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

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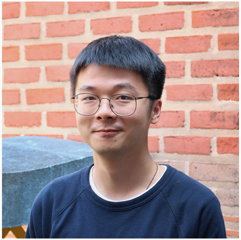
Collaborators

Tim Warburton (VT)

Mario Bencomo (postdoc, adjoints)

Philip Wu (GPU + shallow water)

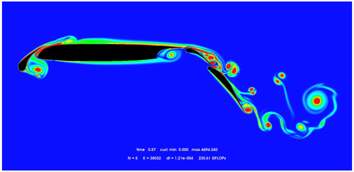


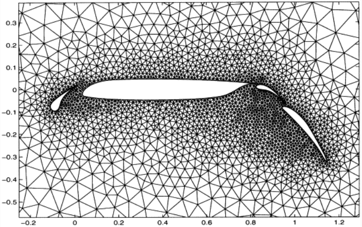
Yimin Lin (GPU + compressible flow)

Christina Taylor (implicit + ROMs?)

High order finite element methods for hyperbolic PDEs

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





Mesh from Slawig 2001.

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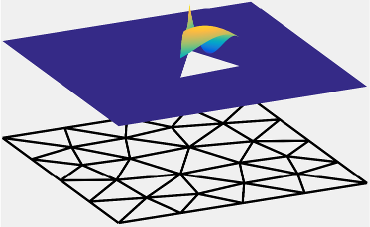
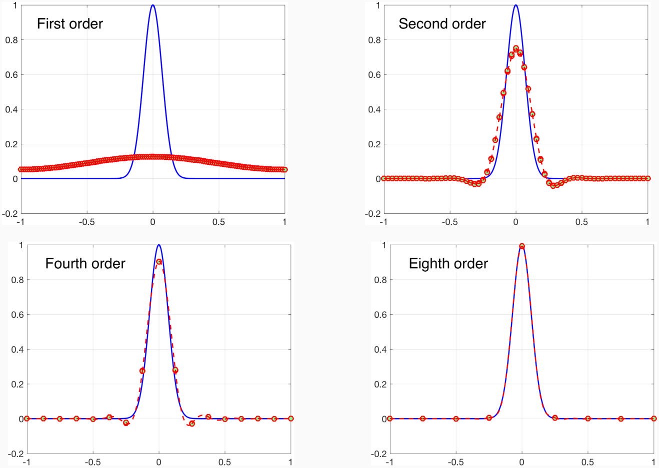
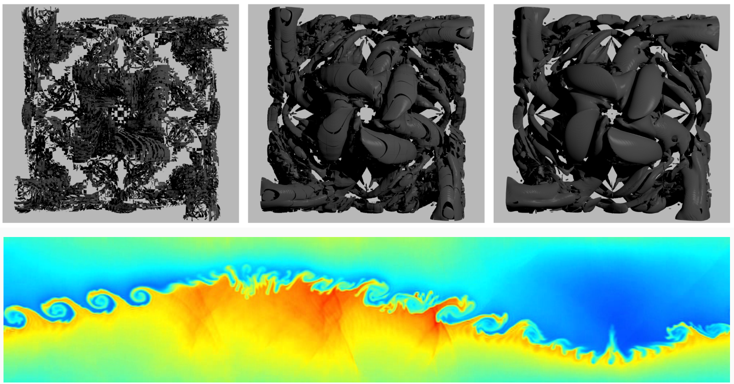


Why high order accuracy?



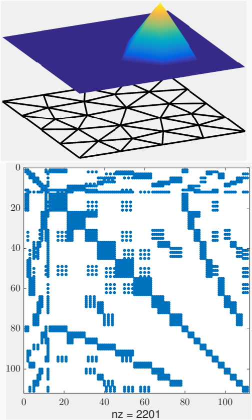
High order accurate resolution of propagating vortices and waves.

Why high order accuracy?

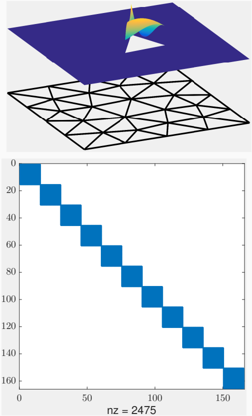


2nd, 4th, and 16th order Taylor-Green (top), 8th order Kelvin-Helmholtz (bottom). Vorticular structures and acoustic waves are both sensitive to numerical dissipation. Results from Beck and Gassner (2013) and Per-Olof Persson's website.

Why discontinuous Galerkin methods?



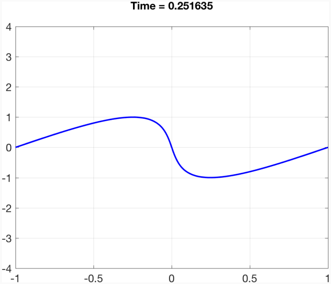
(a) High order FEM



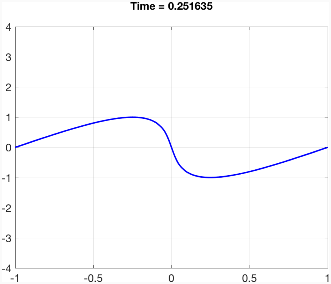
(b) High order DG

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

Why *not* high order DG methods?



(a) Exact solution



(b) 8th order DG

High order methods blow up for under-resolved solutions of nonlinear conservation laws (e.g., shocks and turbulence).

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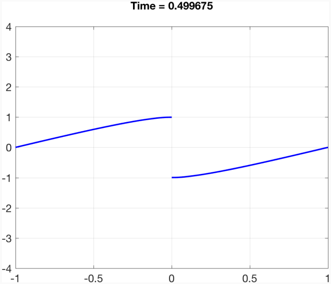

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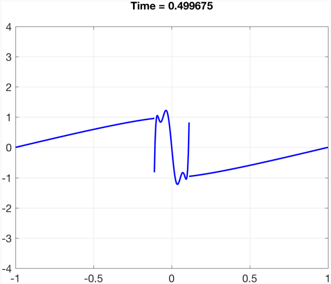

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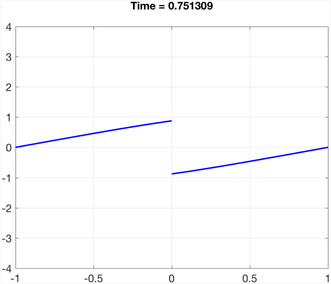

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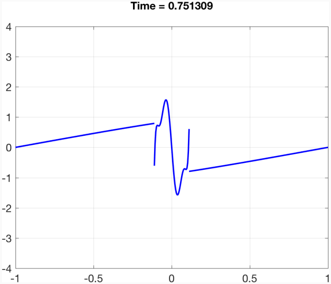

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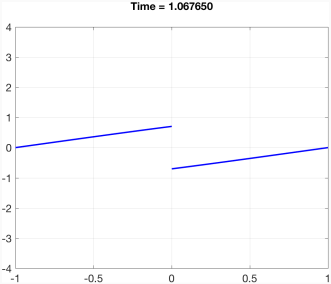

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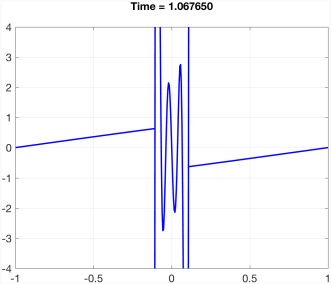


(b) 8th order DG

High order methods blow up for under-resolved solutions of nonlinear conservation laws (e.g., shocks and turbulence).

Why entropy stability for high order schemes?

In practice, high order schemes need solution regularization (e.g., artificial viscosity, filtering, slope limiting).

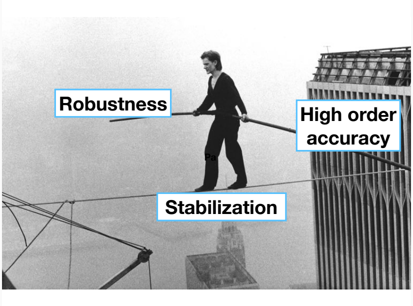
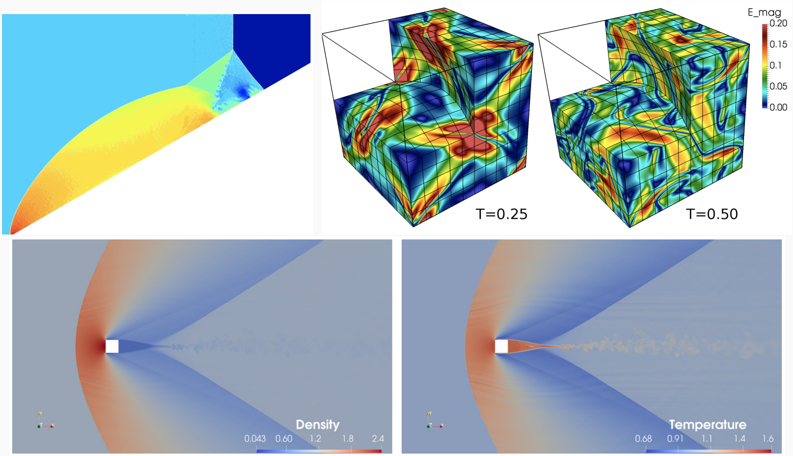


Image adapted from "Man On Wire" (2008)

- Goal: stability independent of solution regularization.
- Entropy stable schemes: improve robustness without reducing accuracy.

Finite volume methods: Tadmor, Chandrashekar, Ray, Svard, Fjordholm, Mishra, LeFloch, Rohde, ...
High order tensor product elements: Fisher, Carpenter, Gassner, Winters, Kopriva, Persson, ...
High order general elements: Chen and Shu, Crean, Hicken, Del Rey Fernandez, Zingg, ...

Examples of high order entropy stable simulations



All simulations run without artificial viscosity, filtering, or slope limiting.

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

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

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

Entropy conservative/stable finite volume methods

Entropy stability for nonlinear problems

- Energy balance for nonlinear conservation laws (Burgers', shallow water, compressible Euler + Navier-Stokes).

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

- Continuous entropy inequality: convex entropy function $S(\boldsymbol{u})$, "entropy potential" $\psi(\boldsymbol{u})$, entropy variables $\boldsymbol{v}(\boldsymbol{u})$

$$\int_\Omega \boldsymbol{v}^T \left(\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x}\right) = 0, \qquad \boxed{\boldsymbol{v}(\boldsymbol{u}) = \frac{\partial S}{\partial \boldsymbol{u}}}$$

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

Entropy conservative finite volume methods

- Finite volume scheme:

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{dt}} + \frac{\boldsymbol{f}_S(\mathbf{u}_{i+1}, \mathbf{u}_i) - \boldsymbol{f}_S(\mathbf{u}_{i+1}, \mathbf{u}_i)}{h} = \mathbf{0}.$$

- Take $\boldsymbol{f}_S$ to be an entropy conservative numerical flux

$$\begin{aligned} \boldsymbol{f}_S(\boldsymbol{u}, \boldsymbol{u}) &= \boldsymbol{f}(\boldsymbol{u}), && \text{(consistency)} \\ \boldsymbol{f}_S(\boldsymbol{u}, \boldsymbol{v}) &= \boldsymbol{f}_S(\boldsymbol{v}, \boldsymbol{u}), && \text{(symmetry)} \\ (\boldsymbol{v}_L - \boldsymbol{v}_R)^T \boldsymbol{f}_S(\boldsymbol{u}_L, \boldsymbol{u}_R) &= \psi_L - \psi_R, && \text{(conservation).} \end{aligned}$$

- Can show numerical scheme conserves entropy

$$\int_\Omega \frac{\partial S(\boldsymbol{u})}{\partial t} \approx \sum_i h \frac{\mathrm{d}S(\mathbf{u}_i)}{\mathrm{dt}} = 0.$$

Tadmor (1987). *The numerical viscosity of entropy stable schemes for systems of conservation laws.*

Entropy stable finite volume methods

- Finite volume scheme with dissipation $\mathbf{d}(\mathbf{u})$:

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{dt}} + \frac{\boldsymbol{f}_S(\mathbf{u}_{i+1}, \mathbf{u}_i) - \boldsymbol{f}_S(\mathbf{u}_{i+1}, \mathbf{u}_i)}{h} = \mathbf{d}(\mathbf{u}).$$

- Take $\boldsymbol{f}_S$ to be an entropy conservative numerical flux

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- Can show numerical scheme dissipates entropy

$$\int_\Omega \frac{\partial S(\boldsymbol{u})}{\partial t} \approx \sum_i h \frac{\mathrm{d}S(\mathbf{u}_i)}{\mathrm{dt}} = \mathbf{v}^T \mathbf{d}(\mathbf{u}) \overset{?}{\leq} 0.$$

Tadmor (1987). *The numerical viscosity of entropy stable schemes for systems of conservation laws.*

Example of EC fluxes (compressible Euler equations)

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

$$
\begin{aligned}
f_S^1(\boldsymbol{u}_L, \boldsymbol{u}_R) &= \{\{\rho\}\}^{\log} \{\{u\}\} \\
f_S^2(\boldsymbol{u}_L, \boldsymbol{u}_R) &= \{\{u\}\} f_S^1 + p_{\text{avg}} \\
f_S^3(\boldsymbol{u}_L, \boldsymbol{u}_R) &= (E_{\text{avg}} + p_{\text{avg}}) \{\{u\}\},
\end{aligned}
$$

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

- Non-standard logarithmic mean, "inverse temperature" β

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

Chandreshekar (2013), *Kinetic energy preserving and entropy stable finite volume schemes for the compressible Euler and Navier-Stokes equations.*

Matrix reformulation using Hadamard products

Hadamard product of two matrices $\mathbf{A} \circ \mathbf{B}$

$$\begin{bmatrix} \mathbf{A}_{11} & \dots & \mathbf{A}_{1n} \\ \vdots & \ddots & \vdots \\ \mathbf{A}_{n1} & \dots & \mathbf{A}_{nn} \end{bmatrix} \circ \begin{bmatrix} \mathbf{B}_{11} & \dots & \mathbf{B}_{1n} \\ \vdots & \ddots & \vdots \\ \mathbf{B}_{n1} & \dots & \mathbf{B}_{nn} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{11}\mathbf{B}_{11} & \dots & \mathbf{A}_{1n}\mathbf{B}_{1n} \\ \vdots & \ddots & \vdots \\ \mathbf{A}_{n1}\mathbf{B}_{n1} & \dots & \mathbf{A}_{nn}\mathbf{B}_{nn} \end{bmatrix}.$$

Rewrite an N-point (periodic) finite volume scheme as

$$\frac{\mathrm{d}}{\mathrm{dt}} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_N \end{bmatrix} + \frac{1}{h} \begin{bmatrix} \boldsymbol{f}_S(\mathbf{u}_1, \mathbf{u}_2) - \boldsymbol{f}_S(\mathbf{u}_N, \mathbf{u}_1) \\ \boldsymbol{f}_S(\mathbf{u}_2, \mathbf{u}_3) - \boldsymbol{f}_S(\mathbf{u}_1, \mathbf{u}_2) \\ \vdots \\ \boldsymbol{f}_S(\mathbf{u}_N, \mathbf{u}_1) - \boldsymbol{f}_S(\mathbf{u}_{N-1}, \mathbf{u}_N) \end{bmatrix} = \mathbf{0}.$$

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$$h\frac{\mathrm{d}}{\mathrm{dt}} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_N \end{bmatrix} + \begin{bmatrix} \mathbf{F}_{1,2} - \mathbf{F}_{1,N} \\ \mathbf{F}_{2,3} - \mathbf{F}_{2,1} \\ \vdots \\ \mathbf{F}_{N,1} - \mathbf{F}_{N,N-1} \end{bmatrix} = \mathbf{0}, \qquad \mathbf{F}_{ij} = \boldsymbol{f}_S(\mathbf{u}_i, \mathbf{u}_j).$$

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$$\begin{bmatrix} \mathbf{F}_{1,2} - \mathbf{F}_{1,N} \\ \mathbf{F}_{2,3} - \mathbf{F}_{2,1} \\ \vdots \\ \mathbf{F}_{N,1} - \mathbf{F}_{N,N-1} \end{bmatrix} = \left(\begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & 1 \\ 1 & & -1 & 0 \end{bmatrix} \circ \begin{bmatrix} \mathbf{F}_{1,1} & \dots & \mathbf{F}_{1,N} \\ \vdots & \ddots & \vdots \\ \mathbf{F}_{N,1} & \dots & \mathbf{F}_{N,N} \end{bmatrix} \right) \mathbf{1}.$$

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Rewrite an N-point (periodic) finite volume scheme as

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Interpretation using finite difference matrices

Let $\mathbf{M} = h\mathbf{I}$. Can reformulate entropy conservative finite volumes as

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + 2\left(\mathbf{Q} \circ \mathbf{F}\right)\mathbf{1} = \mathbf{0}, \qquad \mathbf{Q} = \frac{1}{2}\begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & 1 \\ 1 & & -1 & 0 \end{bmatrix}$$

Note: $\mathbf{M}^{-1}\mathbf{Q}$ is a 2nd order (periodic) differentiation matrix.

Key observation: generalizable beyond finite volumes

Entropy conservation for any $\underbrace{\mathbf{Q} = -\mathbf{Q}^T}_{\text{skew-symmetry}}$ and $\underbrace{\mathbf{Q}\mathbf{1} = \mathbf{0}}_{\text{conservative}}$!

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Boundary conditions and summation-by-parts (SBP) property

Boundary conditions: choose appropriate "ghost" values $\mathbf{u}_1^+, \mathbf{u}_N^+$

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + 2\left(\mathbf{Q} \circ \mathbf{F}\right)\mathbf{1} + \mathbf{B}\begin{bmatrix} \boldsymbol{f}_S(\mathbf{u}_1^+, \mathbf{u}_1) - \boldsymbol{f}(\mathbf{u}_1) \\ \mathbf{0} \\ \boldsymbol{f}_S(\mathbf{u}_N^+, \mathbf{u}_N) - \boldsymbol{f}(\mathbf{u}_N) \end{bmatrix} = \mathbf{0}.$$

Entropy stable if $\mathbf{Q}$ satisfies a summation-by-parts (SBP) property

$$\mathbf{Q} = \frac{1}{2}\begin{bmatrix} -1 & 1 & & 0 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & 1 \\ & & -1 & 1 \end{bmatrix}, \qquad \mathbf{Q}+\mathbf{Q}^T = \mathbf{B} = \begin{bmatrix} -1 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}.$$

Main innovation: fully algebraic proof of entropy stability

- Discrete analogue of the entropy identity

$$\boxed{\int_{-1}^{1} \boldsymbol{v}^T \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = \mathbf{v}^T \boldsymbol{f}(\mathbf{u}) - \psi(\mathbf{u})\Big|_{-1}^{1}} \iff \boxed{\begin{aligned} &\mathbf{v}^T \left(2\mathbf{Q} \circ \mathbf{F}\right) \mathbf{1} \\ &= \mathbf{1}^T \mathbf{B} \left(\mathbf{v}^T \boldsymbol{f}(\mathbf{u}) - \psi(\mathbf{u})\right) \end{aligned}}$$

- Key step in proof: use entropy conservative property of flux on skew-symmetric form of $\mathbf{v}^T \left(2\mathbf{Q} \circ \mathbf{F}\right) \mathbf{1}$

$$\mathbf{v}^T \left(\left(\mathbf{Q} - \mathbf{Q}^T\right) \circ \mathbf{F}\right) \mathbf{1} = \sum_{ij} \mathbf{Q}_{ij} \underbrace{\left(\mathbf{v}_i - \mathbf{v}_j\right)^T \boldsymbol{f}_S\left(\mathbf{u}_i, \mathbf{u}_j\right)}_{\left(\psi(\mathbf{u}_i) - \psi(\mathbf{u}_j)\right)}$$

Tadmor (1987), Carpenter et al. (2014), Gassner, Winters, and Kopriva (2016).

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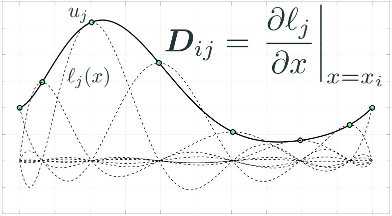
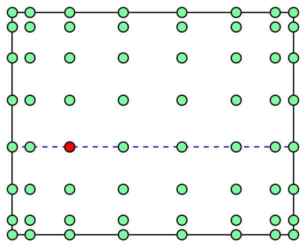
Tadmor (1987), Carpenter et al. (2014), Gassner, Winters, and Kopriva (2016).

Extension to high order summation by parts (SBP) schemes





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

$$\sum_j \mathbf{D}_{ij} = 0 \quad \Longrightarrow \quad \mathbf{D}\mathbf{1} = \mathbf{0}.$$

- Lobatto quadrature nodes recover summation-by-parts (SBP) property! Let $\mathbf{M}$ = lumped diagonal mass matrix:

$$\mathbf{Q} = \mathbf{M}\mathbf{D}, \qquad \boxed{\mathbf{Q} + \mathbf{Q}^T = \mathbf{B}}.$$

Extension to high order DG methods (e.g., multiple elements)

- If $\mathbf{Q}$ is conservative $(\mathbf{Q1} = \mathbf{0})$ and satisfies summation-by-parts (SBP) property, then DG formulation is entropy *conservative*

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

- Generalizes to arbitrarily high polynomial degree N.
- Adding interface dissipation (e.g., Lax-Friedrichs) yields an entropy stable DG scheme.

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

Fisher and Carpenter (2014), Gassner, Winters, and Kopriva (2016), Chen and Shu (2017), etc.

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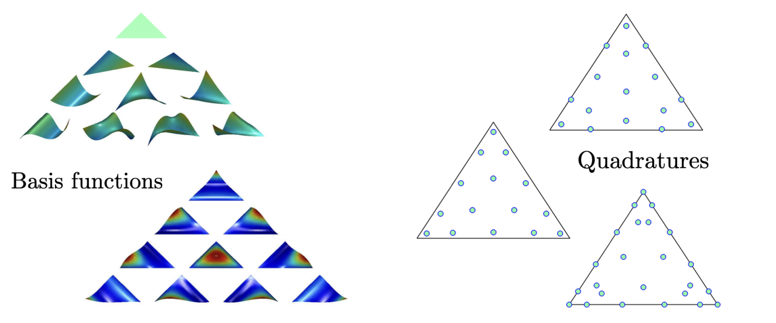
Entropy stable modal discontinuous Galerkin formulations

Why "modal" formulations?

Nodal formulations: tied to a specific set of nodes.
"Modal" formulations: arbitrary basis functions and quadrature.



Enables use of standard tools in finite elements.

Figures from http://www2.compute.dtu.dk/ apek/DGFEMCourse2009/Lecture05.pdf.

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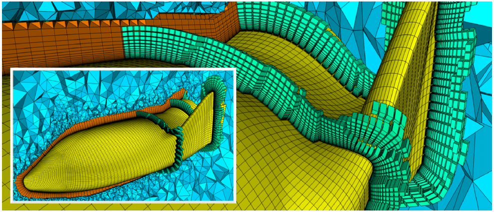

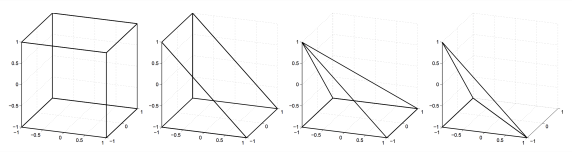

Applicable for any type of reference element.

https://www.pointwise.com/news/2014/Hybrid-Hex-Tet-Meshing-Latest-Pointwise-Release.html.

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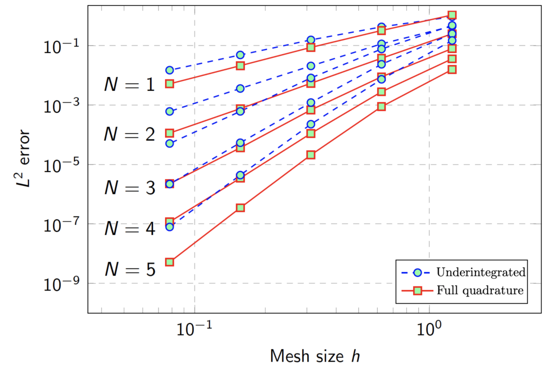

Can avoid *underintegration errors* for nonlinear terms + curved elements.

Wu, Chan, Kubatko (2020). *High-order ESDG methods for the shallow water equations ...*

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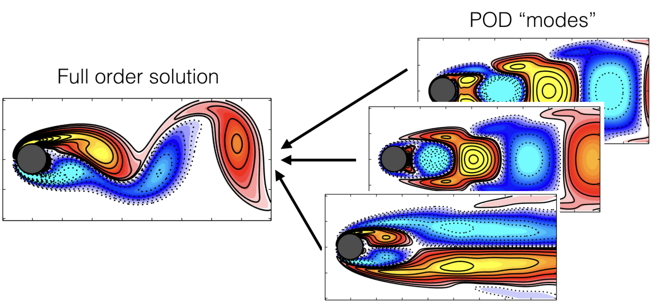

Projection-based reduced order models: learn basis functions from data.

Figure adapted from Brunton, Proctor, Kutz (2016), *Discovering governing equations from data* . . . .

Challenge 1 for modal formulations: entropy projection

- Test functions must be polynomial. Entropy variables are not.

- If $\boldsymbol{u}_N$ is polynomial, testing with L^2 projection of entropy variables $\Pi_N \boldsymbol{v}\left(\boldsymbol{u}_N\right)$ recovers rate of change of entropy

$$\int_{D^k} \Pi_N \boldsymbol{v}\left(\boldsymbol{u}_N\right)^T \frac{\partial \boldsymbol{u}_N}{\partial t} = \int_{D^k} \underbrace{\boldsymbol{v}\left(\boldsymbol{u}_N\right)^T}_{\frac{\partial S(\boldsymbol{u})}{\partial \boldsymbol{u}}} \frac{\partial \boldsymbol{u}_N}{\partial t} = \int_{D^k} \frac{\partial S(\boldsymbol{u}_N)}{\partial t}$$

- For consistency, must also evaluate fluxes using projected entropy variables $\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(\Pi_N \boldsymbol{v}\left(\boldsymbol{u}_N\right)\right)$.

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

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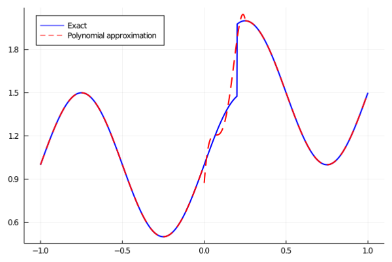
Illustration of entropy projection: $N = 4$, 8 elements



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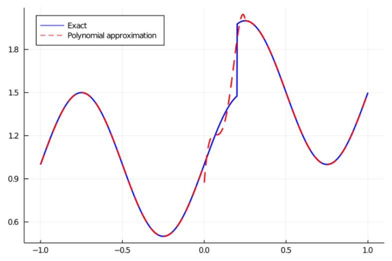

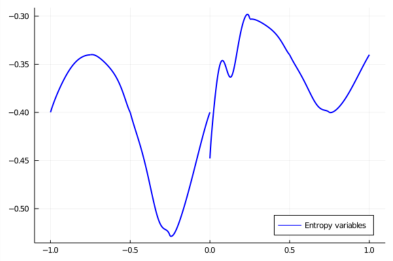

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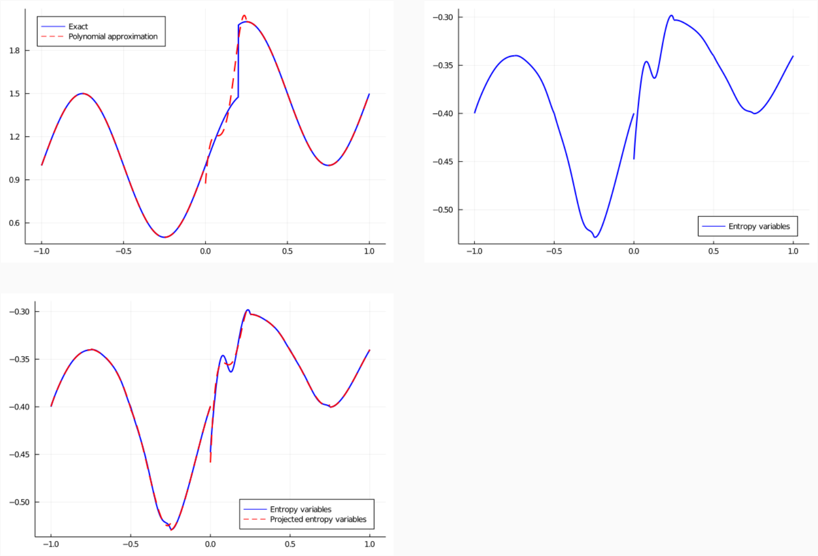

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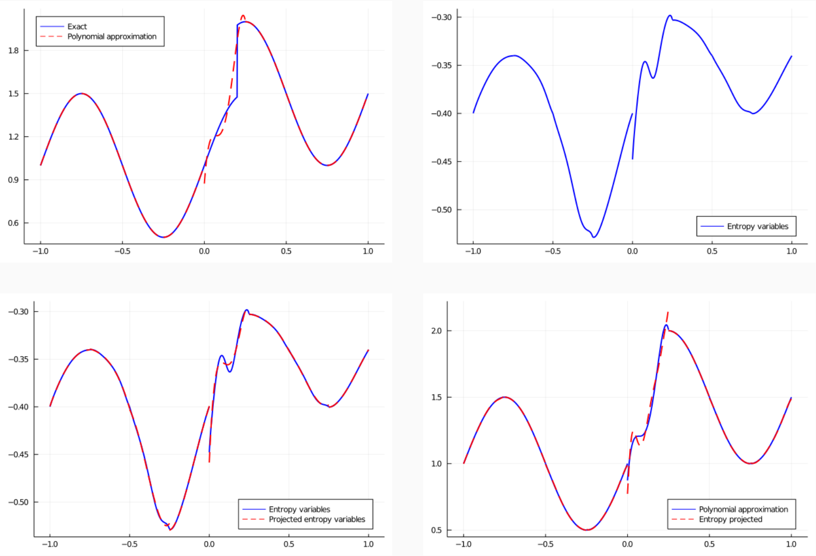
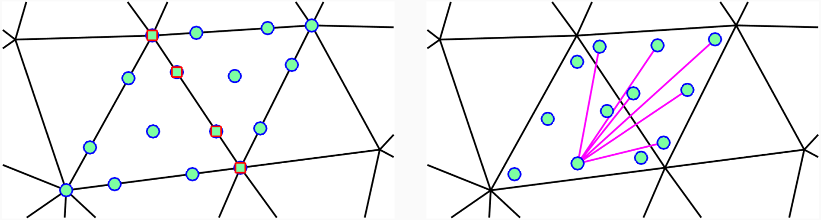


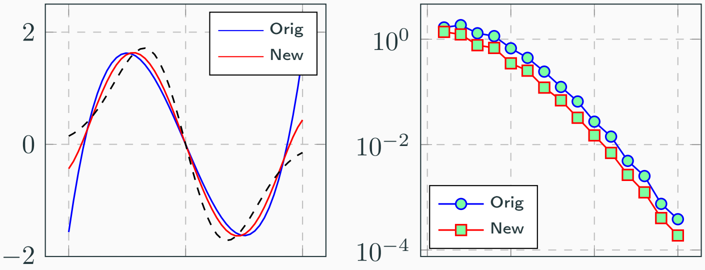
Challenge 2 for modal formulations: interface coupling



Entropy stable interface coupling with/without boundary nodes

- Interface fluxes must be designed to cancel other boundary terms in the discrete entropy balance.
- Entropy stable interface fluxes previously involved all-to-all coupling between nodes on different elements.

Efficient interface fluxes via "hybridization"



(a) Approximated derivatives **(b)** L^2 error, degree $N = 1, \ldots, 15$

- Use an expanded *hybridized* SBP operator, where **E** is a face extrapolation matrix.

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

- Akin to adding correction terms similar to "$\mathbf{E}f(\mathbf{u}) - f(\mathbf{E}\mathbf{u})$".

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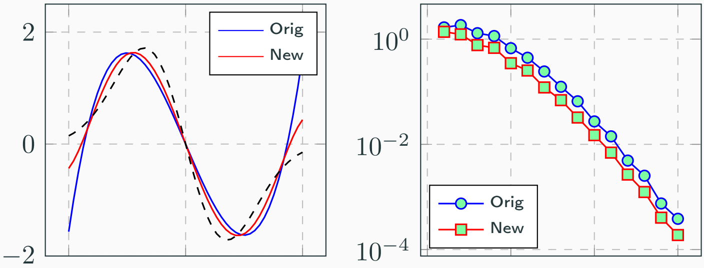

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$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + 2\left(\mathbf{Q} \circ \mathbf{F}\right)\mathbf{1} + \mathbf{B}\left(\mathbf{f}^* - \boldsymbol{f}(\mathbf{u})\right) = 0.$$

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

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- Entropy stability if conservative ($\mathbf{Q}_h\mathbf{1} = \mathbf{0}$). Equivalent to weak SBP condition related to quadrature accuracy.

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

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

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

Entropy stable schemes using hybridized SBP operators

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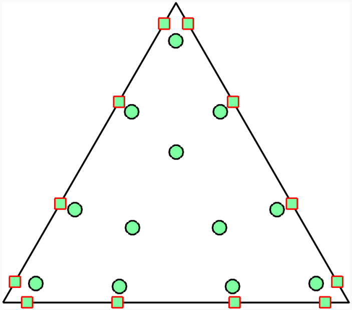
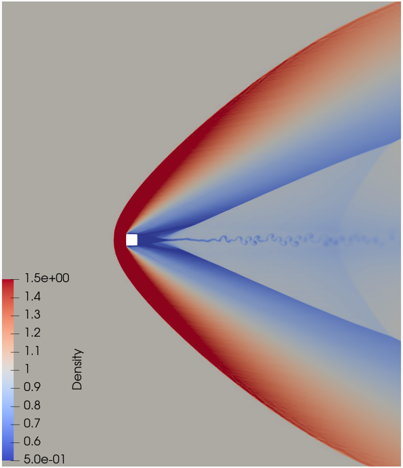
- Degree N polynomial approximation + degree $\geq 2N$ volume/face quadratures.
- Uniform 32×32 mesh: degree $N = 3$, CFL $.125$, only dissipation from DG interface penalization.



Results computed on larger periodic domain ("natural" boundary conditions not entropy stable).

Recent applications of the modal ESDG formulation

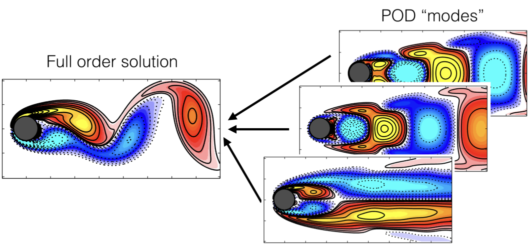


Degree $N = 3$, 16574 triangular elements (~ 4 per cylinder side). $T_{\text{final}} = 100$, $\mathrm{Re} = 10^4$, $\mathrm{Ma} = 1.5$.

- Quad/hex non-conforming meshes (with Bencomo, Fernandez, Carpenter)
- Shallow water + networks (with Wu, Kubatko)
- $\Longleftarrow$ Compressible Navier-Stokes (with Lin, Warburton)
- Reduced order modeling
- Jacobian matrices, time-implicit solvers (with Taylor)

Reduced order modeling

Projection-based reduced order models (ROMs)



- Goal: reduce cost of many-query scenarios.
- 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, but not for nonlinear hyperbolic problems!

Figure adapted from Brunton, Proctor, Kutz (2016), *Discovering governing equations from data . . . .*

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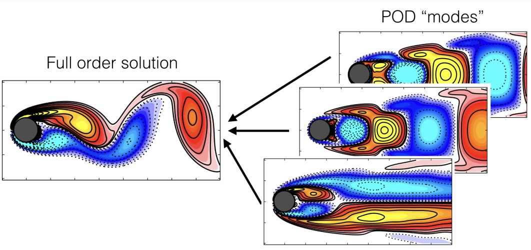

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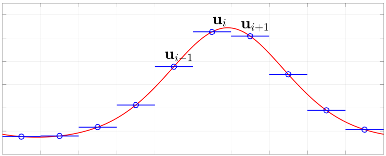
Full order model: entropy stable finite volumes



- Discretize integrated form of nonlinear conservation law

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

- Let $\boldsymbol{M} = (\Delta x)\boldsymbol{I}$, assume periodicity

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

Naive POD-Galerkin procedure

- (Offline) POD from solution component snapshots.
- (Online) Galerkin projection of the matrix system

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

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

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

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

Evaluating nonlinear ROM terms dominates costs

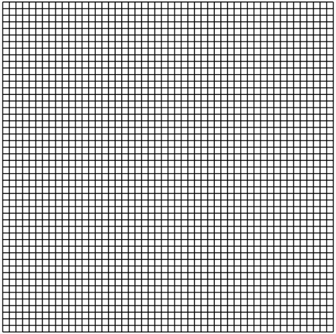
Problem: cost of evaluating ROM nonlinear terms scales with number of grid points! Cost still scales with size of full order model.

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

- Hyper-reduction approximates nonlinear evaluations.

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

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



Hernandez et al., Bui/Willcox, Chantarantabut/Sorensen, Farhat et al. Patera/Yano, ...

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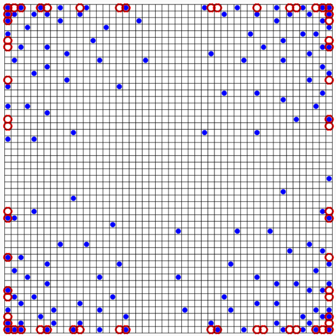

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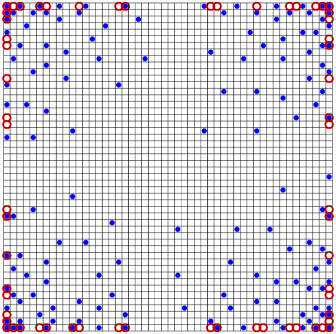
$$\widetilde{\mathbf{u}} = \boldsymbol{u}\left(\mathbf{V}\mathbf{V}^{\dagger}\boldsymbol{v}\left(\mathbf{V}\mathbf{u}_N\right)\right), \qquad 2\left(\mathbf{Q} \circ \mathbf{F}\right)\mathbf{1}$$

- Hyper-reduction approximates nonlinear evaluations.

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

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



Hernandez et al., Bui/Willcox, Chantarantabut/Sorensen, Farhat et al. Patera/Yano, ...

Entropy stability and standard hyper-reduction

- Hyper-reduce $(\mathbf{Q} \circ \mathbf{F})$: construct "sampled" $\mathbf{Q}_s$ from $\mathbf{Q}$.
- Must preserve $\mathbf{Q}_s = -\mathbf{Q}_s^T$ 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 $\mathbf{Q}_e$.

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

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

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

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Two-step hyper-reduction: compress and project

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

$$\mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t, \qquad \mathbf{V}_t = \operatorname{orth}\left(\begin{bmatrix} \mathbf{V} & \mathbf{1} & \mathbf{QV} \end{bmatrix}\right)$$

- Step 2: use projection to determine coefficients in test basis

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

i.e., $\mathbf{P}_t$ uses hyper-reduced points/weights to project onto $\mathbf{V}_t$.

- Step 3: define

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

Then, $\mathbf{Q}_s$ is accurate, skew-symmetric, and conservative!

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Hyper-reduction: empirical cubature

- Construct approximate quadrature to integrates target space to some tolerance.
- Target space motivated by inner products of POD basis: most accurate + smallest number of points in practice

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

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Summary: entropy stable ROMs on periodic domains

- "Compress and project" hyper-reduction of $(\mathbf{Q} \circ \mathbf{F})$
  - 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:

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

$$\mathbf{F}_{ij} = \boldsymbol{f}_S \left(\widetilde{\mathbf{u}}_i, \widetilde{\mathbf{u}}_j \right), \quad \widetilde{\mathbf{u}} = \boldsymbol{u} \left(\mathbf{V}(\mathcal{I},:) \mathbf{P} \boldsymbol{v} \left(\mathbf{V}\mathbf{u}_N \right) \right),$$

where $\mathbf{P}$ is the projection onto POD modes.

- No free lunch: $O(N_s^2)$ vs $O(N_s)$ flux evaluations for ROM!

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Non-periodic boundary conditions

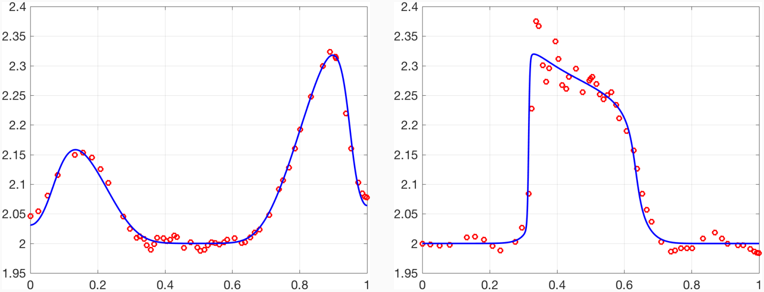
- Weakly impose BCs using hybridized SBP operators
- Can add entropy-dissipative penalization terms (e.g., Lax-Friedrichs penalization).
- In dimensions $d > 1$, entropy stability requires weak SBP property with surface interpolation matrix $\mathbf{V}_f$ + hyper-reduced surface weights $\mathbf{w}_f$.

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

Enforce conditions using constrained hyper-reduction + LP.

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 $\epsilon = 2 \times 10^{-4}$, 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

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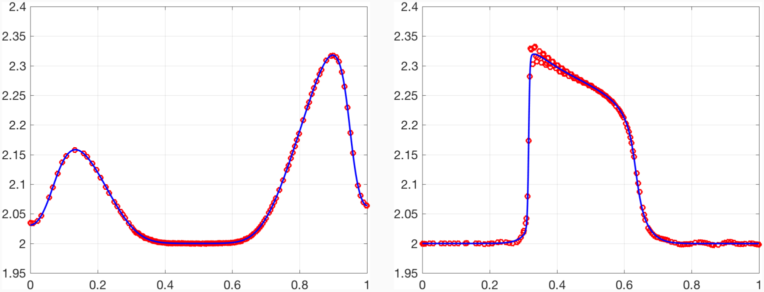

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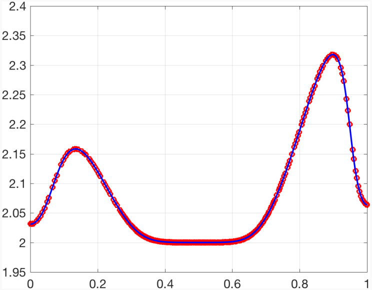

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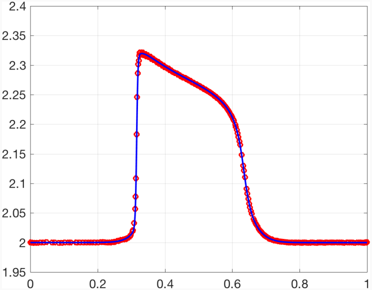

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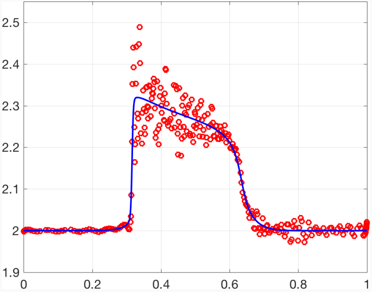
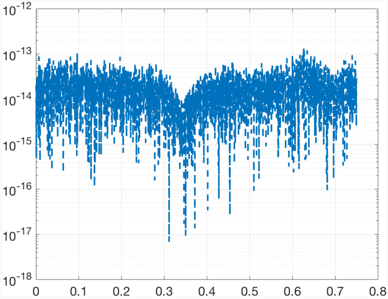
Entropy conservation test



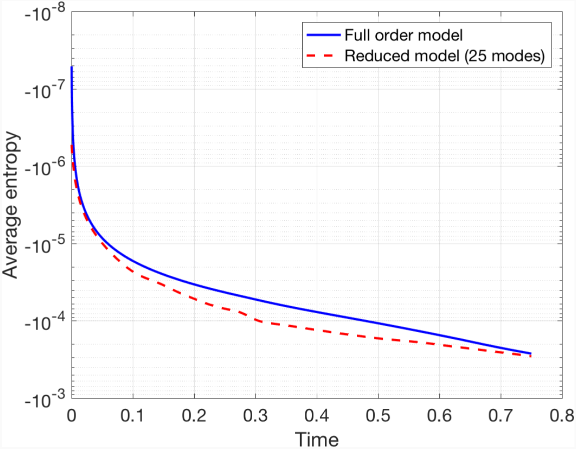
(a) Density ρ (125 modes, no viscosity)



(b) Convective entropy contribution

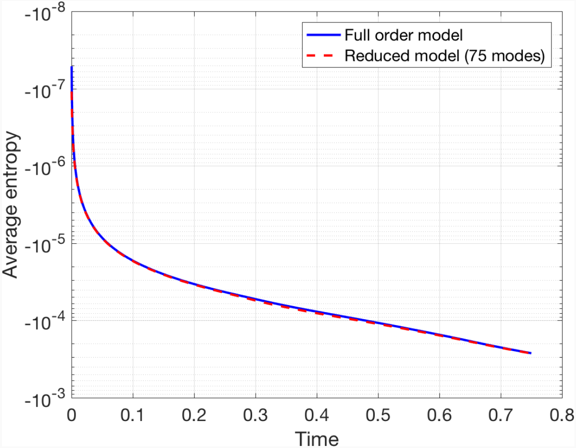
Figure 1: Reduced order solution and convective entropy RHS contribution $\left|\mathbf{v}_N^T \mathbf{V}_h^T \left(\mathbf{Q}_h \circ \mathbf{F}\right) \mathbf{1}\right|$ for the case of zero viscosity.

Evolution of average entropy



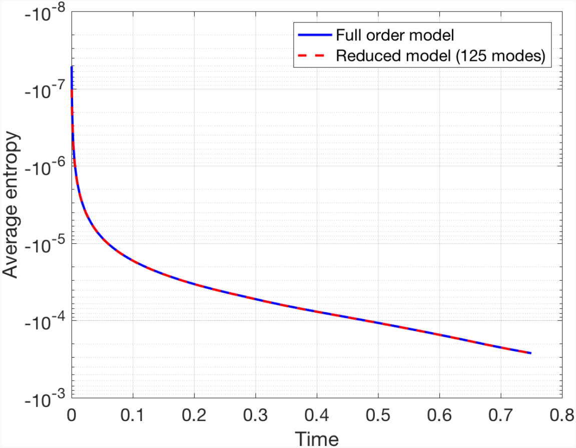
Average entropy over time (25 modes).

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

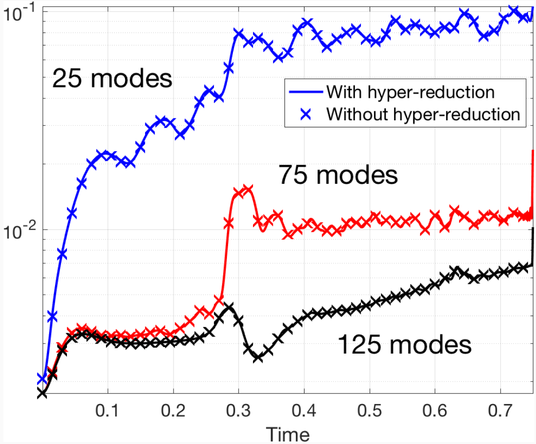
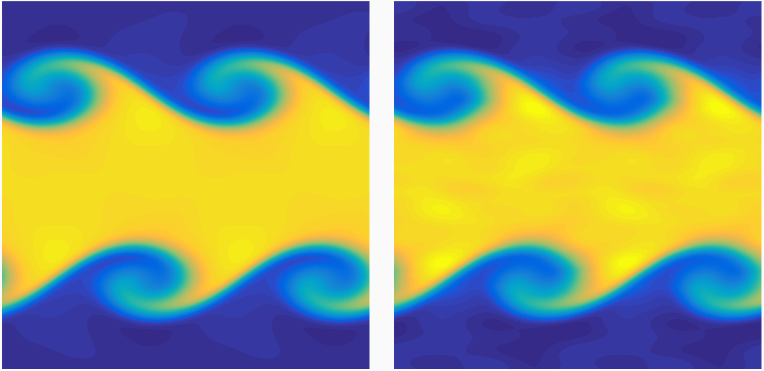


Figure 2: Error over time for a $K = 2500$ FOM and ROM with $25, 75, 125$ modes.

Smoothed 2D Kelvin-Helmholtz instability



(a) Density, full order model **(b)** Reduced order model

FOM with 40000 points, viscosity $\epsilon = 10^{-3}$. ROM with 75 modes, 884 reduced quadrature points, 1.02% relative L^2 error at $T = 3$.

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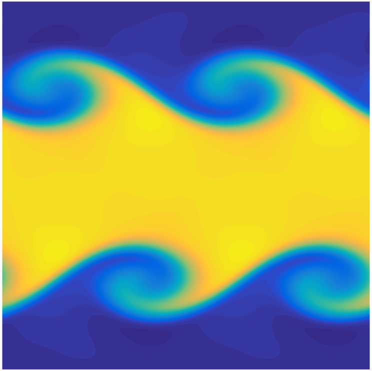
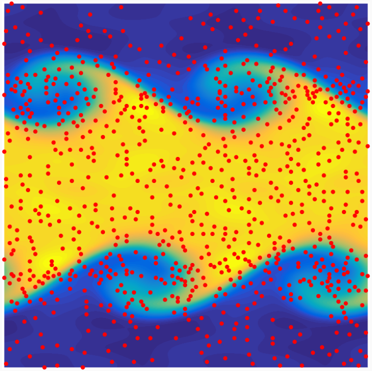


(c) Density, full order model



(d) ROM w/reduced quad. points

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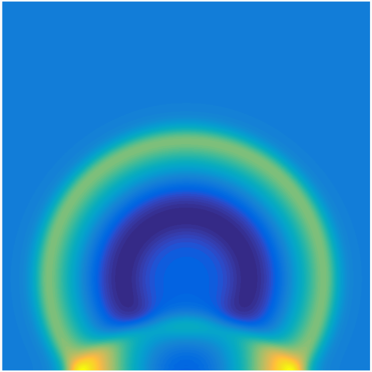
2D Gaussian pulse with reflective wall



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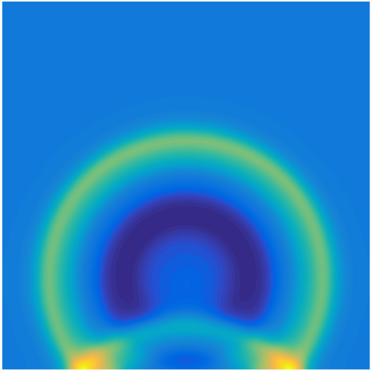

(b) Reduced order model

FOM with 10000 points, viscosity $\epsilon = 10^{-3}$. ROM with 25 modes, 306 reduced volume points, 82 reduced surface points, $.57\%$ error at $T = .25$.

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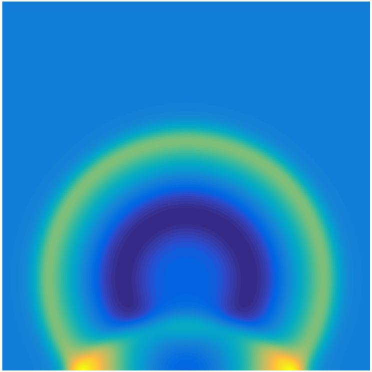

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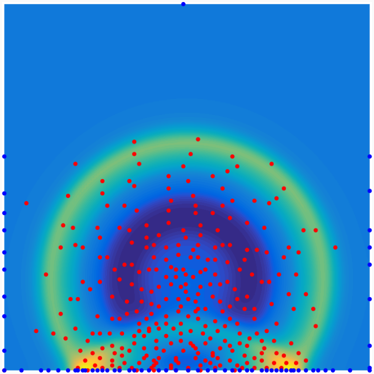

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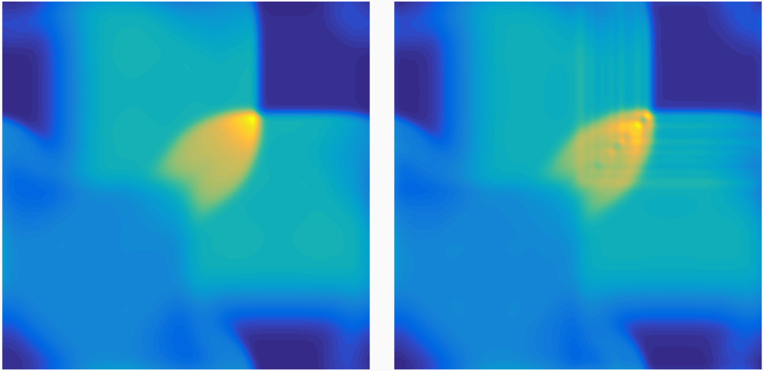
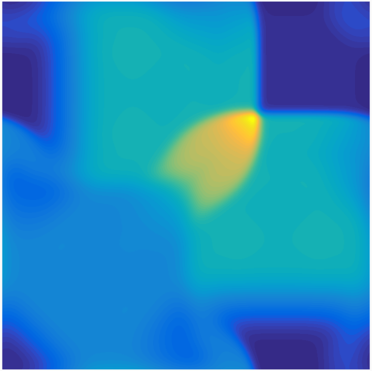
2D Riemann problem on periodic domain



(a) Full order model **(b)** Reduced order model, 50 modes

FOM with 40000 points, viscosity $\epsilon = 5 \times 10^{-3}$, $T = .25$. ROM with 50 modes, 812 reduced quadrature points, 3.278% relative L^2 error.

2D Riemann problem on periodic domain



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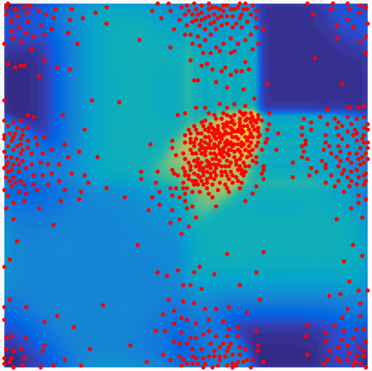

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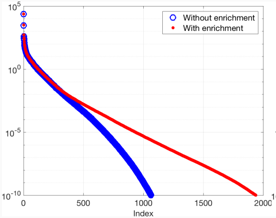
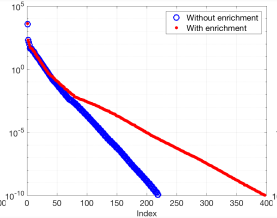
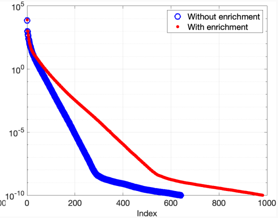
Singular value decay with entropy variable enrichment



(a) KH instability
(75 modes used)



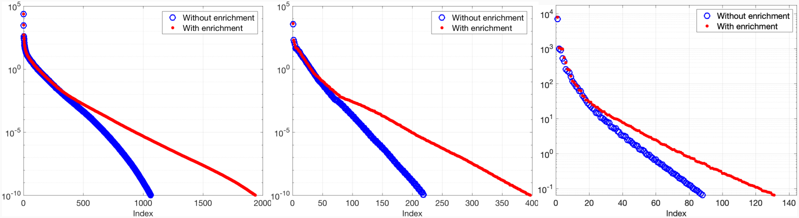
(b) Gaussian pulse
(25 modes used)



(c) Riemann problem
(50 modes used)

Decay of solution snapshot singular values with entropy variable enrichment is slower for transport or shock solutions.

Singular value decay with entropy variable enrichment



(d) KH instability (75 modes used)

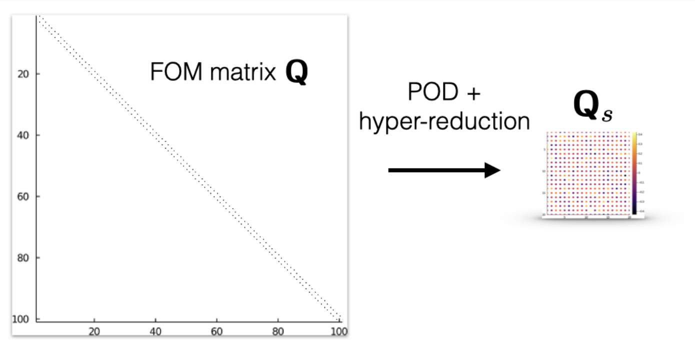
(e) Gaussian pulse (25 modes used)

(f) Riemann problem (50 modes used)

Decay of solution snapshot singular values with entropy variable enrichment is slower for transport or shock solutions.

Cost tradeoffs for entropy stable ROMs

Main cost for explicit time-stepping: computing Hadamard product $(\mathbf{Q} \circ \mathbf{F})\,\mathbf{1} \Longrightarrow \sum_j \mathbf{Q}_{ij} \boldsymbol{f}_S(\mathbf{u}_i, \mathbf{u}_j)$ on the fly.



$\boxed{\mathbf{Q}_s \text{ smaller but dense: } (\mathbf{Q}_s \circ \mathbf{F})\,\mathbf{1} \text{ can be more expensive!}}$

Reduced order modeling

Implicit time-stepping, efficient computation of Jacobian matrices

Current methods for computing Jacobian matrices

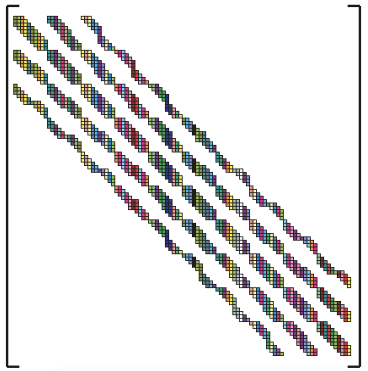


Figure from Gebremedhin, Manne, Pothen (2005), *What color is your Jacobian? Graph coloring for computing derivatives.*

- Implicit time-stepping: compute Jacobian matrices using automatic differentiation (AD)
- Graph coloring reduces costs, but only for sparse matrices
- Cost of AD scales with input and output dimensions.

Jacobian matrices for flux differencing (with C. Taylor)

Theorem

Assume $\mathbf{Q} = \pm\mathbf{Q}^T$. *Consider a scalar "collocation" discretization*

$$\mathbf{r}(\mathbf{u}) = (\mathbf{Q} \circ \mathbf{F})\,\mathbf{1}, \qquad \mathbf{F}_{ij} = f_S(\mathbf{u}_i, \mathbf{u}_j).$$

The Jacobian matrix is then

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}\mathbf{u}} = (\mathbf{Q} \circ \partial\mathbf{F}_R) \pm \operatorname{diag}\left(\mathbf{1}^T\left(\mathbf{Q} \circ \partial\mathbf{F}_R\right)\right),$$
$$(\partial\mathbf{F}_R)_{ij} = \left.\frac{\partial f_S(u_L, u_R)}{\partial u_R}\right|_{\mathbf{u}_i, \mathbf{u}_j}.$$

AD is efficient for $O(1)$ inputs/outputs!

Separates discretization matrix $\mathbf{Q}$ and AD for flux contributions

Computational timings

Jacobian timings for $f_S(u_L, u_R) = \frac{1}{6}\left(u_L^2 + u_L u_R + u_R^2\right)$ and dense differentiation matrices $\mathbf{Q} \in \mathbb{R}^{N\times N}$.

	N = 10	N = 25	N = 50
Direct automatic differentiation	5.666	60.388	373.633
`FiniteDiff.jl`	1.429	17.324	125.894
Jacobian formula (analytic deriv.)	.209	1.005	3.249
Jacobian formula (AD flux deriv.)	.210	1.030	3.259
Evaluation of $\mathbf{f}(\mathbf{u})$ (reference)	.120	.623	2.403

Summary and future work

- Entropy stable modal formulations and reduced order modeling improve robustness while retaining accuracy.
- Next steps: implicit time-stepping for ROMs.

This work is supported by the NSF under awards
DMS-1719818, DMS-1712639, and DMS-CAREER-1943186.

Thank you! Questions?

Chan, Taylor (2020). *Efficient computation of Jacobian matrices for ES-SBP schemes.*

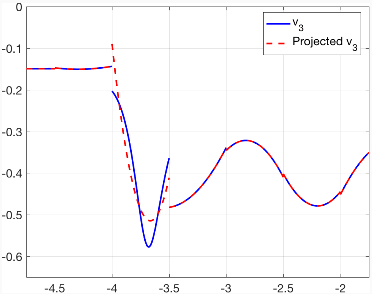
Chan (2020). *Entropy stable reduced order modeling of nonlinear conservation laws.*

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

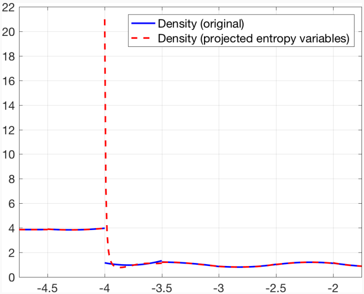
Additional slides

Loss of control with the entropy projection

- For $(N+1)$-point Lobatto, $\widetilde{\boldsymbol{u}} = \boldsymbol{u}$ at nodal points.
- For $(N+2)$-point Gauss, discrepancy between $\boldsymbol{v}(\boldsymbol{u})$ and projection on the boundary of elements.
- Still need positivity of thermodynamic quantities for stability!



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



(b) $\rho(x), \rho\left(\left(\Pi_N \boldsymbol{v}\right)(x)\right)$

Taylor-Green vortex

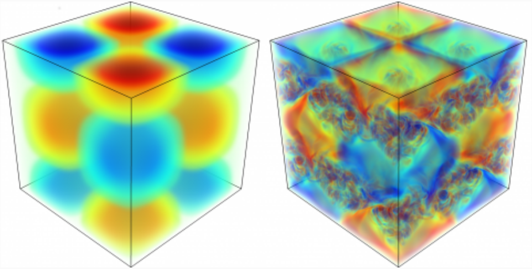
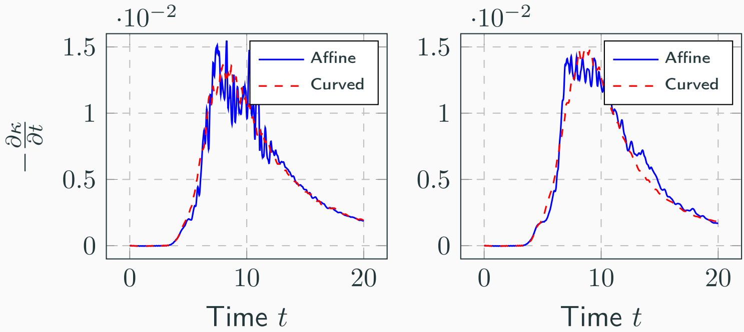


Figure 3: Isocontours of z-vorticity for Taylor-Green at $t = 0, 10$ seconds.

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

https://how4.cenaero.be/content/bs1-dns-taylor-green-vortex-re1600.

3D inviscid Taylor-Green vortex

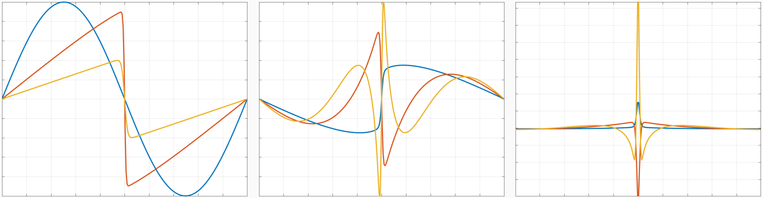


(a) GLL collocation **(b)** Gauss collocation

Figure 4: Kinetic energy dissipation rate for entropy stable GLL and Gauss collocation schemes with $N = 7$ and $h = \pi/8$.

Accuracy of the expanded test basis

- If $\mathbf{V}_t = \mathrm{orth}\left(\begin{bmatrix}\mathbf{V} & \mathbf{1}\end{bmatrix}\right)$, then the modes $\mathbf{V}_t$ can sample $\mathbf{QV}$ very poorly, e.g., $\mathbf{V}_t^T\mathbf{QV}_t \approx \mathbf{0}$!



(a) Shock snapshots **(b)** Modes (**V** columns) **(c)** Mode derivatives **QV**

- Fix: further expand the test basis $\mathbf{V}_t$ by adding $\mathbf{QV}$

$$\mathbf{V}_t = \mathrm{orth}\left(\begin{bmatrix}\mathbf{V} & \mathbf{1} & \mathbf{QV}\end{bmatrix}\right), \qquad \mathbf{V}_t^T\mathbf{QV}_t \in \mathbb{R}^{(2N+1)\times(2N+1)}.$$

Carlberg, Barone, Antil (2017). *Galerkin v. LSPG projection in nonlinear model reduction.*