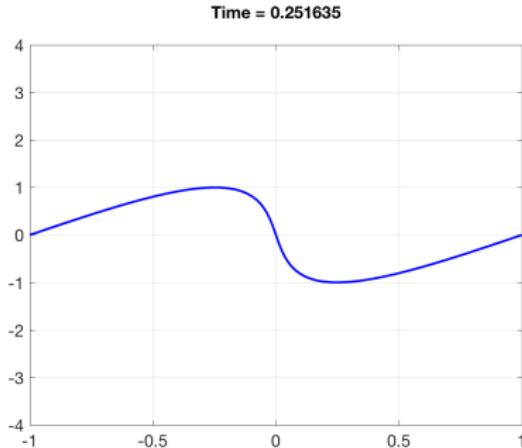
(a) High order FEM



(b) High order DG

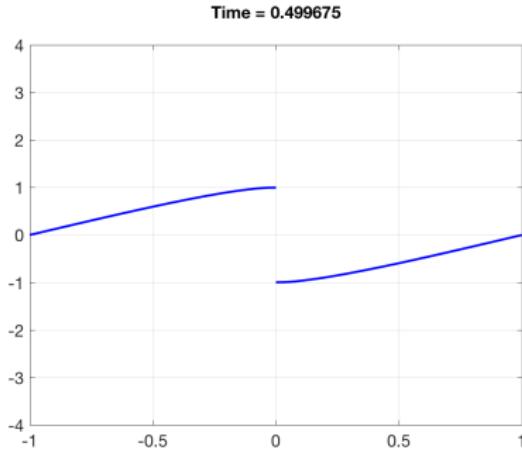
The DG mass matrix is easily invertible for explicit time-stepping.

Why *not* high order DG methods?

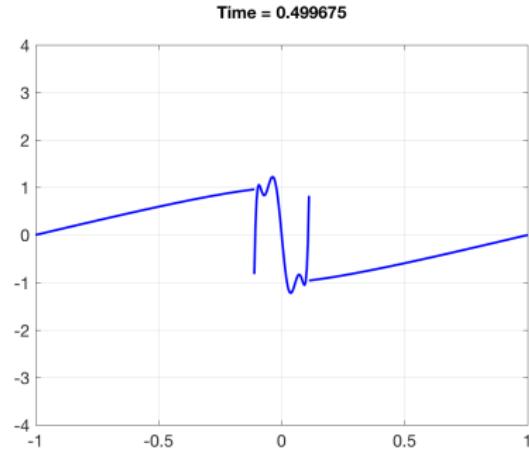


- High order methods blow up for under-resolved solutions of **nonlinear conservation laws** (e.g., shocks and turbulence).
- Instability tied to loss of the **chain rule + quadrature error**.

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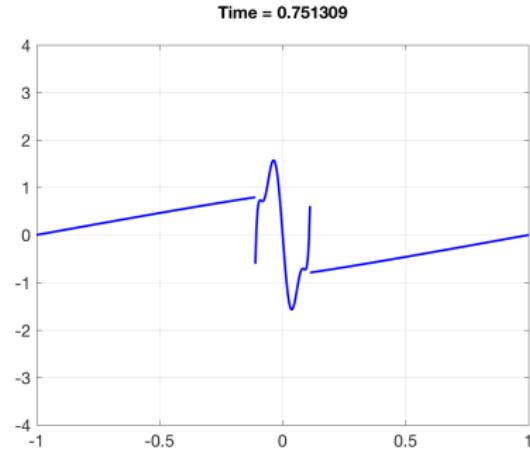
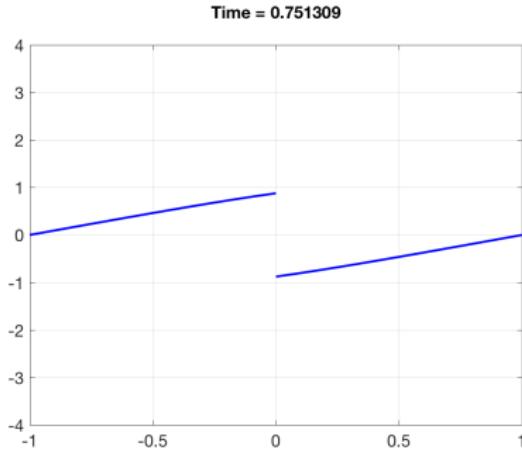
(a) Exact solution



(b) 8th order DG

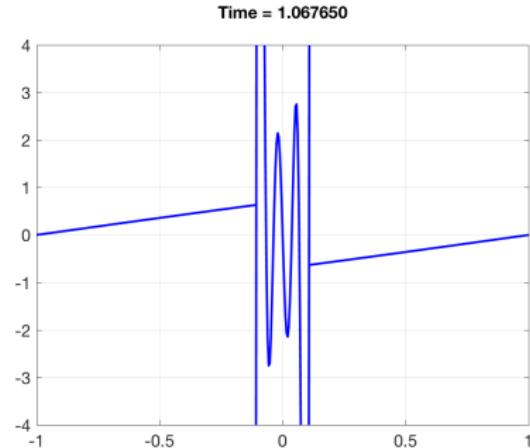
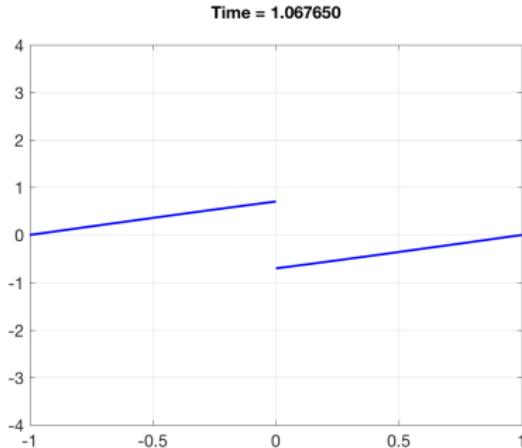
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Entropy stability for nonlinear problems

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

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

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

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

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

Talk outline

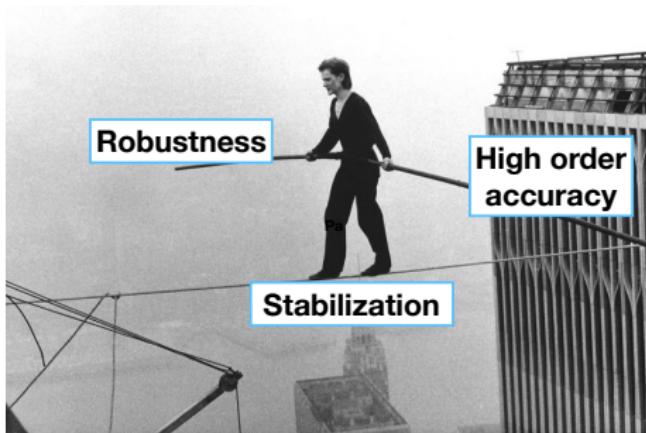
- 1 Entropy stable nodal summation-by-parts (SBP) schemes
- 2 Modal entropy stable DG formulations
- 3 Applications of modal formulations
 - Triangles and tetrahedra: full integration
 - Quad and hex meshes: new collocation schemes
 - Reduced order modeling

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Discretely entropy stable schemes

Goal: improve robustness by enforcing a discrete entropy inequality.



- Aim for stability independently of artificial viscosity, limiters.
- *Mechanical* approach to stability based on algebraic discretization properties.

Image adapted from "Man On Wire" (2008)

Finite volume methods: Tadmor, Chandrashekhar, Ray, Svard, Fjordholm, Mishra, LeFloch, Rohde, ...

High order tensor product elements: Fisher, Carpenter, Gassner, Winters, Kopriva, Hindenlang, Persson, Pazner, ...

High order general elements: Chen and Shu, Crean, Hicken, DCDR Fernandez, Zingg, ...

Discretely entropy stable schemes: main ideas

- Continuous and semi-discrete systems

$$\boxed{\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} - \epsilon \frac{\partial^2 \mathbf{u}}{\partial x^2} = 0} \quad \Rightarrow \quad \boxed{\mathbf{M} \frac{d\mathbf{u}}{dt} + \mathbf{f}_x(\mathbf{u}) + \epsilon \mathbf{d}(\mathbf{u}) = \mathbf{0}}$$

- Test with discrete entropy variables, use chain rule in time

$$\underbrace{\mathbf{v}^T \mathbf{M} \frac{d\mathbf{u}}{dt}}_{\mathbf{1}^T \mathbf{M} \frac{dS(\mathbf{u})}{dt}} + \mathbf{v}^T \mathbf{f}_x(\mathbf{u}) + \epsilon \mathbf{v}^T \mathbf{d}(\mathbf{u}) = 0$$

- Construct discretization s.t. (for periodic boundary conditions)

$$\boxed{\begin{aligned} \mathbf{v}^T \mathbf{f}_x(\mathbf{u}) &= 0 \\ \mathbf{v}^T \mathbf{d}(\mathbf{u}) &\geq 0 \end{aligned}} \quad \Rightarrow \quad \mathbf{1}^T \mathbf{M} \frac{dS(\mathbf{u})}{dt} = -\epsilon \mathbf{v}^T \mathbf{d}(\mathbf{u}) \leq 0.$$

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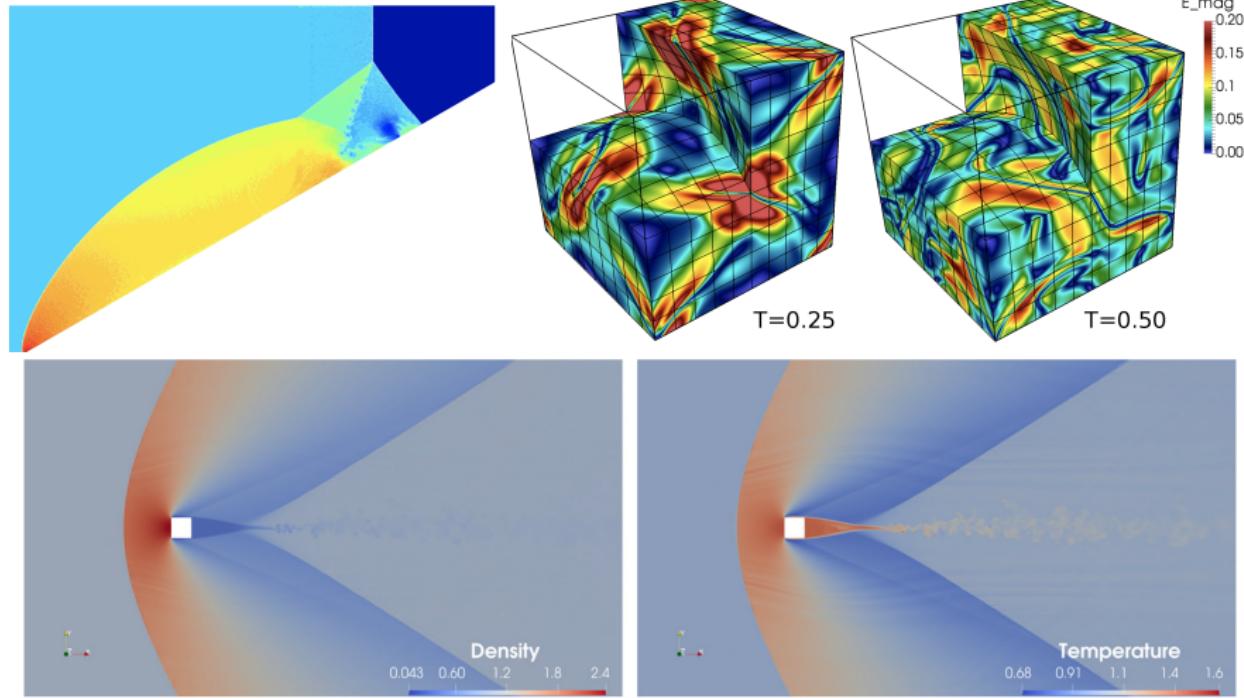
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Examples of high order entropy stable simulations

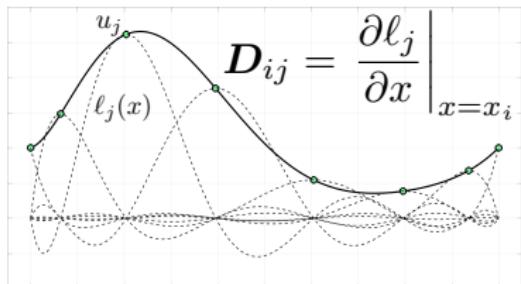


Chen, Shu (2017). *Entropy stable high order DG methods with suitable quadrature rules for hyperbolic conservation laws*.

Bohm et al. (2019). *An entropy stable nodal DG method for the resistive MHD equations. Part I*.

Dalcin et al. (2019). *Conservative and entropy stable solid wall BCs for the compressible NS equations*.

Nodal DG, summation-by-parts, flux differencing



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

- Nodal differentiation matrix \mathbf{D} has zero row sums

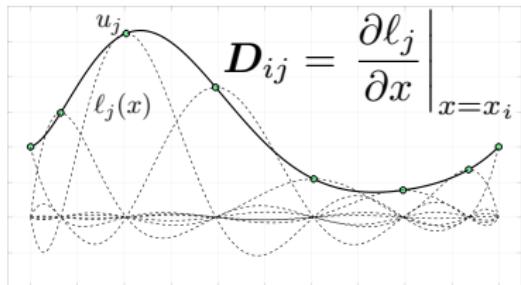
$$\mathbf{D}\mathbf{1} = 0 \quad \Rightarrow \quad \sum_j \mathbf{D}_{ij} = 0, \quad (\text{exact for constants})$$

- Lobatto nodes mimic integration by parts (summation-by-parts)

$$\mathbf{Q} = \mathbf{MD}, \quad \mathbf{M} \text{ diag. mass matrix,}$$

$$\boxed{\mathbf{Q} = \mathbf{B} - \mathbf{Q}^T}.$$

Nodal DG, summation-by-parts, flux differencing



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- Nodal “collocation” over a single element:

$$\int \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} v(x) \approx \mathbf{Q} \mathbf{f}(\mathbf{u}) \quad \Rightarrow \quad \sum_j \mathbf{Q}_{ij} \mathbf{f}(\mathbf{u}_j).$$

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

$$\sum_j \mathbf{Q}_{ij} \mathbf{f}(\mathbf{u}_j) = \sum_j \mathbf{Q}_{ij} 2\mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_j) \quad \Rightarrow \quad \boxed{2(\mathbf{Q} \circ \mathbf{F}) \mathbf{1} = 0.}$$

Flux differencing and entropy conservative fluxes

- Applying a difference matrix \mathbf{Q} to $\mathbf{f}(\mathbf{u})$ can be interpreted as **flux differencing** on a central flux

$$\boxed{\mathbf{Q}\mathbf{f}(\mathbf{u})} \iff \boxed{2(\mathbf{Q} \circ \mathbf{F})\mathbf{1} = 0}, \quad \text{if } \mathbf{F}_{ij} = \frac{1}{2} (\mathbf{f}(\mathbf{u}_i) + \mathbf{f}(\mathbf{u}_j)).$$

- Main idea: use Tadmor's entropy conservative numerical flux for \mathbf{f}_S

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

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

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

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Entropy stable nodal DG: a brief summary

- If \mathbf{Q} satisfies $\mathbf{Q}\mathbf{1} = \mathbf{0}$ and the **summation-by-parts (SBP)** property, then the following (local) formulation is entropy *conservative*

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + 2(\mathbf{Q} \circ \mathbf{F}) \mathbf{1} + \mathbf{B} \left(\underbrace{\mathbf{f}_S(\mathbf{u}^+, \mathbf{u})}_{\text{interface flux } \mathbf{f}^*} - \mathbf{f}(\mathbf{u}) \right) = \mathbf{0}$$

- Add interface dissipation (e.g., Lax-Friedrichs) for entropy *stability*.

$$\mathbf{f}_S(\mathbf{u}^+, \mathbf{u}) \rightarrow \mathbf{f}_S(\mathbf{u}^+, \mathbf{u}) - \frac{\lambda}{2} [\![\mathbf{u}]\!], \quad \lambda > 0.$$

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Main innovation of entropy stable SBP schemes

- Discrete analogue of the entropy identity

$$\boxed{\int_{-1}^1 \mathbf{v}^T \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \mathbf{v}^T \mathbf{f}(\mathbf{u}) - \psi(\mathbf{u}) \Big|_{-1}^1} \quad \iff$$

$$\begin{aligned} & \mathbf{v}^T (2\mathbf{Q} \circ \mathbf{F}) \mathbf{1} \\ &= \mathbf{1}^T \mathbf{B} (\mathbf{v}^T \mathbf{f}(\mathbf{u}) - \psi) \end{aligned}$$

- Expand $\mathbf{v}^T (2\mathbf{Q} \circ \mathbf{F}) \mathbf{1}$ using the SBP property $\mathbf{Q} = \mathbf{B} - \mathbf{Q}^T$

$$\mathbf{v}^T (2\mathbf{Q} \circ \mathbf{F}) \mathbf{1}$$

- Manipulate volume term using properties of \mathbf{Q} and \mathbf{f}_S .

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Main innovation of entropy stable SBP schemes

- Discrete analogue of the entropy identity

$$\int_{-1}^1 \mathbf{v}^T \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \mathbf{v}^T \mathbf{f}(\mathbf{u}) - \psi(\mathbf{u}) \Big|_{-1}^1 \quad \Longleftrightarrow$$

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Talk outline

1 Entropy stable nodal summation-by-parts (SBP) schemes

2 Modal entropy stable DG formulations

3 Applications of modal formulations

- Triangles and tetrahedra: full integration
- Quad and hex meshes: new collocation schemes
- Reduced order modeling

Why “modal” formulations?

Nodal formulations: tied to a specific polynomial quadrature rule.
“Modal” formulations: designed for arbitrary bases and quadratures.

- Nodal formulations typically *underintegrate*. More accurate quadrature reduces aliasing for nonlinear terms + curved elements.
- Accommodate non-polynomial basis functions:
 - Pyramid elements, physical-frame bases, splines
 - Projection-based reduced order modeling
- Extensions of (and connections with) traditional SBP operators.

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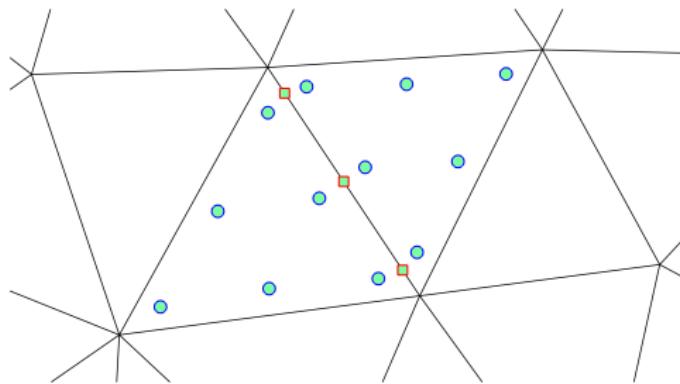
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Challenges for modal formulations

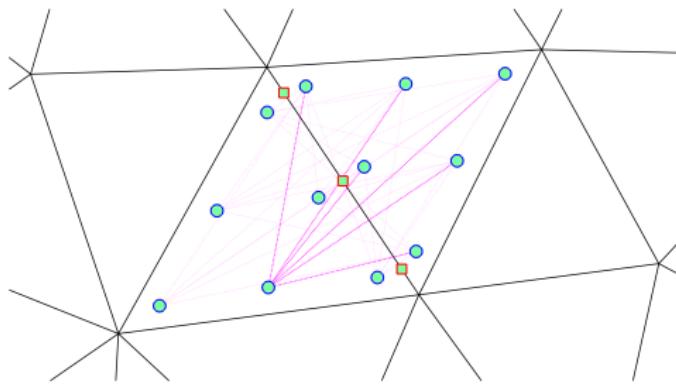
- Challenge 1: entropy variables are not contained in the finite element test space! If $\mathbf{u} \in P^N$, then in general, $\mathbf{v}(\mathbf{u}) \notin P^N$.
- Challenge 2: inter-element coupling more complicated and expensive.



Standard DG coupling (through face points)

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Entropy stable DG coupling (all-to-all)

Challenge 1: entropy projection

- DG: cannot test with entropy variables, only with polynomials.
- Let \mathbf{u}_N be a polynomial. Testing with the L^2 projection of the entropy variables $P_N \mathbf{v}(\mathbf{u}_N)$ recovers evolution of entropy

$$\int_{D^k} P_N \mathbf{v}(\mathbf{u}_N)^T \frac{\partial \mathbf{u}_N}{\partial t} = \int_{D^k} \underbrace{\mathbf{v}(\mathbf{u}_N)^T}_{\frac{\partial S(\mathbf{u})}{\partial \mathbf{u}}} \frac{\partial \mathbf{u}_N}{\partial t} = \int_{D^k} \frac{\partial S(\mathbf{u}_N)}{\partial t}$$

- For consistency with the test function $P_N \mathbf{v}(\mathbf{u}_N)$, spatial formulation is evaluated using projected entropy variables $\tilde{\mathbf{u}} = \mathbf{u}(P_N \mathbf{v}(\mathbf{u}_N))$.

$$(\mathbf{v}_i - \mathbf{v}_j)^T \mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_j) \neq \psi(\mathbf{u}_i) - \psi(\mathbf{u}_j) \quad \text{if } \mathbf{v}_i \neq \mathbf{v}(\mathbf{u}_i).$$

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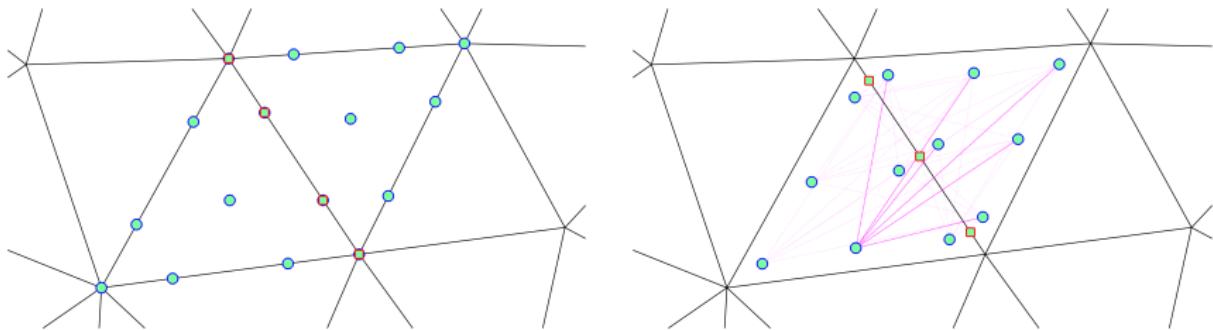
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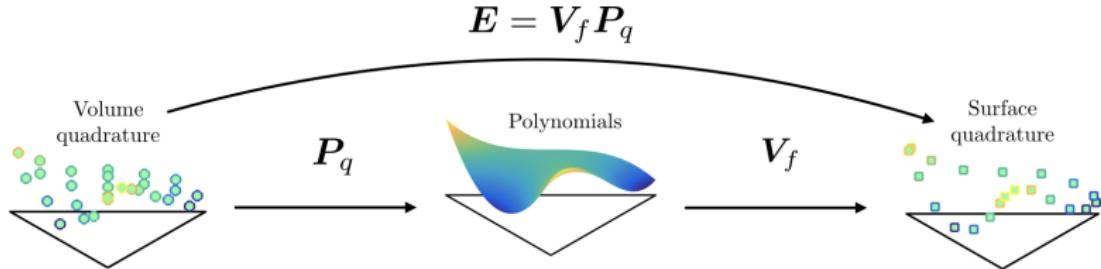
Challenge 2: efficient interface fluxes



Entropy stable interface coupling with/without boundary nodes

- For general formulations, \mathbf{Q} satisfies a **generalized** SBP property
- $$\mathbf{Q} + \mathbf{Q}^T = \mathbf{E}^T \mathbf{B} \mathbf{E}, \quad \mathbf{E} = \text{interpolates volume to surface}$$
- Proof of entropy stability: SBP converts volume terms into boundary terms, which **must cancel with interface flux terms**.

Construction of \mathbf{Q} , \mathbf{E} for DG methods

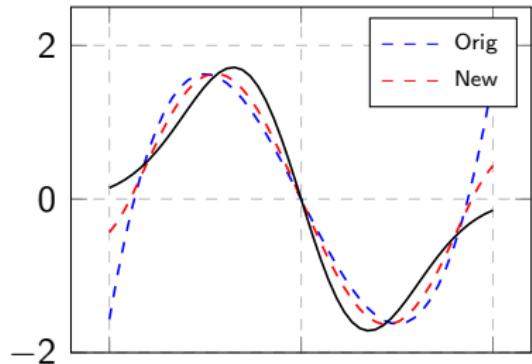


- Let $\mathbf{V}_q, \mathbf{V}_f$ interpolate to quadrature, $\mathbf{W} = \text{diag. weight matrix}$.
- Define nodal operator $\mathbf{Q} = \mathbf{P}_q^T \widehat{\mathbf{Q}} \mathbf{P}_q$ through a “modal” operator $\widehat{\mathbf{Q}}$

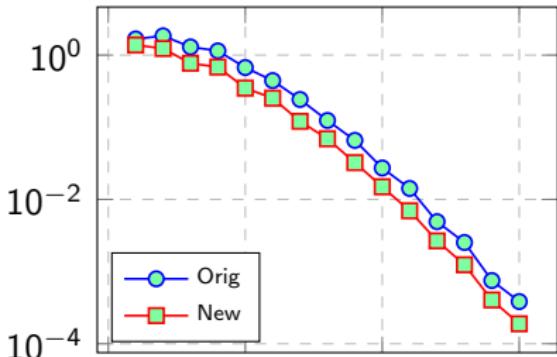
$$\widehat{\mathbf{Q}}_{ij} = \int \frac{\partial \phi_j}{\partial x} \phi_i, \quad \mathbf{P}_q = \mathbf{M}^{-1} \mathbf{V}_q^T \mathbf{W}, \quad \mathbf{M} = \mathbf{V}_q^T \mathbf{W} \mathbf{V}_q,$$

- If $\mathbf{Q} + \mathbf{Q}^T = \mathbf{E}^T \mathbf{B} \mathbf{E}$ (generalized SBP property), then interface fluxes must also involve *dense* \mathbf{E} for entropy stability (all-to-all coupling)!

Efficient interface fluxes via “hybridization”



(a) Approximated derivatives

(b) L^2 error for degrees $N = 1, \dots, 15$

- Use a *hybridized* (block) SBP operator + flux differencing.

$$\mathbf{Q}_h = \frac{1}{2} \begin{bmatrix} \mathbf{Q} - \mathbf{Q}^T & \mathbf{E}^T \mathbf{B} \\ -\mathbf{B} \mathbf{E} & \mathbf{B} \end{bmatrix}, \quad \frac{\partial}{\partial x} \approx \mathbf{M}^{-1} \begin{bmatrix} \mathbf{V}_q \\ \mathbf{V}_f \end{bmatrix}^T \mathbf{Q}_h$$

Entropy stable schemes using hybridized SBP operators

- Replace SBP operator with hybridized SBP operator

$$\mathbf{M} \frac{d\mathbf{u}_h}{dt} + 2(\mathbf{Q} \circ \mathbf{F}) \mathbf{1} + \mathbf{B} (\mathbf{f}^* - \mathbf{f}(\mathbf{u})) = 0.$$

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

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

- Entropy stability if $\mathbf{Q}_h \mathbf{1} = \mathbf{0} \Rightarrow$ equivalent to either GSBP or **weak** SBP condition related to quadrature accuracy.

$$\mathbf{Q} + \mathbf{Q}^T = \mathbf{E}^T \mathbf{B} \mathbf{E} \quad \Rightarrow \quad \mathbf{Q}^T \mathbf{1} = \mathbf{E}^T \mathbf{B} \mathbf{1} \quad (\text{weaker conditions})$$

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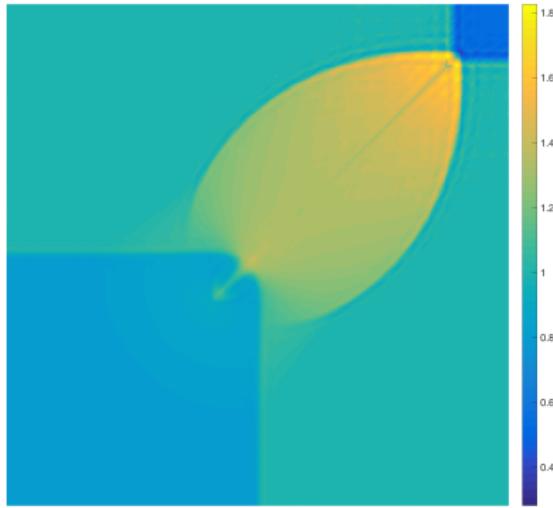
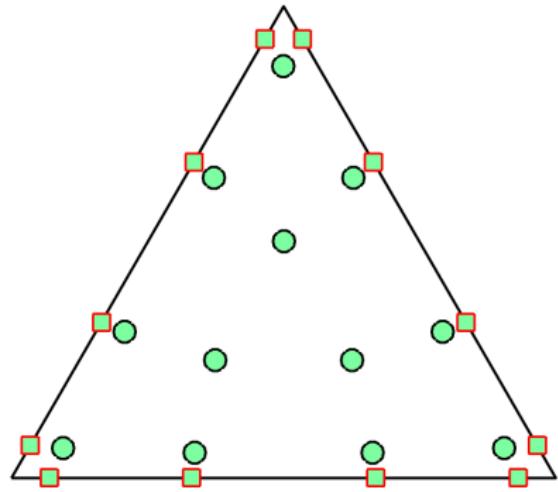
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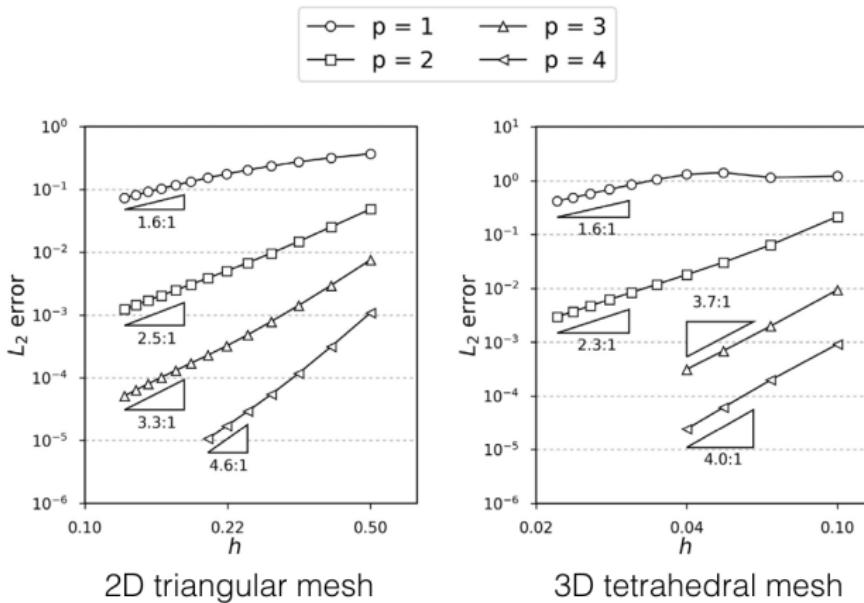
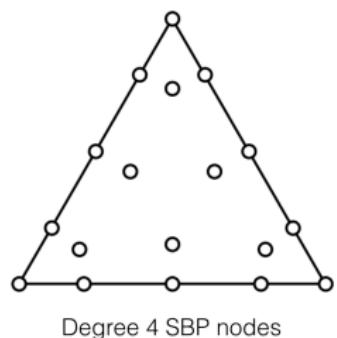
Triangles: 2D Riemann problem

- Approximation space P^N , degree $\geq 2N$ volume/face quadratures
(most SBP operators use under-integrated degree $2N - 1$ quadrature)
- Uniform 32×32 mesh: $N = 3$, CFL .125, Lax-Friedrichs stabilization.



Results computed on larger periodic domain ("natural" boundary conditions unstable).

Curved simplicial meshes (with Lucas Wilcox)

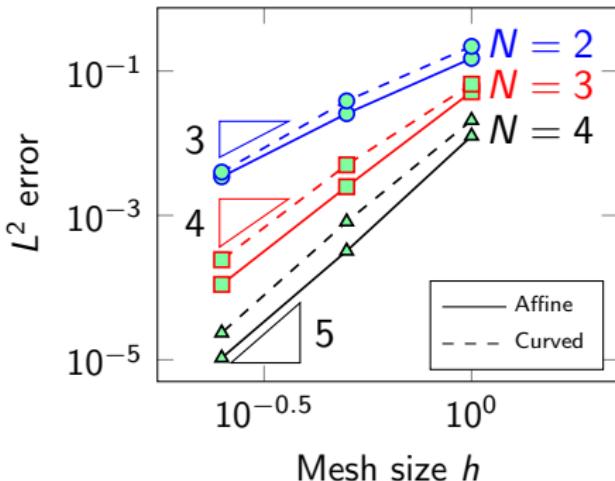


Sub-optimal rates for under-integrated nodal SBP schemes (Crean et al. 2018).

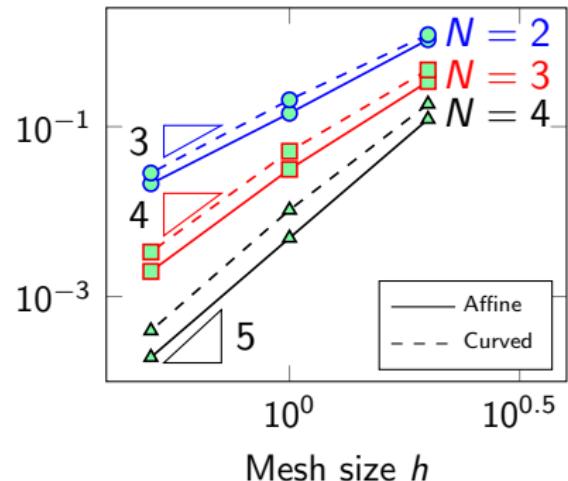
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(a) 2D triangular mesh



(b) 3D tetrahedral mesh

Accurate numerical integration restores optimal rates of convergence.

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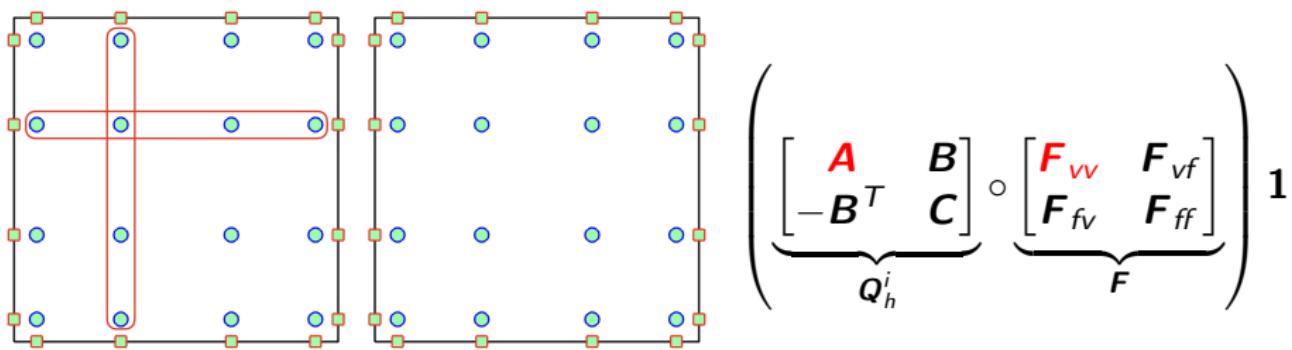
Entropy stable Gauss collocation on tensor product elements (with MH Carpenter + DCDR Fernandez)

$$\left(\begin{bmatrix} A & B \\ -B^T & C \end{bmatrix} \circ \begin{bmatrix} F_{vv} & F_{vf} \\ F_{fv} & F_{ff} \end{bmatrix} \right) \mathbf{1}$$

$$Q_h^i$$

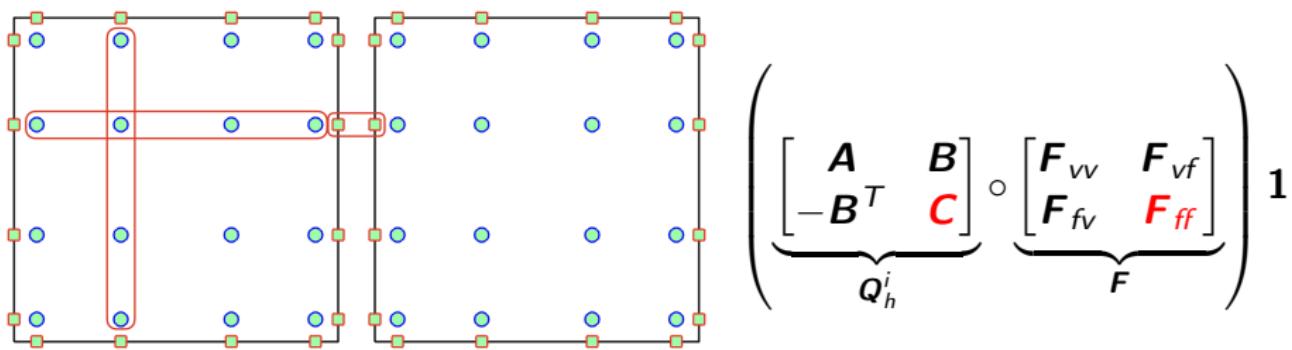
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- Tensor product $(N + 1)$ -point Gauss quadrature for integrals.
- Advantage of hexes vs. tets: simplifies to **collocation**, Kronecker product reduces flux evaluations from $O(N^6)$ to $O(N^4)$ in 3D.

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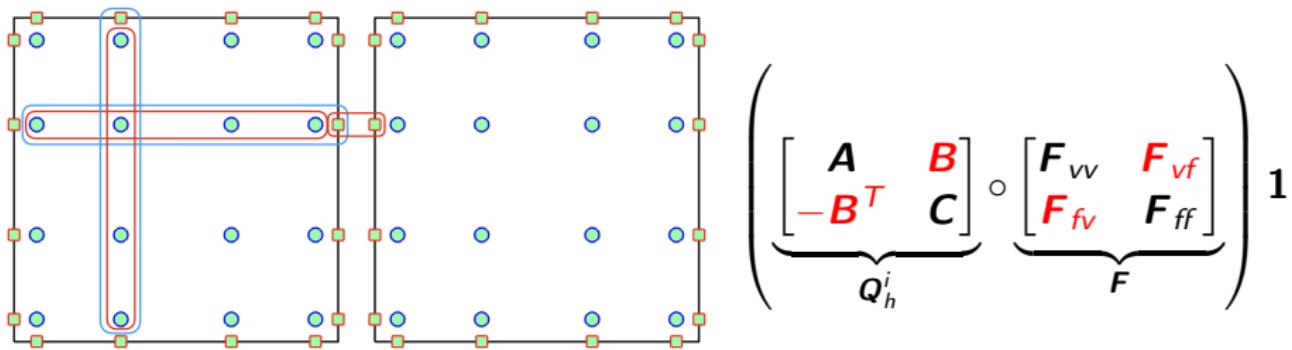
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Entropy stable Gauss collocation on tensor product elements (with MH Carpenter + DCDR Fernandez)



- Hexahedral elements: tensor product polynomial basis
- Tensor product $(N + 1)$ -point Gauss quadrature for integrals.
- Advantage of hexes vs. tets: simplifies to **collocation**, Kronecker product reduces flux evaluations from $O(N^6)$ to $O(N^4)$ in 3D.

Gauss quadrature improves errors on warped meshes

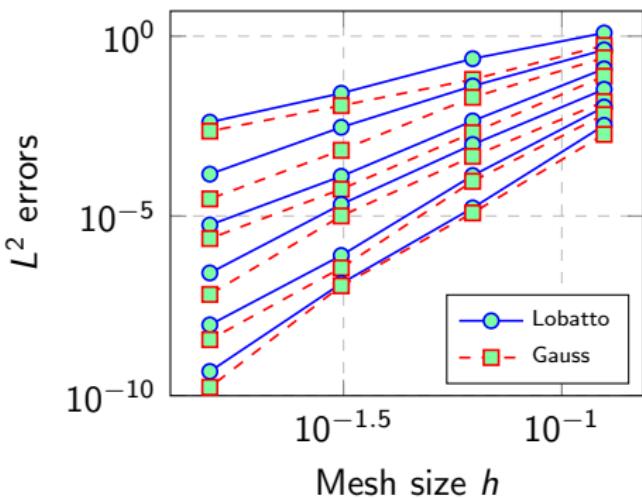
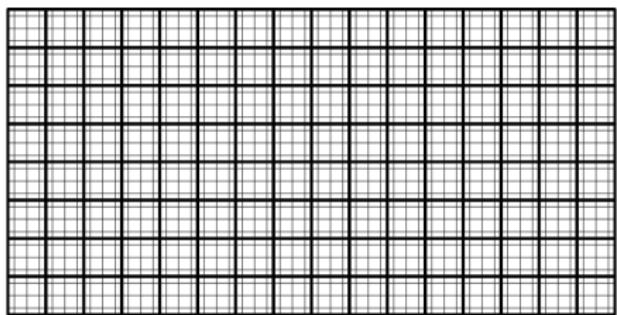


Figure: L^2 errors for the 2D isentropic vortex at time $T = 5$ for degree $N = 2, \dots, 7$ Lobatto and Gauss collocation schemes (similar behavior in 3D).

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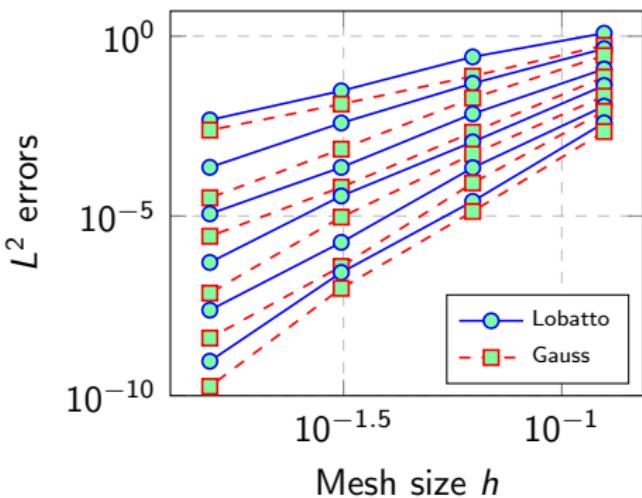
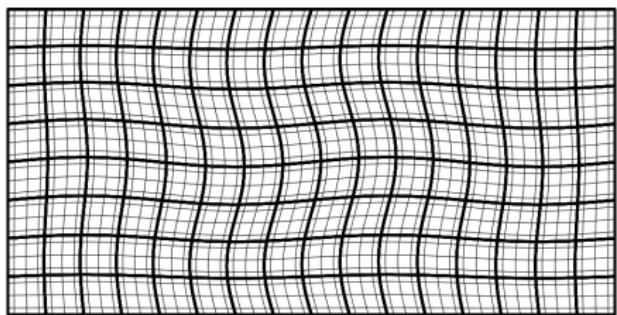


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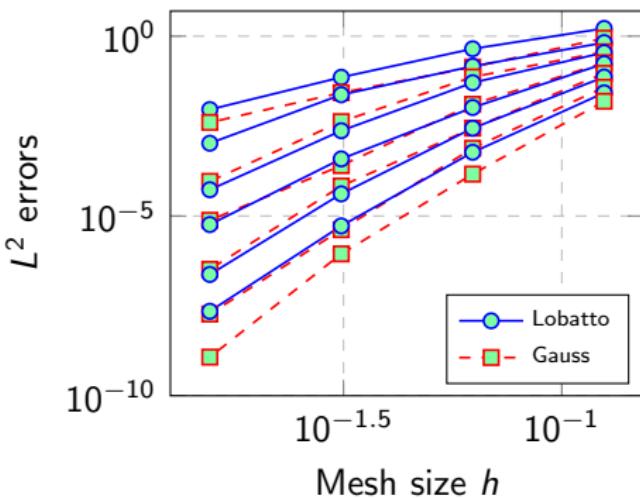
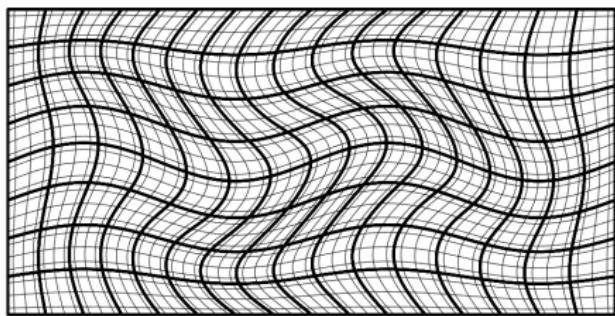


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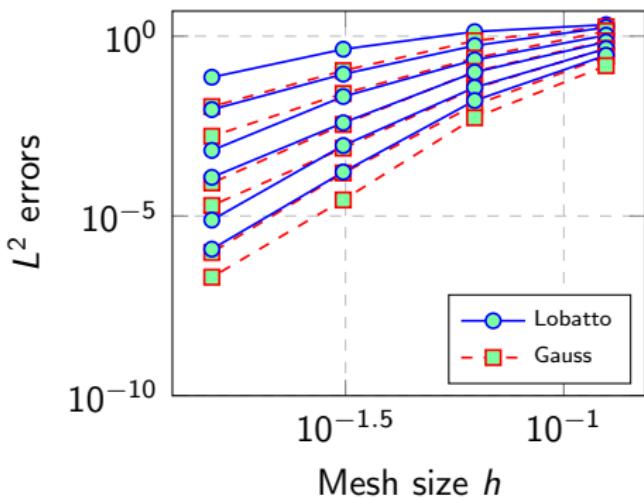
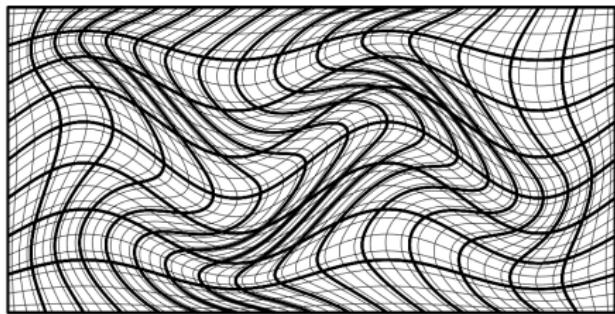


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Shock vortex interaction

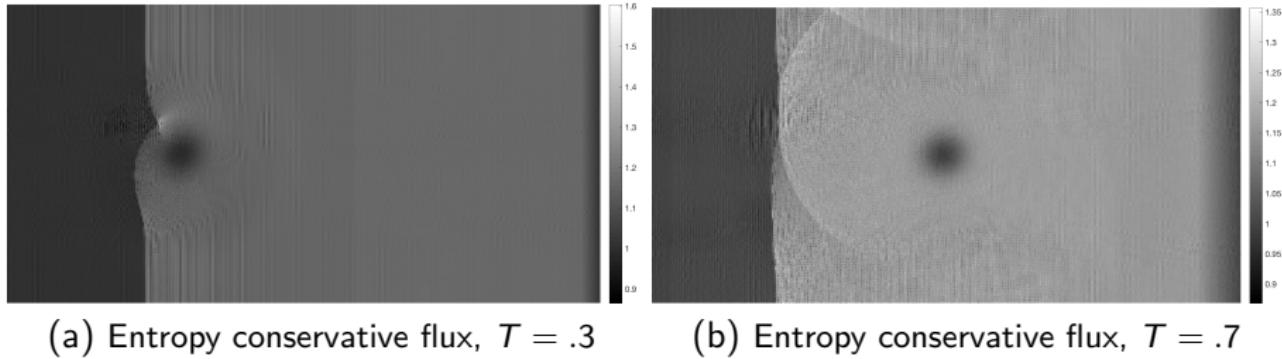


Figure: Shock vortex interaction problem using high order entropy stable Gauss collocation schemes with $N = 4, h = 1/100$.

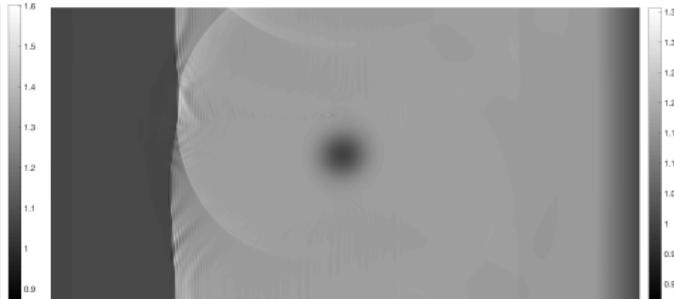
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Shock vortex interaction



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



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

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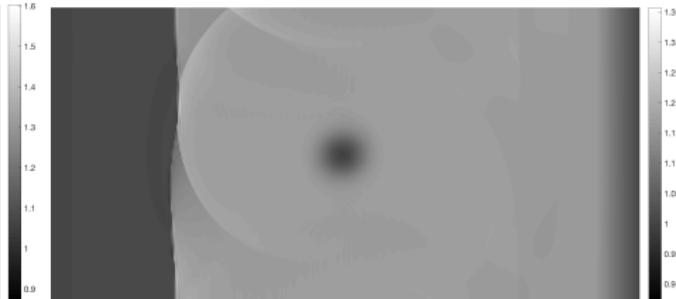
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(a) Matrix dissipation flux, $T = .3$



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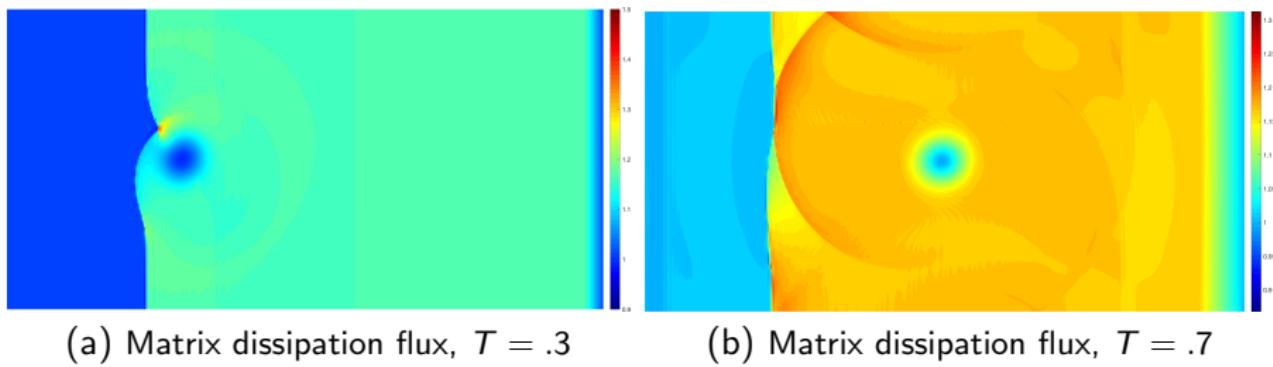
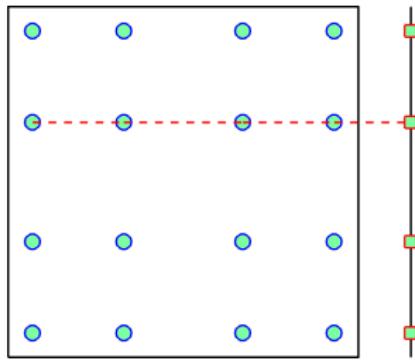


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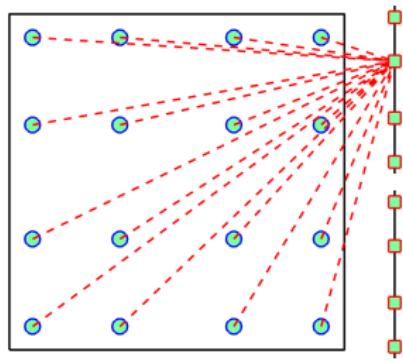
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Non-conforming interfaces (with DCDR Fernandez)



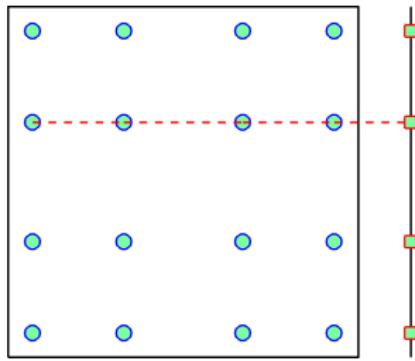
(a) Conforming surface quadrature nodes



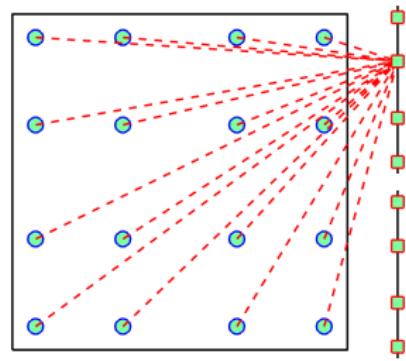
(b) Non-conforming surface nodes

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

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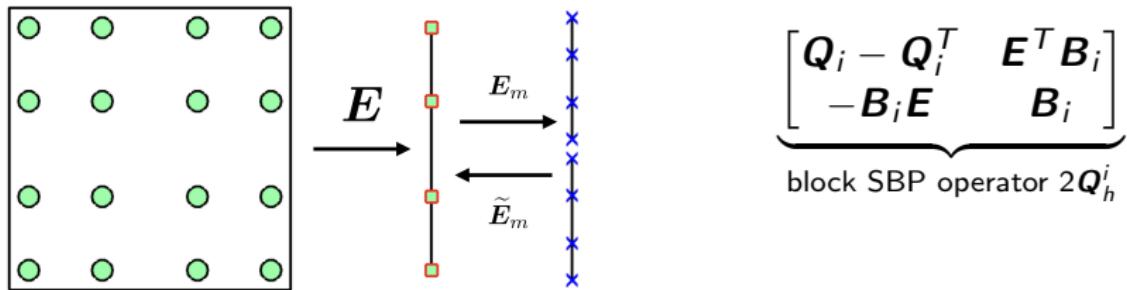
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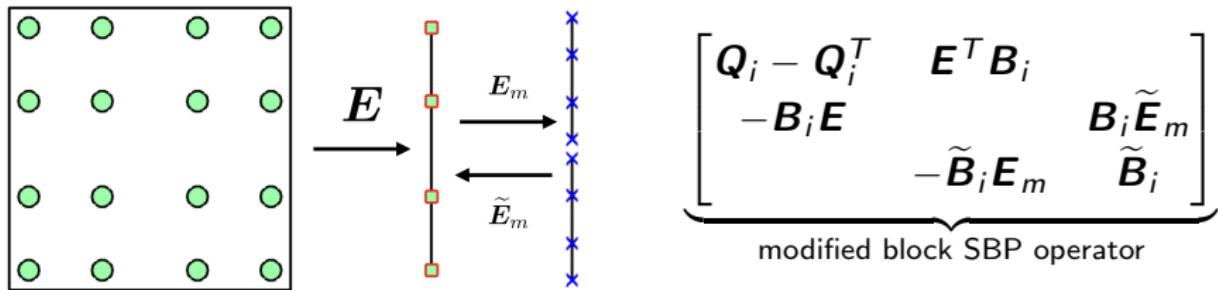
A mortar-based hybridized SBP operator



- Define transfer operators $\mathbf{E}_m, \tilde{\mathbf{E}}_m$ between conforming and non-conforming (mortar) nodes.
- Modify the hybridized SBP volume term:

$$\sum_{i=1}^d \begin{bmatrix} \mathbf{I} \\ \mathbf{E} \end{bmatrix}^T \left(\begin{bmatrix} \mathbf{Q}_i - \mathbf{Q}_i^T & \mathbf{E}^T \mathbf{B}_i \\ -\mathbf{B}_i \mathbf{E} & \mathbf{B}_i \end{bmatrix} \circ \mathbf{F}_i \right) \mathbf{1}$$

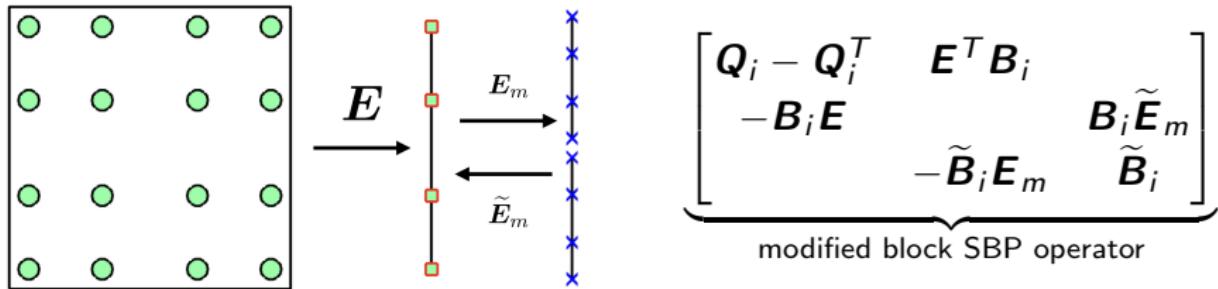
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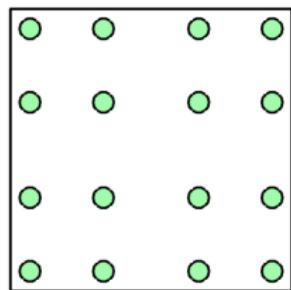
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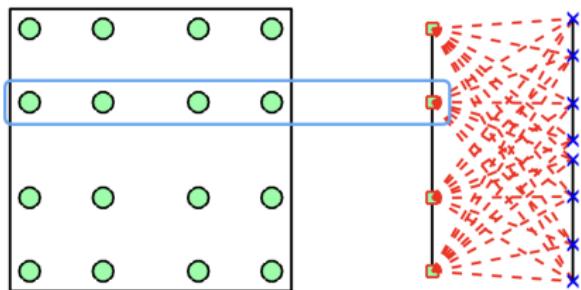
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An efficient mortar reformulation



(a) Mortar operators



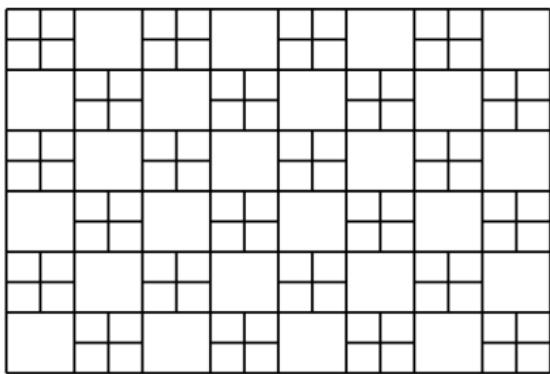
(b) Volume + surface + mortar coupling

$$\boldsymbol{M} \frac{d\boldsymbol{u}}{dt} + \sum_{i=1}^d \begin{bmatrix} \boldsymbol{I} \\ \boldsymbol{E} \end{bmatrix}^T (2\boldsymbol{Q}_h^i \circ \boldsymbol{F}_i) \boldsymbol{1} + \boldsymbol{E}^T \boldsymbol{B}_i \tilde{\boldsymbol{f}}_i^* = 0$$

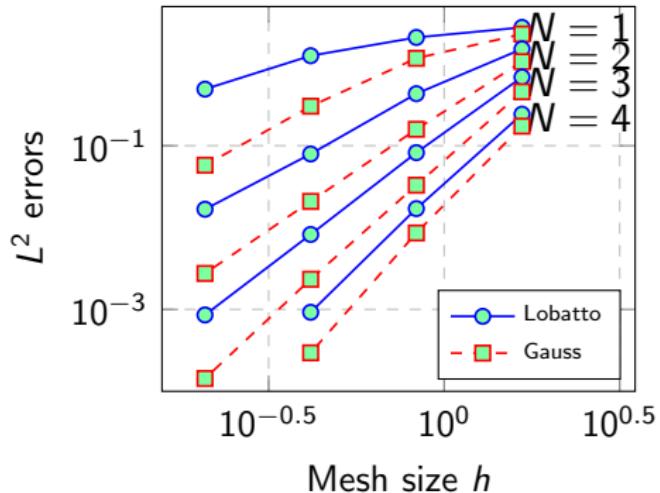
$$\tilde{\boldsymbol{f}}_i^* = \tilde{\boldsymbol{E}}_m (\boldsymbol{f}_i^* - \boldsymbol{f}_i(\boldsymbol{u})) + (\tilde{\boldsymbol{E}}_m \circ \boldsymbol{F}_{i,sm}) \boldsymbol{1} - \tilde{\boldsymbol{E}}_m (\boldsymbol{E}_m \circ \boldsymbol{F}_{i,ms}) \boldsymbol{1}$$

Reformulate as an entropy stable correction to the numerical flux.

Numerical results: non-conforming meshes



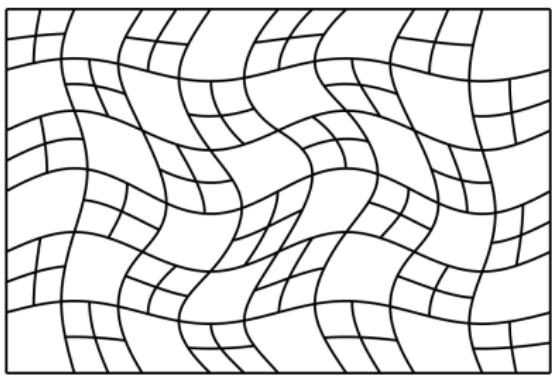
(a) Coarse non-conforming mesh



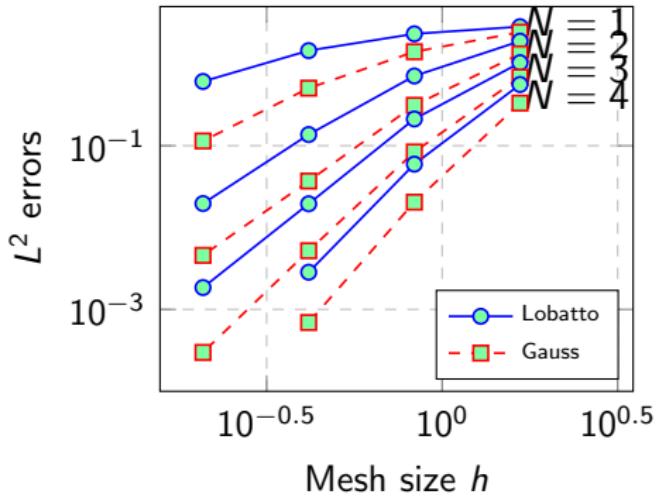
(b) Sub-optimal rates if under-integrated

The skew symmetric formulation is entropy stable for both Lobatto and Gauss quadrature, but Lobatto is $O(h^N)$ while Gauss is $O(h^{N+1})$.

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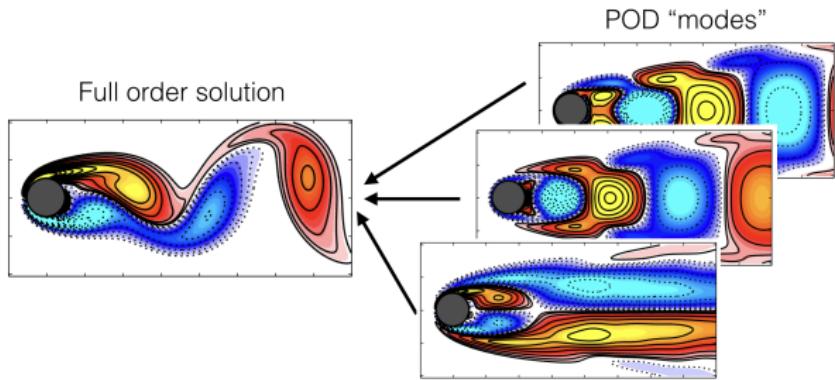
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Talk outline

- 1 Entropy stable nodal summation-by-parts (SBP) schemes
- 2 Modal entropy stable DG formulations
- 3 Applications of modal formulations
 - Triangles and tetrahedra: full integration
 - Quad and hex meshes: new collocation schemes
 - Reduced order modeling

Projection-based reduced order models (ROMs)

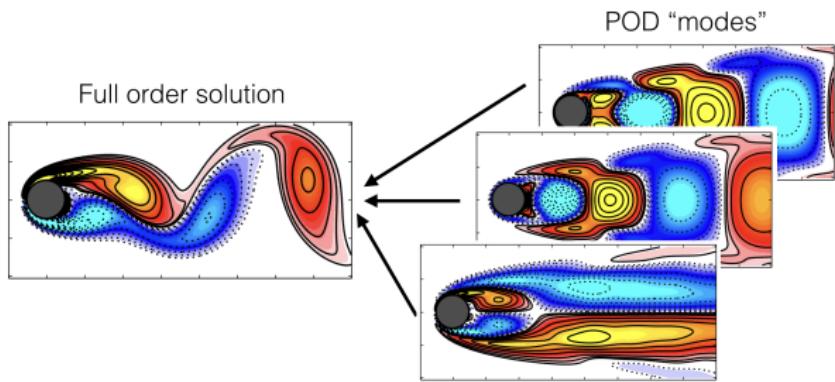


- Goal: reduce cost of many-query scenarios (design space exploration).
- Main steps: **offline** training phase with full order model (FOM), cheap **online** phase with reduced order model (ROM).

Challenge: ROMs inherit stability of FOM for elliptic PDEs,
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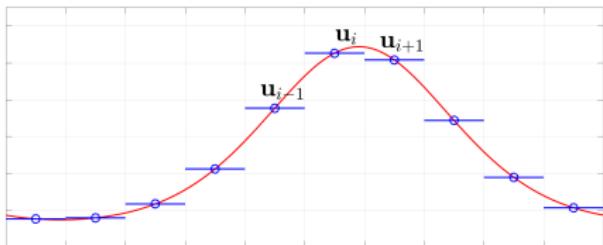


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Full order model: entropy stable finite volumes



- Discretize integrated form of nonlinear conservation law

$$\Delta x \frac{d\mathbf{u}_i}{dt} + \mathbf{f}_S(\mathbf{u}_{i+1}, \mathbf{u}_i) - \mathbf{f}_S(\mathbf{u}_i, \mathbf{u}_{i-1}) = 0, \quad \text{interior } i.$$

- Matrix formulation: let $\mathbf{M} = (\Delta x)\mathbf{I}$, and (assuming periodicity)

$$\mathbf{M} \frac{d\mathbf{u}}{dt} + 2(\mathbf{Q} \circ \mathbf{F})\mathbf{1} + \underbrace{\epsilon \mathbf{K} \mathbf{u}}_{\text{art. viscosity}} = 0, \quad \mathbf{Q} = \frac{1}{2} \begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & 1 \\ 1 & & -1 & 0 \end{bmatrix}$$

Naive POD-Galerkin procedure

- (Offline) compute POD basis from solution component snapshots.

$$\mathbf{V} = \begin{bmatrix} | & & | \\ \phi_1 & \dots & \phi_N \\ | & & | \end{bmatrix}, \quad \phi_i^T \phi_j = 0, \quad \mathbf{u} \approx \mathbf{V} \mathbf{u}_N.$$

- (Online) Galerkin projection of the matrix system

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

- (Online) Entropy projection results in an entropy stable ROM

$$\tilde{\mathbf{u}} = \mathbf{u} \left(\mathbf{V} \mathbf{V}^\dagger \mathbf{v} (\mathbf{V} \mathbf{u}_N) \right), \quad (\mathbf{F})_{ij} = \mathbf{f}_S(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j).$$

For accuracy, compute POD basis from snapshots of both conservative and entropy variables.

Evaluating nonlinear ROM terms dominates costs

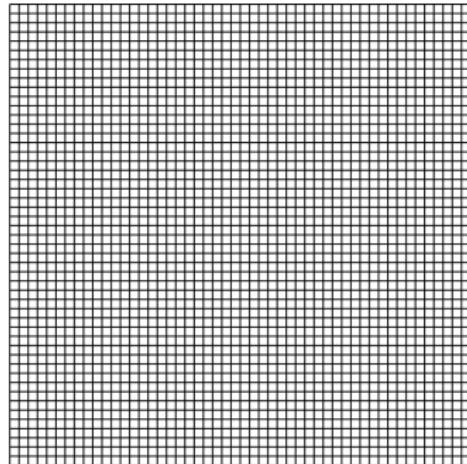
Problem: cost of evaluating ROM nonlinear terms scales with **number of grid points**! Cost still scales with size of full order model.

$$\tilde{\mathbf{u}} = \mathbf{u} \left(\mathbf{V} \mathbf{V}^\dagger \mathbf{v} (\mathbf{V} \mathbf{u}_N) \right), \quad 2(\mathbf{Q} \circ \mathbf{F}) \mathbf{1}$$

- Hyper-reduction reduces costs by approximating nonlinear evaluations.

$$\mathbf{V}^T g(\mathbf{V} \mathbf{u}_N) \approx \underbrace{\mathbf{V}(\mathcal{I}, :)^T}_{\text{sampled rows}} \mathbf{W} g(\mathbf{V}(\mathcal{I}, :) \mathbf{u}_N)$$

- Examples: gappy POD, DEIM, empirical cubature, ECSW, ...



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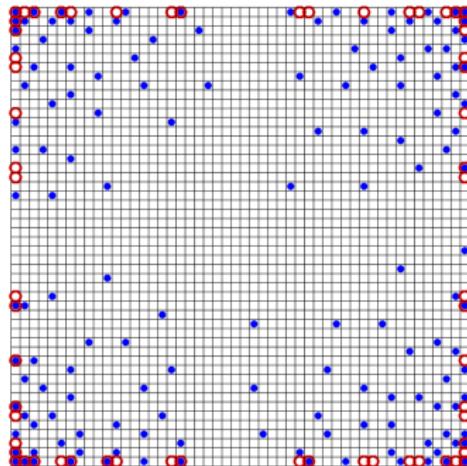
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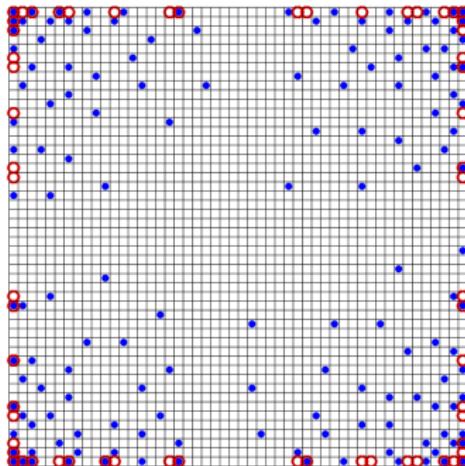
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- Examples: gappy POD, DEIM, empirical cubature, ECSW, ...



Entropy stability and standard hyper-reduction

- How to hyper-reduce $(\mathbf{Q} \circ \mathbf{F})$? Construct a *sampled* matrix \mathbf{Q}_s from \mathbf{Q} . Need $\mathbf{Q}_s = -\mathbf{Q}_s^T$ and $\mathbf{Q}_s \mathbf{1} = \mathbf{0}$ for entropy stability.
- Options: sub-sample rows and columns of full matrix \mathbf{Q} or approximate \mathbf{Q} by weighted sum of local skew matrices \mathbf{Q}_e .

$$\mathbf{Q} = \sum_{e=1}^K \mathbf{Q}_e \approx \mathbf{Q}_s = \sum_{e=1}^K \mathbf{w}_e \mathbf{Q}_e, \quad \mathbf{w} \text{ sparse.}$$

Problems: either \mathbf{Q}_s loses skew-symmetry or $\mathbf{Q}_s \mathbf{1} \neq \mathbf{0}$.

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Two-step hyper-reduction: compress and project

- Step 1: construct a *modal* \mathbf{Q} using an expanded “test” basis \mathbf{V}_t

$$\mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t, \quad \mathbf{1} \in \mathcal{R}(\mathbf{V}_t)$$

- Step 2: determine test basis coefficients using hyper-reduced points.

$$\mathbf{M}_t = \mathbf{V}_t(\mathcal{I}, :)^T \mathbf{W} \mathbf{V}_t(\mathcal{I}, :), \quad \mathbf{P}_t = \mathbf{M}_t^{-1} \mathbf{V}_t(\mathcal{I}, :)^T \mathbf{W}.$$

Here, \mathbf{P}_t is a weighted projection onto the test basis.

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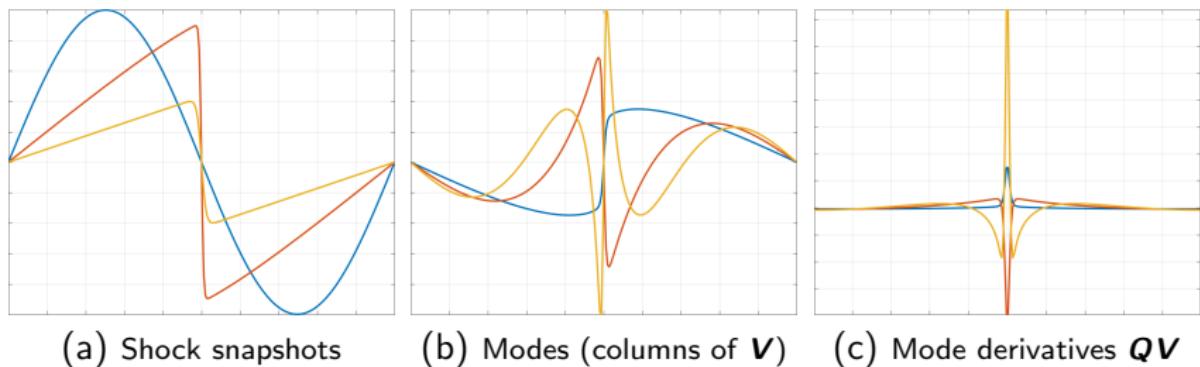
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- Problem: modes \mathbf{V}_t may sample $\mathbf{Q}\mathbf{V}$ very poorly, e.g., $\mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t \approx 0!$



- Fix: sample \mathbf{Q} using an expanded “test” basis \mathbf{V}_t

$$\mathbf{V}_t = \text{orth}([\mathbf{V} \quad \mathbf{1} \quad \mathbf{Q}\mathbf{V}]), \quad \mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t \in \mathbb{R}^{(2N+1) \times (2N+1)}.$$

$\mathbf{Q}_s = \mathbf{P}_t^T (\mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t) \mathbf{P}_t$ is now accurate, $\mathbf{Q}_s = -\mathbf{Q}_s^T$, and $\mathbf{Q}_s \mathbf{1} = \mathbf{0}$.

Hyper-reduction: empirical cubature

- Greedy algorithm constructs an approximate quadrature which integrates a target space to some tolerance.
- Target space motivated by inner products of POD basis: most accurate + smallest number of points in practice

$$\text{Target space} = \text{span} \{ \phi_i(\mathbf{x})\phi_j(\mathbf{x}), \quad 1 \leq i, j \leq N \}.$$

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- Fix: add “**stabilizing**” points which target the near null space of \mathbf{M}_t .

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$$\text{Target space} = \text{span} \{ \phi_i(\mathbf{x})\phi_j(\mathbf{x}), \quad 1 \leq i, j \leq N \}.$$

- Problem: target space ignores rest of expanded test basis. Test mass matrix \mathbf{M}_t may be **singular** \implies projection matrix \mathbf{P}_t ill-defined!
- Fix: add “**stabilizing**” points which target the near null space of \mathbf{M}_t .

Summary: entropy stable ROMs on periodic domains

- Two-step hyper-reduction of $(\mathbf{Q} \circ \mathbf{F})$: compress and project
 - Compress \mathbf{Q} onto expanded test basis spanning $\mathbf{1}$, \mathbf{V} , and \mathbf{QV} .
 - Project hyper-reduced point values onto modes of test basis

$$\mathbf{Q}_s = \mathbf{P}_t^T \left(\mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t \right) \mathbf{P}_t$$

- Entropy stable reduced order model with hyper-reduction:

$$\mathbf{V}(\mathcal{I}, :)^T \mathbf{W} \mathbf{V}(\mathcal{I}, :) \frac{d\mathbf{u}_N}{dt} + 2 \mathbf{V}(\mathcal{I}, :)^T (\mathbf{Q}_s \circ \mathbf{F}) \mathbf{1} = 0,$$

$$\mathbf{F}_{ij} = \mathbf{f}_s(\tilde{\mathbf{u}}_i, \tilde{\mathbf{u}}_j), \quad \tilde{\mathbf{u}} = \mathbf{u}(\mathbf{V}(\mathcal{I}, :) \mathbf{P} \mathbf{v}(\mathbf{V} \mathbf{u}_N)),$$

where \mathbf{P} is the hyper-reduced projection onto POD modes.

- No free lunch: $O(N_s^2)$ vs $O(N_s)$ flux evaluations, where $N_s = |\mathcal{I}|$.

Summary: entropy stable ROMs on periodic domains

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- No free lunch: $O(N_s^2)$ vs $O(N_s)$ flux evaluations, where $N_s = |\mathcal{I}|$.

Non-periodic boundary conditions

- Weak boundary conditions using hybridized SBP operators + DG numerical flux.
- Can add entropy-dissipative penalization terms (e.g., Lax-Friedrichs).
- In 2D/3D, entropy stability requires surface quad. weights \mathbf{w}_f to satisfy weak SBP property involving surface interpolation matrix \mathbf{V}_f .

$$\mathbf{V}_t^T \mathbf{Q}_x^T \mathbf{1} = \mathbf{V}_f^T (\mathbf{n}_x \circ \mathbf{w}_f),$$

$$\mathbf{V}_t^T \mathbf{Q}_y^T \mathbf{1} = \mathbf{V}_f^T (\mathbf{n}_y \circ \mathbf{w}_f).$$

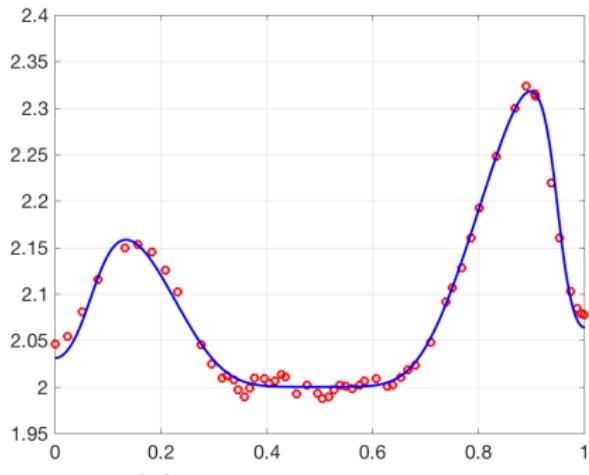
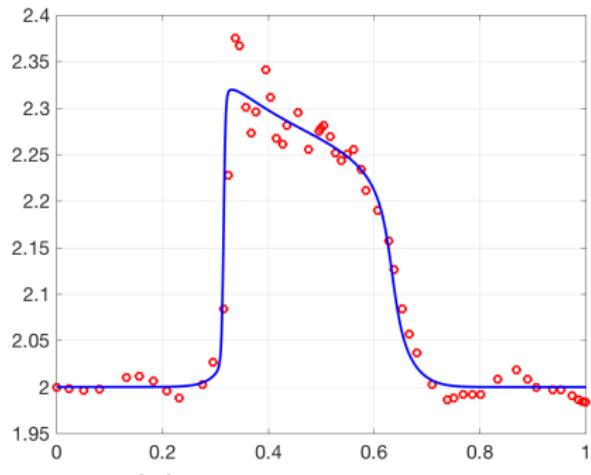
Enforce conditions using constrained LP hyper-reduction.

Patera and Yano (2017). *An LP empirical quadrature procedure for parametrized functions*.

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

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

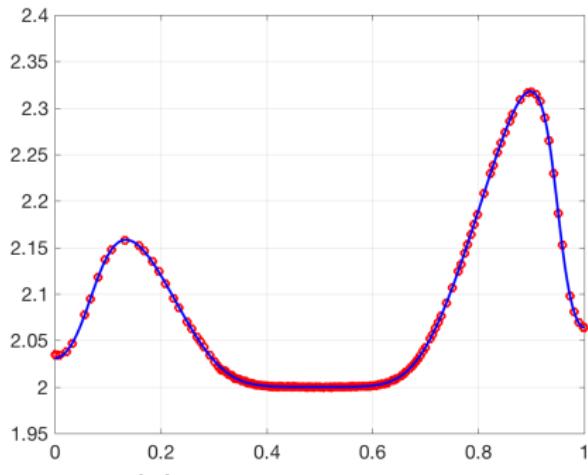
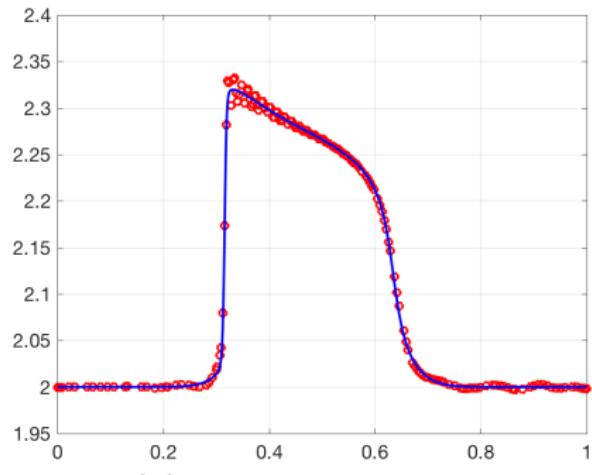
1D Euler with reflective BCs + shock

(a) 25 modes, $T = .25$ (b) 25 modes, $T = .75$

FOM with 2500 grid points, viscosity coefficient $\epsilon = 2e - 4$, ROM with 25 modes.

Number of modes N	25	75	125	175
Number of empirical cubature points	54	158	259	355
Number of stabilizing points	3	21	36	28

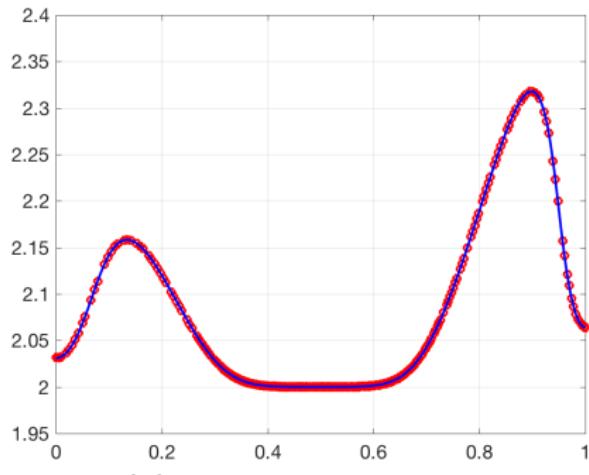
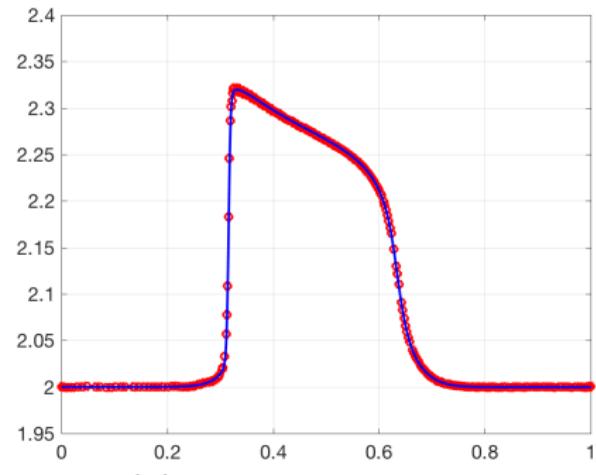
1D Euler with reflective BCs + shock

(a) 75 modes, $T = .25$ (b) 75 modes, $T = .75$

FOM with 2500 grid points, viscosity coefficient $\epsilon = 2e - 4$, ROM with 75 modes.

Number of modes N	25	75	125	175
Number of empirical cubature points	54	158	259	355
Number of stabilizing points	3	21	36	28

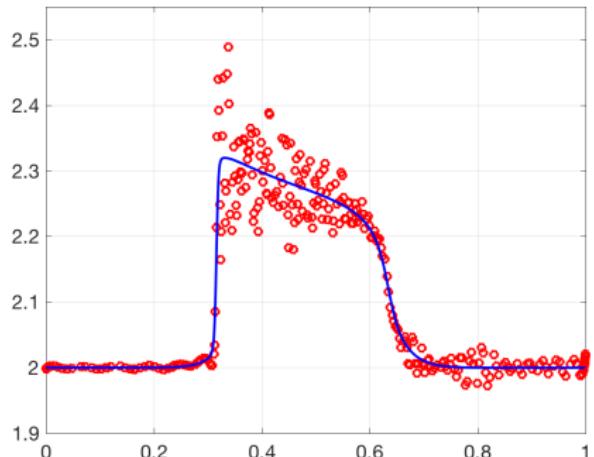
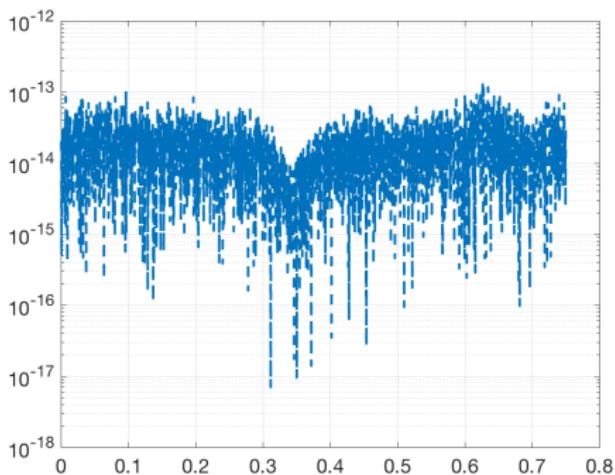
1D Euler with reflective BCs + shock

(a) 125 modes, $T = .25$ (b) 125 modes, $T = .75$

FOM with 2500 grid points, viscosity coefficient $\epsilon = 2e - 4$, ROM with 125 modes.

Number of modes N	25	75	125	175
Number of empirical cubature points	54	158	259	355
Number of stabilizing points	3	21	36	28

Entropy conservation test

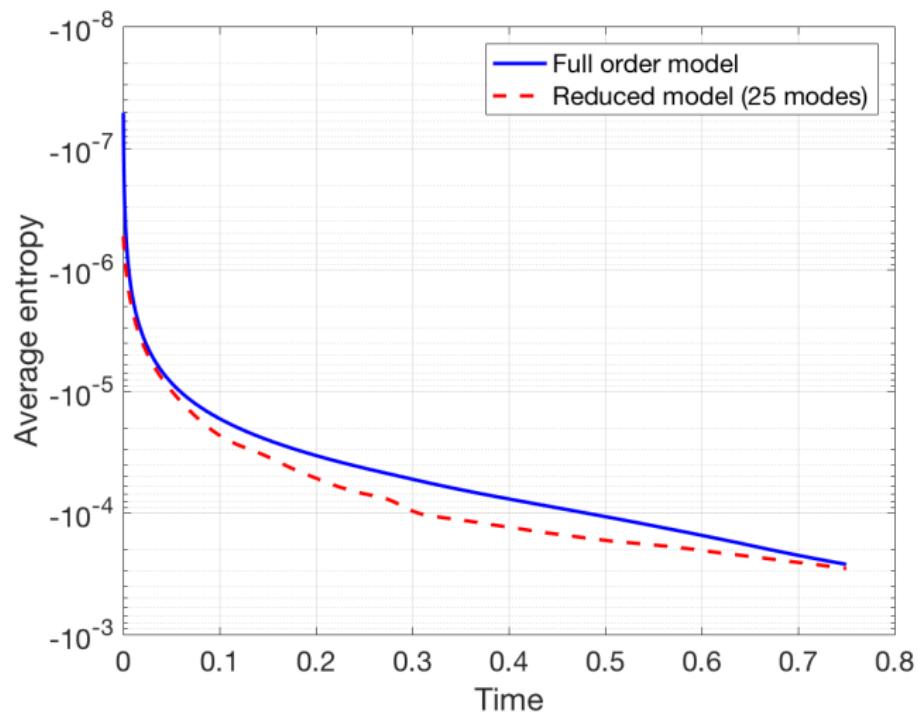
(a) Density ρ (125 modes, no viscosity)

(b) Convective entropy contribution

Figure: Reduced order solution and convective entropy RHS contribution

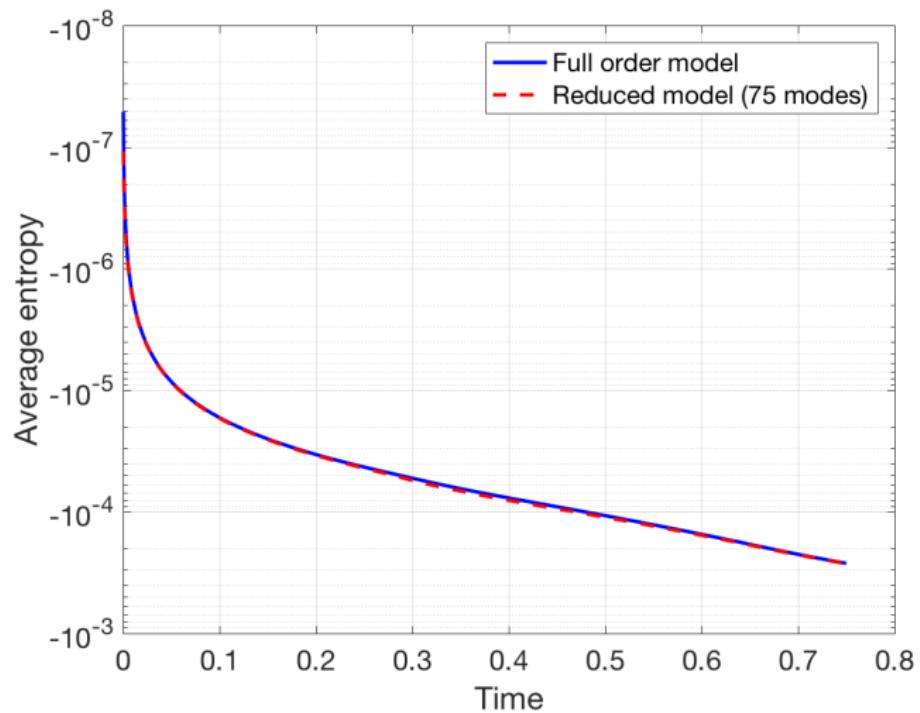
$|\mathbf{v}_N^T \mathbf{V}_h^T (\mathbf{Q}_h \circ \mathbf{F}) \mathbf{1}|$ for the case of zero viscosity.

Evolution of average entropy



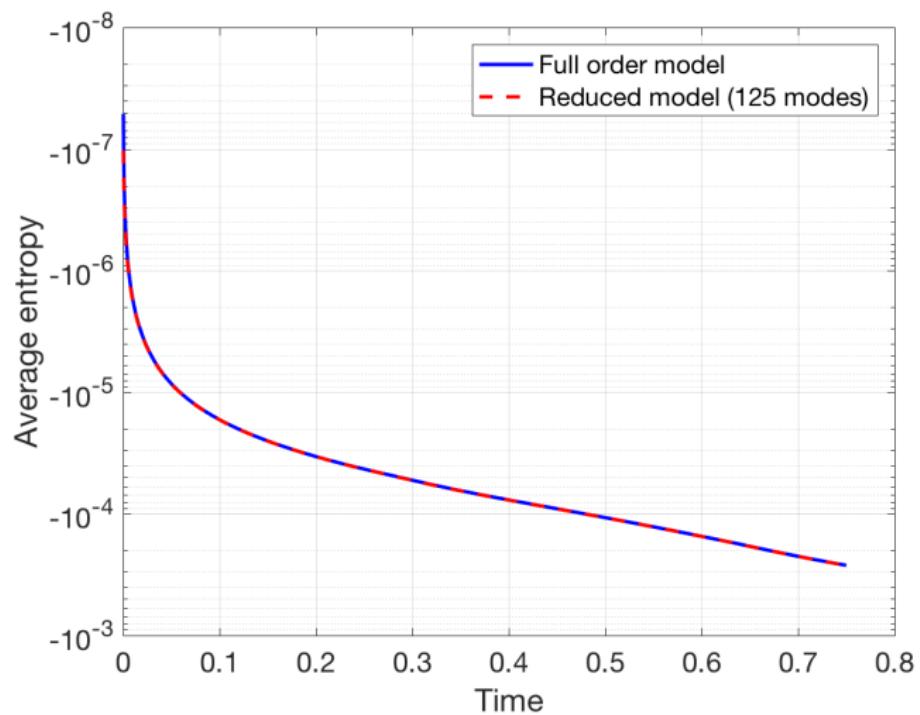
Average entropy over time (25 modes).

Evolution of average entropy



Average entropy over time (75 modes).

Evolution of average entropy



Average entropy over time (125 modes).

Error with and without hyper-reduction

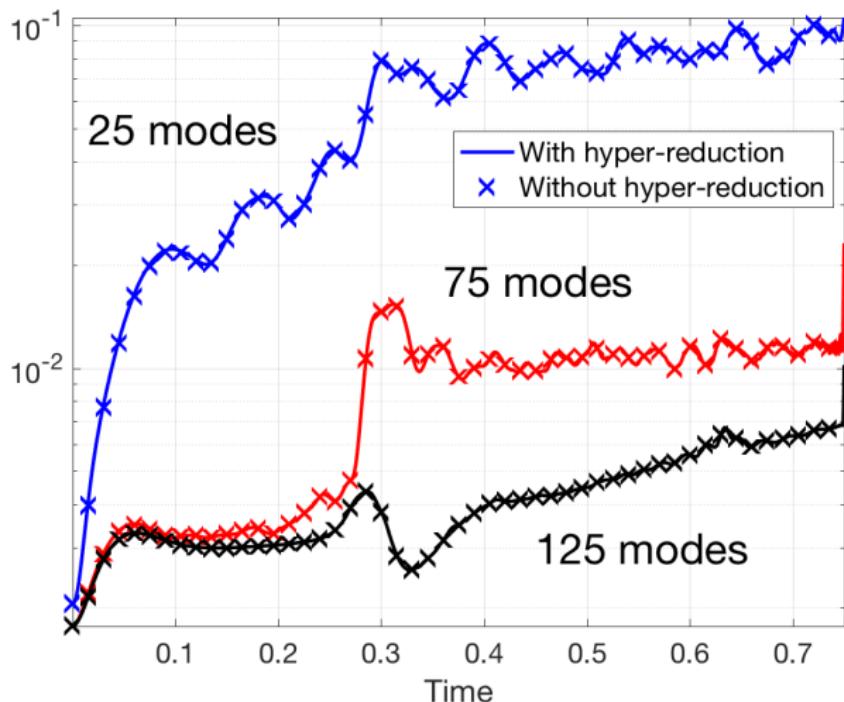
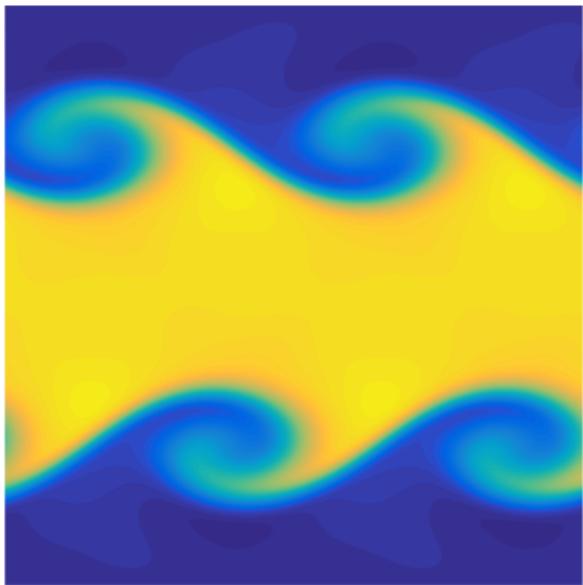
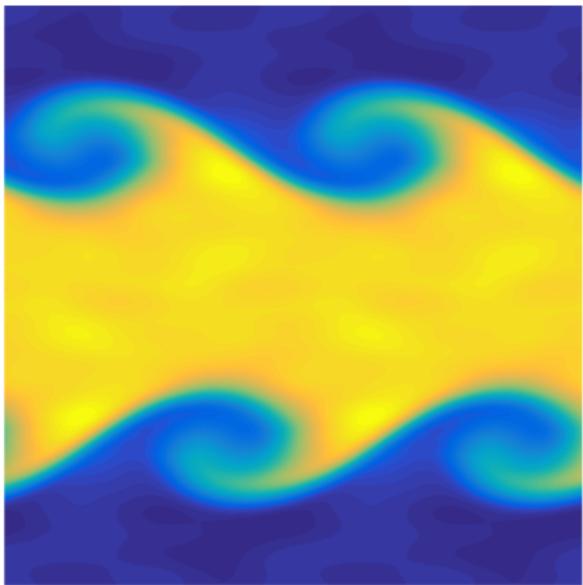


Figure: Error over time for a $K = 2500$ FOM and ROM with 25, 75, 125 modes.

Smoothed 2D Kelvin-Helmholtz instability



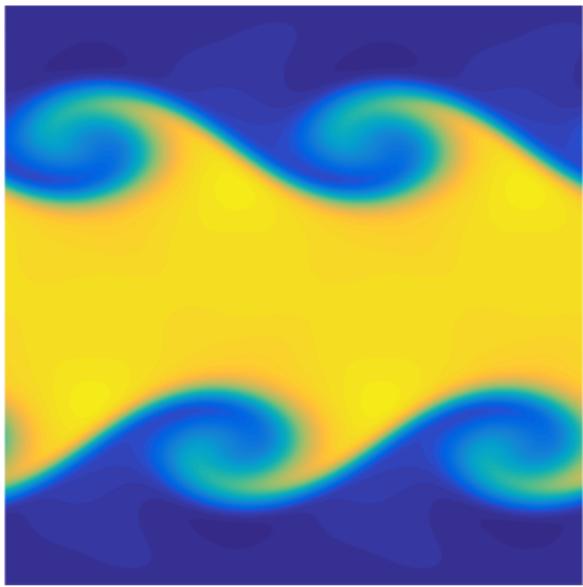
(a) Density, full order model



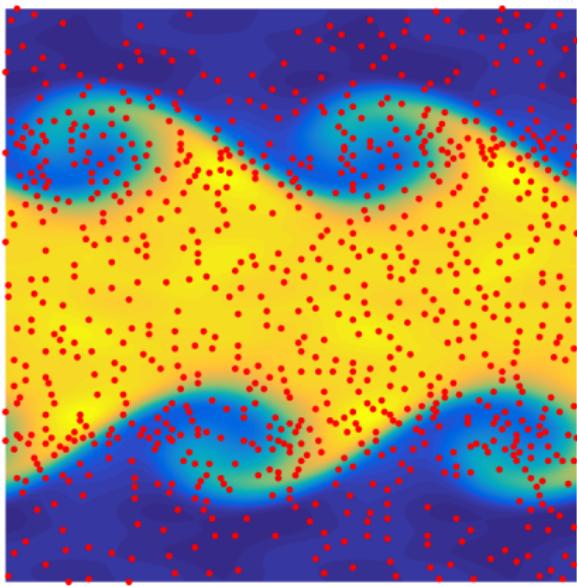
(b) Reduced order model

Figure: Full order model with 40000 points, viscosity $\epsilon = .5\Delta x$. ROM with 75 modes, 865 reduced quadrature points, 1.11% relative L^2 error at $T = 3$.

Smoothed 2D Kelvin-Helmholtz instability



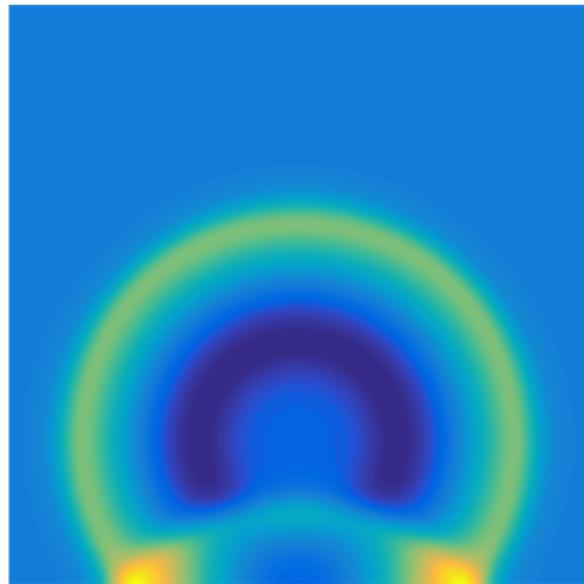
(a) Density, full order model



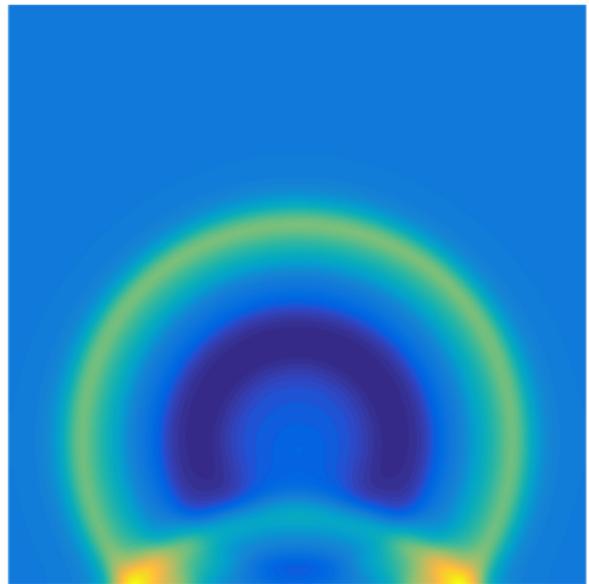
(b) ROM w/reduced quad. points

Figure: Full order model with 40000 points, viscosity $\epsilon = .5\Delta x$. ROM with 75 modes, 865 reduced quadrature points, 1.11% relative L^2 error at $T = 3$.

2D Gaussian pulse with reflective wall



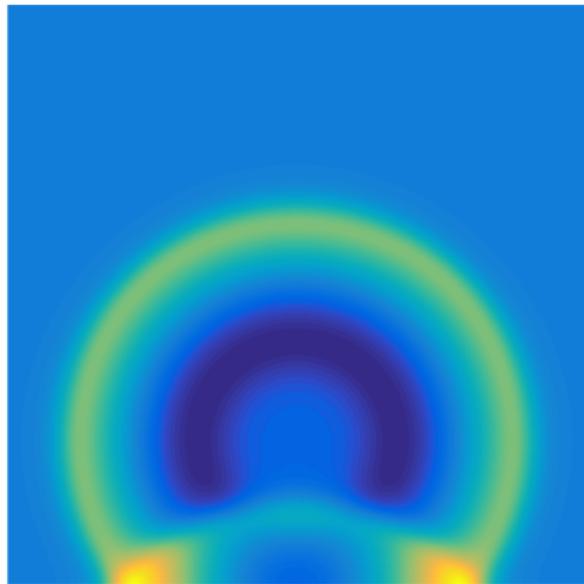
(a) Density, full order model



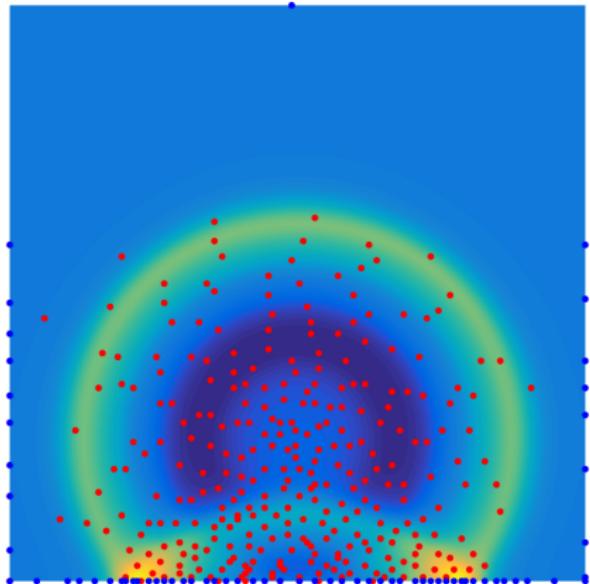
(b) Reduced order model

Figure: FOM with 10000 points, viscosity $\epsilon = .5\Delta x$. ROM with 25 modes, 306 reduced volume points, 82 reduced surface points, .57% error at $T = .25$.

2D Gaussian pulse with reflective wall



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Figure: FOM with 10000 points, viscosity $\epsilon = .5\Delta x$. ROM with 25 modes, 306 reduced volume points, 82 reduced surface points, .57% error at $T = .25$.

Summary and future work

- Entropy stable modal formulations are flexible, with applications to simplicial elements, tensor product elements, and ROMs.
- This work is supported by DMS-1719818 and DMS-1712639.

Thank you! Questions?



-
- Chan (2019). *Entropy stable reduced order modeling of nonlinear conservation laws*.
- 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

Over-integration loses effectiveness without L^2 projection

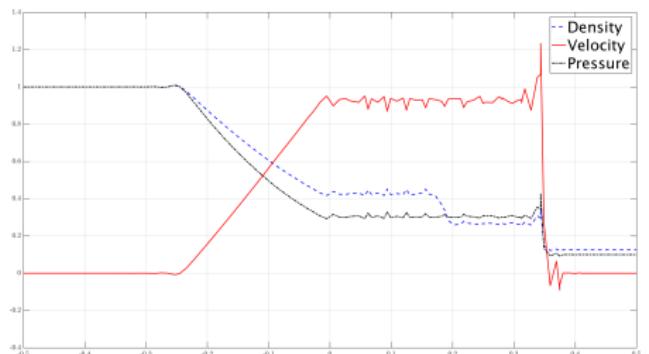
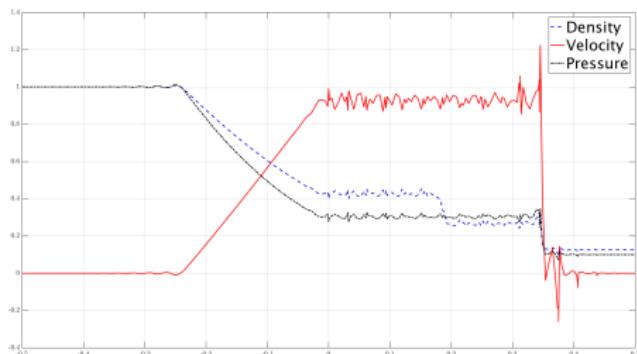
(a) $(N + 1)$ points(b) $(N + 4)$ points

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

Example of EC fluxes (compressible Euler equations)

- Define average $\{\{u\}\} = \frac{1}{2}(u_L + u_R)$. In one dimension:

$$f_S^1(\mathbf{u}_L, \mathbf{u}_R) = \{\{\rho\}\}^{\log} \{\{u\}\}$$

$$f_S^2(\mathbf{u}_L, \mathbf{u}_R) = \{\{u\}\} f_S^1 + p_{\text{avg}}$$

$$f_S^3(\mathbf{u}_L, \mathbf{u}_R) = (E_{\text{avg}} + p_{\text{avg}}) \{\{u\}\},$$

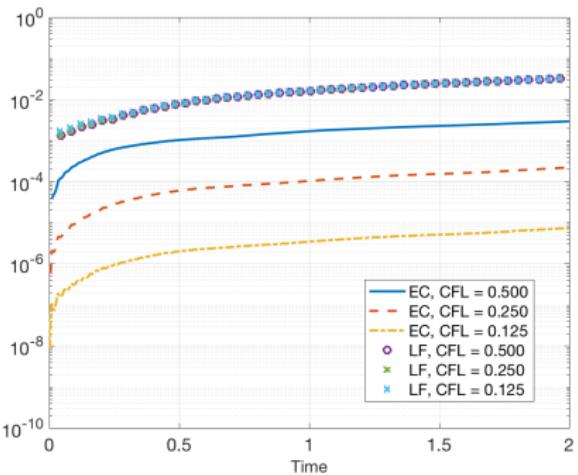
$$p_{\text{avg}} = \frac{\{\{\rho\}\}}{2 \{\{\beta\}\}}, \quad E_{\text{avg}} = \frac{\{\{\rho\}\}^{\log}}{2 \{\{\beta\}\}^{\log} (\gamma - 1)} + \frac{1}{2} u_L u_R.$$

- Non-standard logarithmic mean, “inverse temperature” β

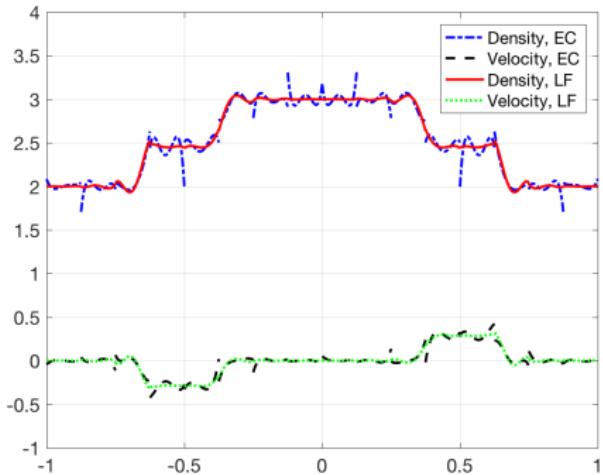
$$\{\{u\}\}^{\log} = \frac{u_L - u_R}{\log u_L - \log u_R}, \quad \beta = \frac{\rho}{2p}.$$

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

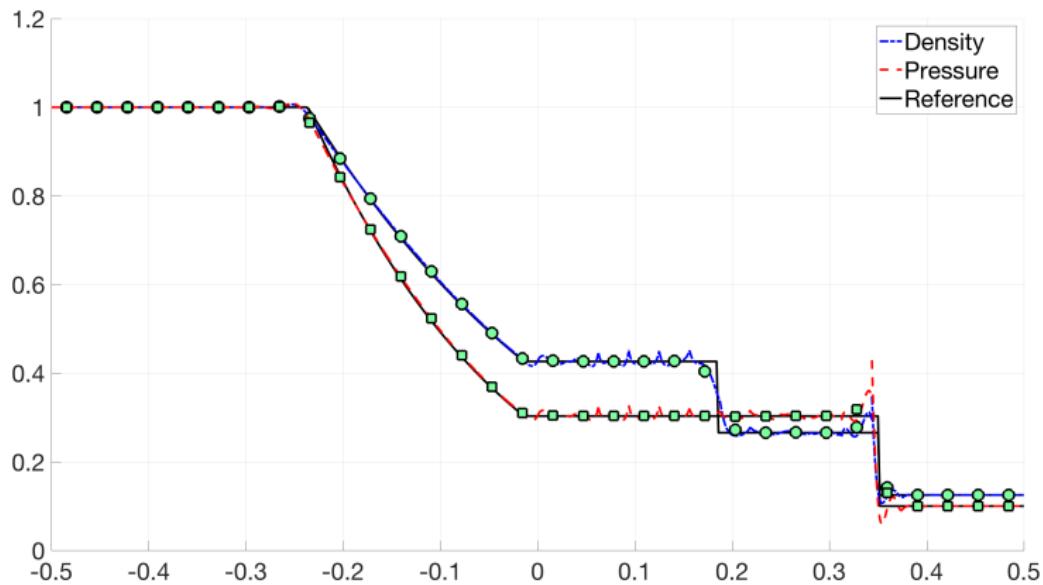


(b) $\rho(x), u(x)$ ($N = 4, K = 16$)

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

1D Sod shock tube

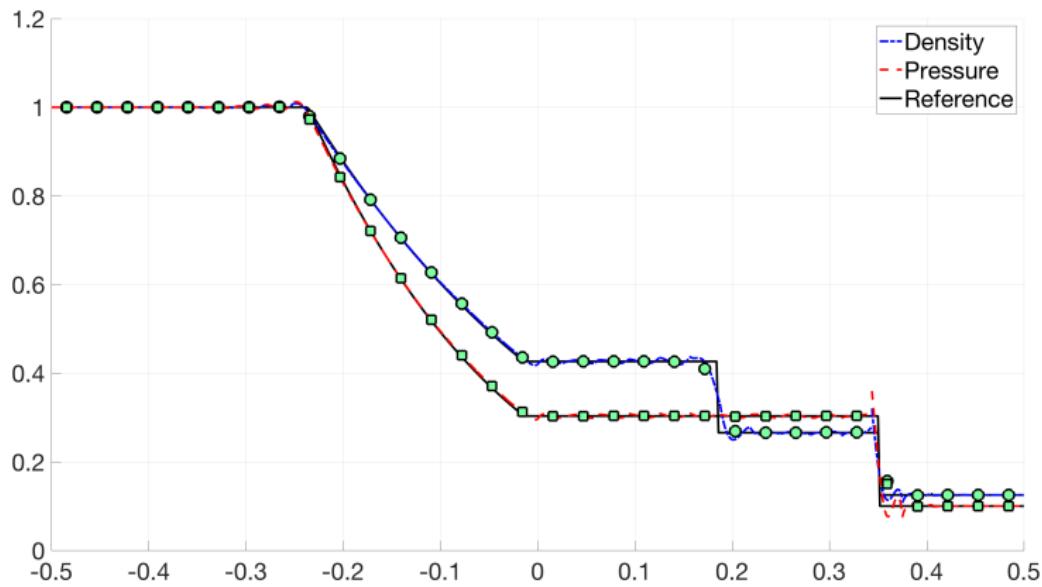
- Circles are cell averages, CFL of .125, LSRK-45 time-stepping.
- Comparison between $(N + 1)$ -point Lobatto and $(N + 2)$ -point Gauss.



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

1D Sod shock tube

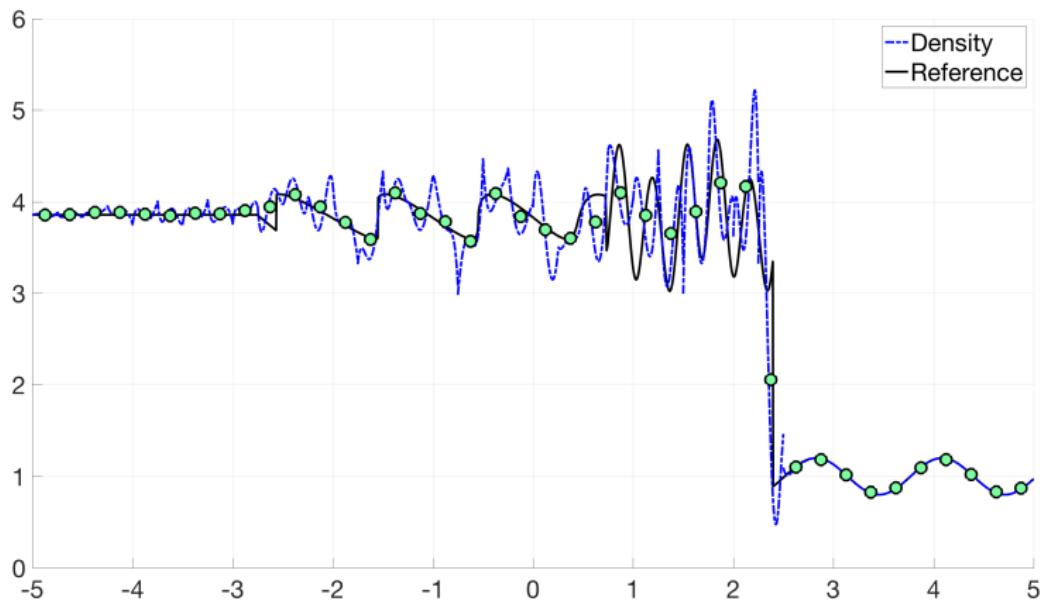
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$N = 4, K = 32, (N + 2)$ point Gauss quadrature.

1D sine-shock interaction

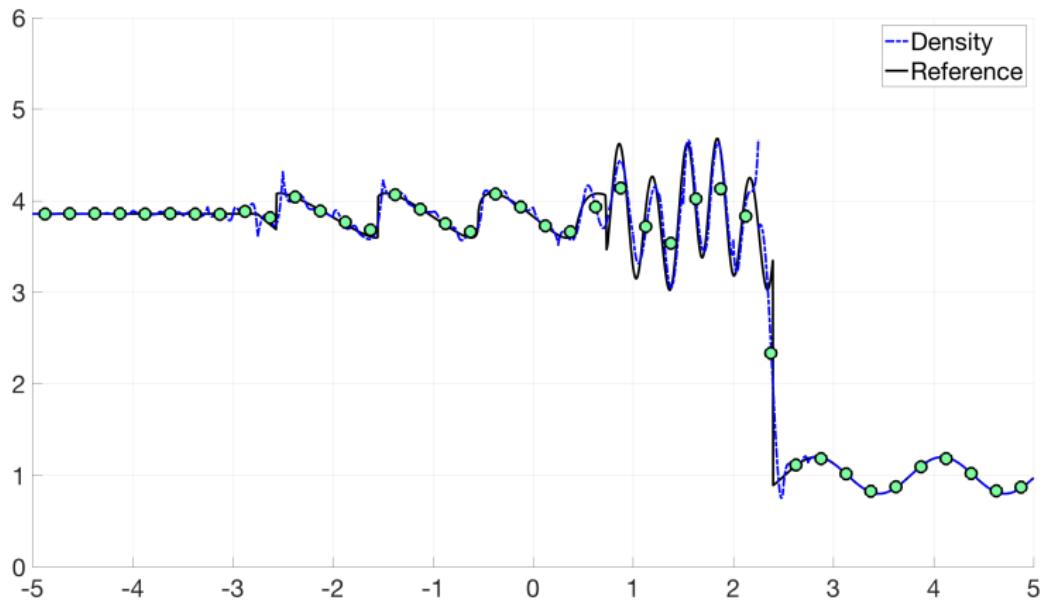
- $(N + 2)$ -point Gauss needs a smaller CFL (.05 vs .125) for stability.



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

1D sine-shock interaction

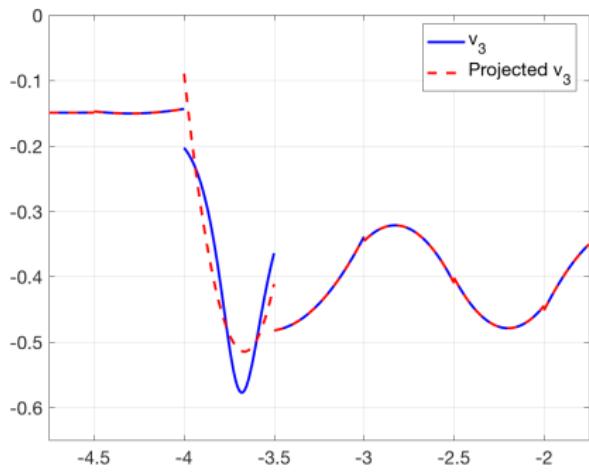
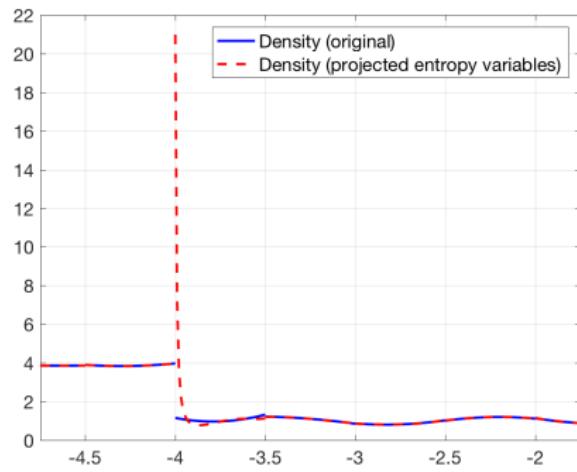
- $(N + 2)$ -point Gauss needs a smaller CFL (.05 vs .125) for stability.



$N = 4, K = 40, \text{CFL} = .05, (N + 2)$ 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) $\rho(x), \rho((P_N \mathbf{v})(x))$

Taylor-Green vortex

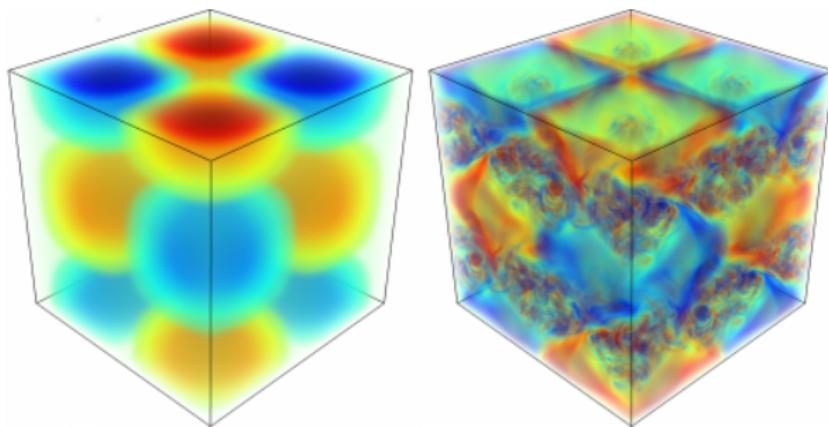


Figure: Isocontours of z -vorticity for Taylor-Green at $t = 0, 10$ seconds.

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

3D inviscid Taylor-Green vortex

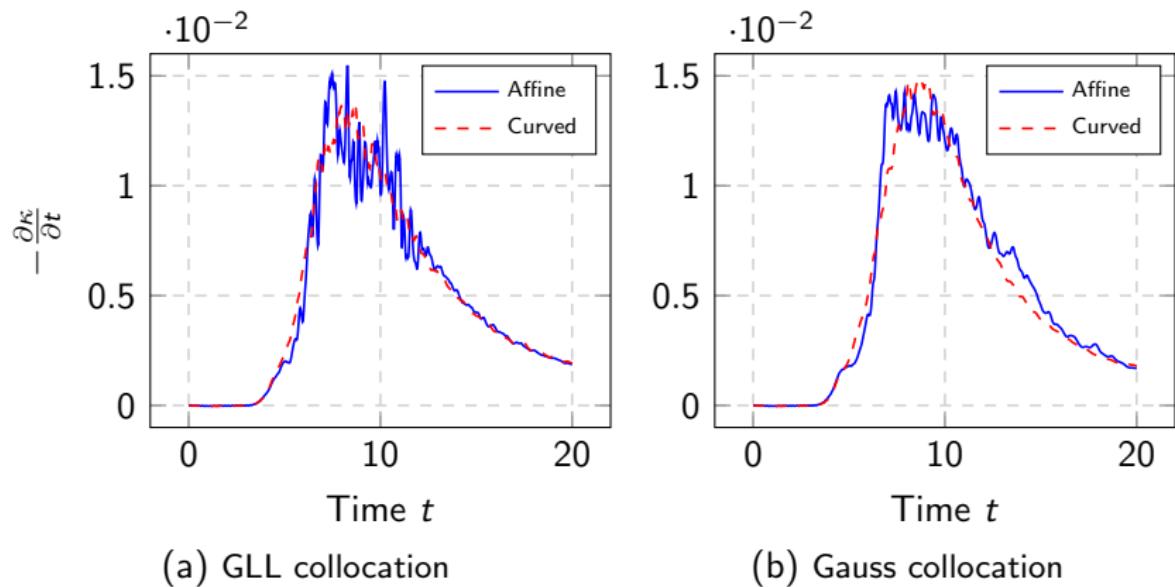


Figure: Kinetic energy dissipation rate for entropy stable GLL and Gauss collocation schemes with $N = 7$ and $h = \pi/8$.

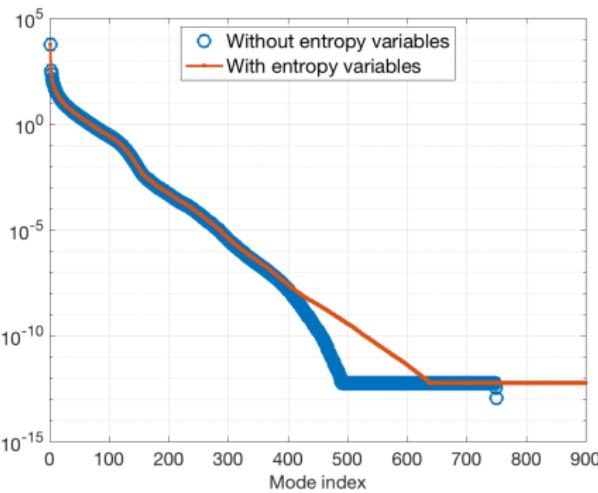
Determining empirical cubature points (ECP) and weights

- Goal: integrate a target basis to some accuracy.
- Offline step: greedy selection of hyper-reduction points
 - Project residual onto remaining rows of basis matrix.
 - Find “most positive” point of projected residual.
 - Solve (nonlinear) least squares for (positive) quadrature weights.
- Target basis: products of modes

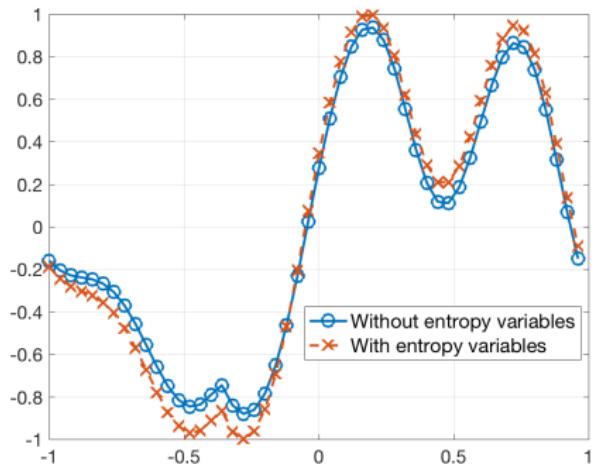
$$\text{span} \left\{ \phi_i(\mathbf{x})\phi_j(\mathbf{x}), \quad 1 \leq i, j \leq N \right\}.$$

Reduce costs by substituting leading POD modes.

Enriching snapshots with entropy variables



(a) Singular values



(b) Fifth singular vector

Figure: Snapshot singular values and reduced basis functions with and without entropy variable enrichment.