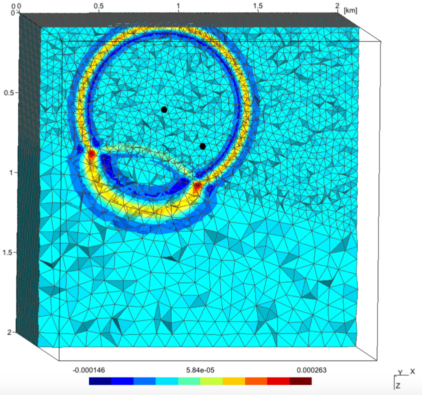
Entropy stable schemes for nonlinear conservation laws: high order discontinuous Galerkin methods and reduced order modeling

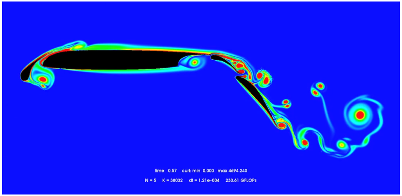
Jesse Chan

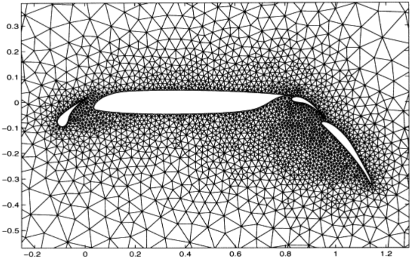
CAAM Colloquium
September 16, 2019

Numerical methods for hyperbolic PDEs



Figures courtesy of T. Warburton, A. Modave.

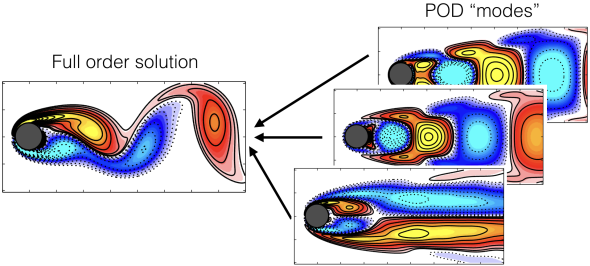




Mesh from Slawig 2001.

Aerodynamics applications: acoustics, vorticular flows, turbulence, shocks.

Projection-based reduced order models (ROMs)



- Reduce costs for many-query scenarios (uncertainty quantification).
- 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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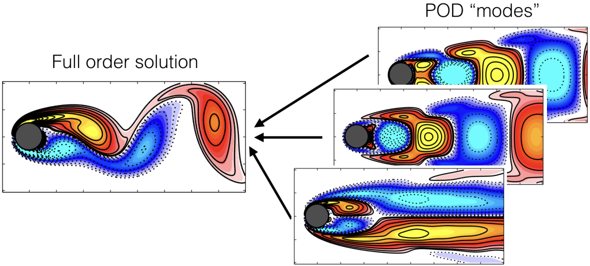

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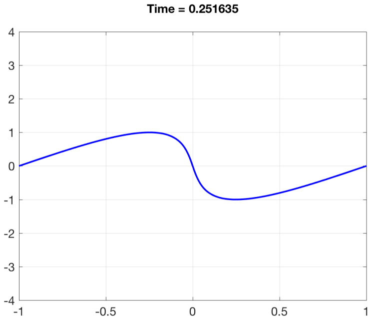
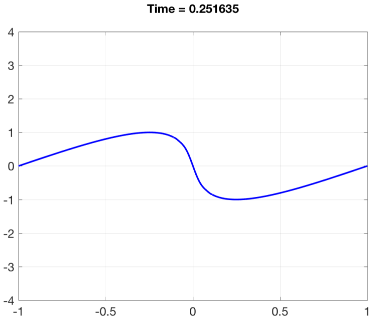
Challenges for nonlinear conservation laws



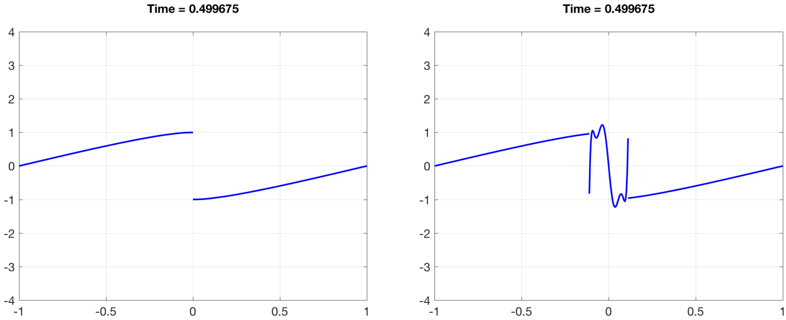
(a) Exact solution



(b) High order DG method

- Advanced numerical 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.

Challenges for nonlinear conservation laws



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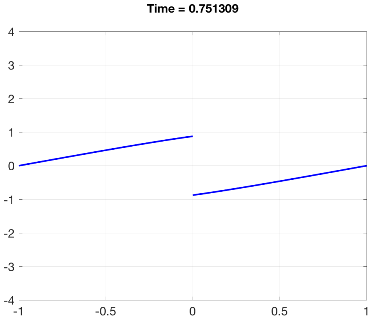

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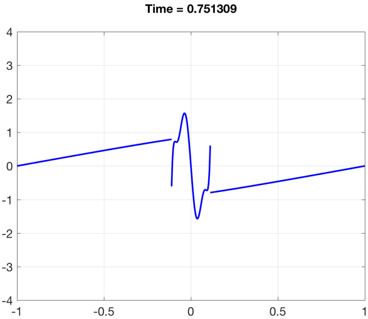

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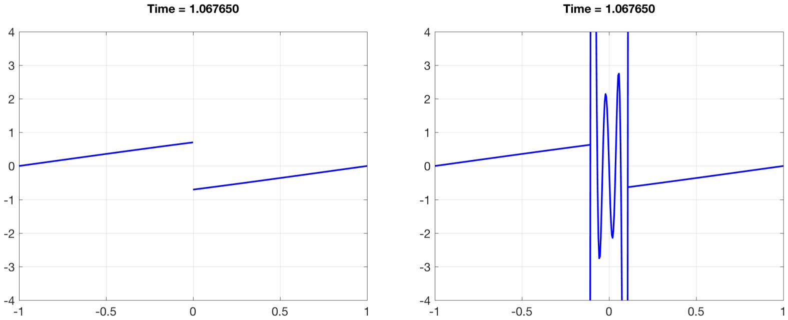

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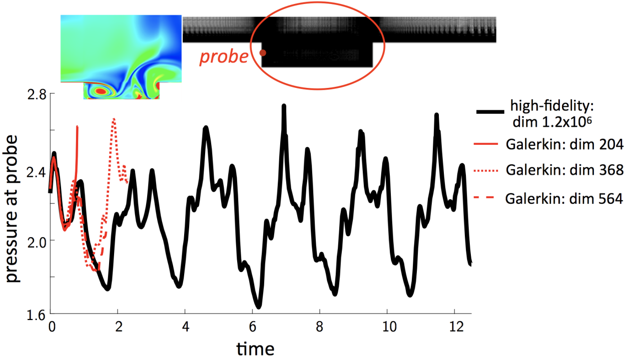


(a) Blowup of ROM from Carlberg, Barone, Antil (2017)

- Advanced numerical 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.

Entropy stability for nonlinear problems

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

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

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

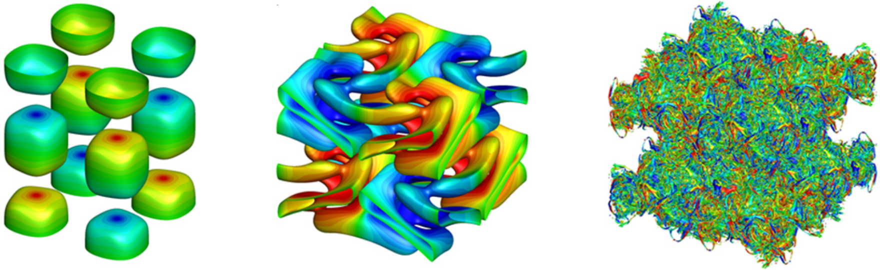
$$\int_\Omega \boldsymbol{v}^T \left(\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x}\right) = 0, \qquad \boxed{\boldsymbol{v}(\boldsymbol{u}) = \frac{\partial S}{\partial \boldsymbol{u}}}$$

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

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

How is instability addressed in practice?

- Asymptotic stability for smooth solutions (not shocks or turbulence!)
- Common fix: stabilize by regularizing (filtering, added dissipation).



Under-resolved solutions: turbulence (inviscid Taylor-Green vortex).

Figures from Beck and Gassner (2012), T. Warburton, Coastal Inlets Research Program (CIRP), "Man on Wire" (2008).

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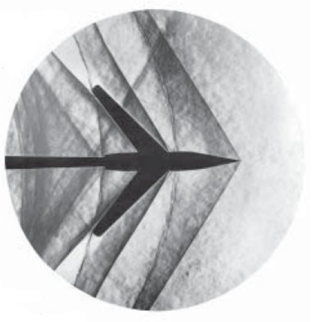

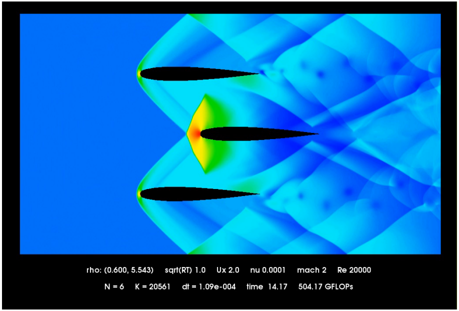

Under-resolved solutions: shock waves.

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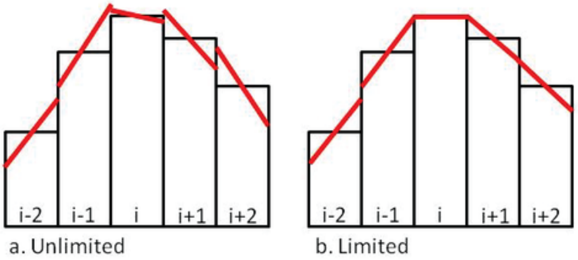

Slope limiting for a finite volume method.

Figures from Beck and Gassner (2012), T. Warburton, Coastal Inlets Research Program (CIRP), "Man on Wire" (2008).

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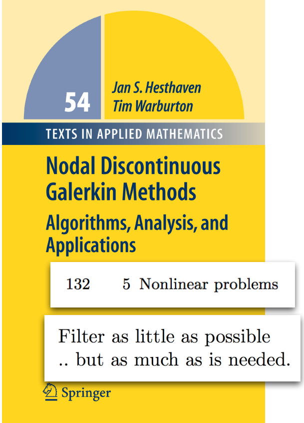

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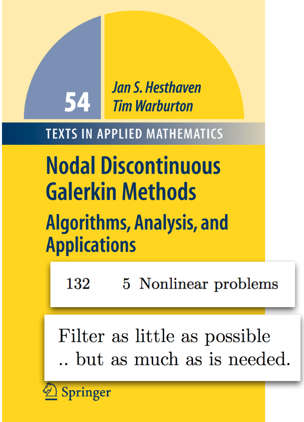

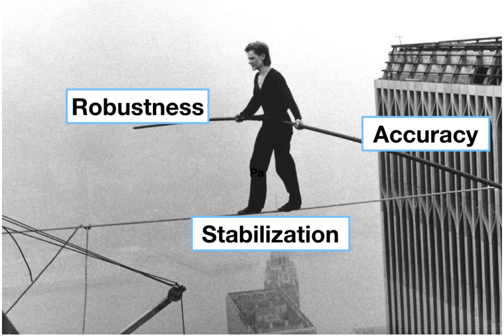

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Discretely entropy stable schemes: main ideas

- Continuous and semi-discrete systems, $\epsilon \geq 0$

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

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

$$\underbrace{\boldsymbol{v}^T\boldsymbol{M}\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{dt}}}_{\boldsymbol{1}^T\boldsymbol{M}\frac{\mathrm{d}S(\boldsymbol{u})}{\mathrm{dt}}} + \boldsymbol{v}^T\boldsymbol{f}_x(\boldsymbol{u}) + \epsilon \boldsymbol{v}^T\boldsymbol{K}\boldsymbol{u} = \boldsymbol{0}$$

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

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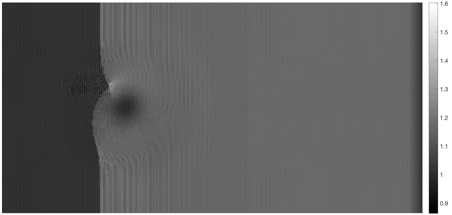
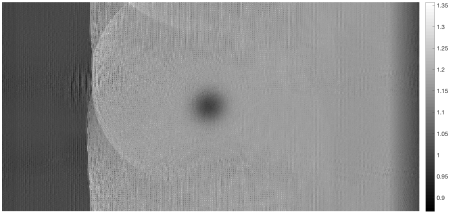
Benefits of entropy stability



(a) No dissipation, $T = .3$



(b) No dissipation, $T = .7$

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

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

Winters, Derigs, Gassner, and Walch (2017). *A uniquely defined entropy stable matrix dissipation operator for high Mach number ideal MHD and compressible Euler simulations.*

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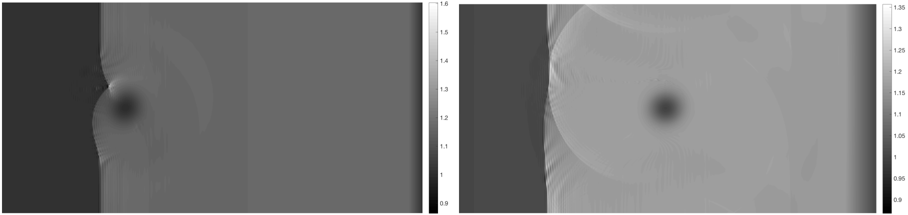

(a) Lax-Friedrichs dissipation, $T = .3$ (b) Lax-Friedrichs dissipation, $T = .7$

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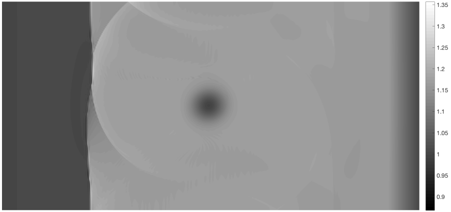
Benefits of entropy stability

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



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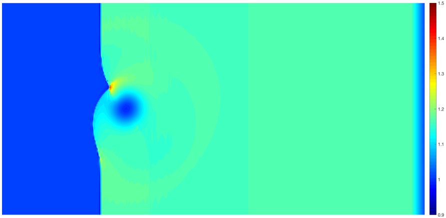

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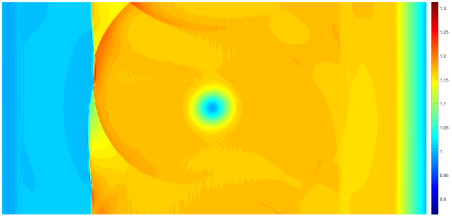

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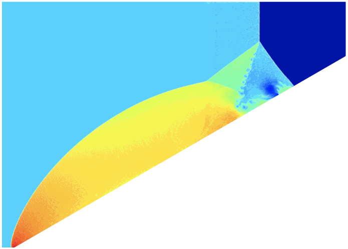
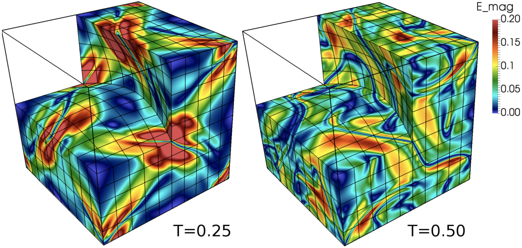
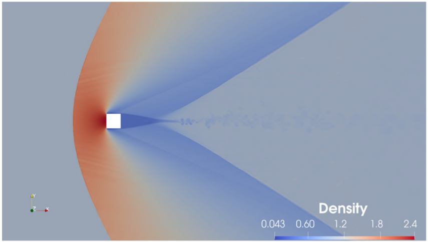
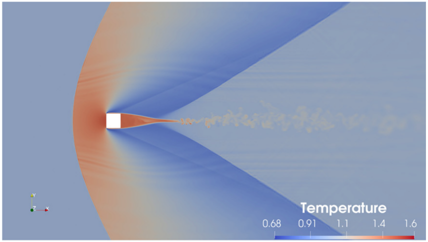
Examples of high order entropy stable simulations









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.*

Scope of this talk, related work

- Goal: semi-discrete entropy inequality + retaining ROM accuracy.
- Combines ideas from:
  - entropy stable finite volume schemes,
  - summation-by-parts (SBP) finite differences,
  - reduced order modeling and hyper-reduction techniques.
- *Accuracy* of reduced bases is an open problem for hyperbolic PDEs!

Finite volumes: Tadmor, Chandrashekar, Ray, Svard, Fjordholm, Mishra, LeFloch, Rohde, ...

SBP: Fisher, Carpenter, Gassner, Winters, Kopriva, Hindenlang, Chen and Shu, Crean and Hicken, DCDR Fernandez, Zingg, Yamaleev, Parsani, Svard, Pazner and Persson, Wintermeyer, Bohm, Friedrich, Schnuke, ...

ROMs: Afkham, Ripamonti, Wang, Hesthaven (2018), Serre, Lafon, Gloerfelt, Bailly (2012), Kalashnikova, Barone, et al. (2014), Carlberg, Choi, Sargsyan (2018), Farhat, Chapman, Avery (2015), ...

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Talk outline

1. An entropy stable full order model
2. Entropy stable reduced order modeling
3. Entropy stable hyper-reduction
   - Non-periodic boundary conditions
4. Numerical experiments

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2 Entropy stable reduced order modeling

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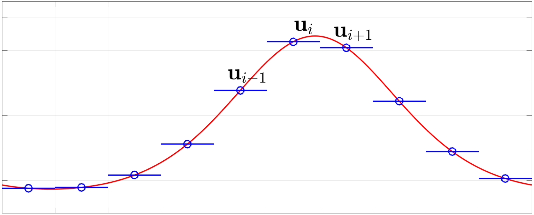
- Non-periodic boundary conditions

4 Numerical experiments

Full order model: entropy stable finite volumes



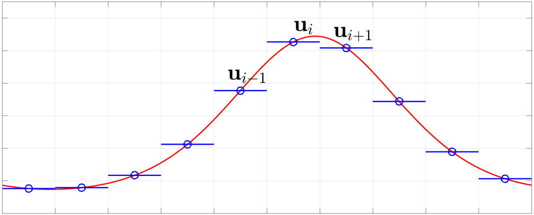
- Integrate conservation law over cell $[x_i, x_{i+1}]$

$$\int_{x_i}^{x_{i+1}} \left(\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} \right) \mathrm{d}x = \mathbf{0}.$$

- Introduce numerical flux $\boldsymbol{f}_S(\boldsymbol{u}_L, \boldsymbol{u}_R)$ at cell interfaces

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

Full order model: entropy stable finite volumes



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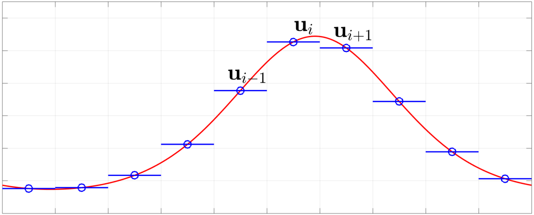

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Entropy conservative numerical fluxes

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

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

- Model problem: compressible Euler equations

$$
\boldsymbol{u} = \begin{bmatrix} \rho \\ \rho u \\ E \end{bmatrix}, \qquad \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = \frac{\partial}{\partial x} \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (E + p) u \end{bmatrix}
$$

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

EC fluxes for the compressible Euler equations

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

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

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

- 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 FV schemes for comp. Euler and NS equations.*

Matrix form of finite volumes

- Finite volume scheme

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

- Matrix formulation: assuming periodicity

$$\boldsymbol{F}_{ij} = \boldsymbol{f}_S\left(\boldsymbol{u}_i, \boldsymbol{u}_j\right), \qquad \Delta x \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{dt}} + 2\left(\boldsymbol{Q} \circ \boldsymbol{F}\right)\boldsymbol{1} + \underbrace{\epsilon \boldsymbol{K}\boldsymbol{u}}_{\text{viscosity}} = 0.$$

- The differentiation matrix $\boldsymbol{Q}$ satisfies $\boldsymbol{Q} = -\boldsymbol{Q}^T$ and $\boldsymbol{Q}\boldsymbol{1} = \boldsymbol{0}$.

$$\boldsymbol{Q} = \frac{1}{2}\begin{bmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & 1 \\ 1 & & -1 & 0 \end{bmatrix}, \qquad \boldsymbol{K} = \frac{1}{\Delta x^2}\begin{bmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & \ddots & \ddots & -1 \\ & & -1 & 1 \end{bmatrix}.$$

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Recovering a semi-discrete entropy balance

- First, show that entropy is *conserved* for the inviscid case. Test with vector of entropy variables $\boldsymbol{v}$

$$\boldsymbol{v}^T\left(\Delta x \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{dt}} + 2\left(\boldsymbol{Q}\circ\boldsymbol{F}\right)\boldsymbol{1}\right) = \boldsymbol{0}.$$

- Use chain rule in time and definition of entropy variables

$$\boldsymbol{v}^T\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{dt}} = \frac{\mathrm{d}S(\boldsymbol{u})}{\mathrm{d}\boldsymbol{u}}^T\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{dt}} = \boldsymbol{1}^T\frac{\mathrm{d}S(\boldsymbol{u})}{\mathrm{dt}}.$$

- If $\boldsymbol{v}^T 2\left(\boldsymbol{Q}\circ\boldsymbol{F}\right)\boldsymbol{1} = 0$, then the average entropy is conserved

$$\Delta x\left(\boldsymbol{1}^T\frac{\mathrm{d}S(\boldsymbol{u})}{\mathrm{dt}}\right) = 0.$$

Main innovation of entropy stable schemes

- Motivation: replicate a discrete analogue of the entropy identity

$$\boxed{\int_{-1}^{1} \boldsymbol{v}^T \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = 0} \Longleftrightarrow \boxed{\boldsymbol{v}^T \left(2\boldsymbol{Q} \circ \boldsymbol{F}\right) \mathbf{1} = 0}$$

- Use $\boldsymbol{Q} = -\boldsymbol{Q}^T$ and $\boldsymbol{Q}\mathbf{1} = \mathbf{0}$ to show $\boldsymbol{v}^T \left(\boldsymbol{Q} \circ \boldsymbol{F}\right) \mathbf{1} = 0$.

$$\begin{aligned} 2\boldsymbol{v}^T \left(\boldsymbol{Q} \circ \boldsymbol{F}\right) \mathbf{1} &= \sum_{ij} 2\boldsymbol{Q}_{ij} \boldsymbol{v}_i^T \boldsymbol{f}_S\left(\boldsymbol{u}_i, \boldsymbol{u}_j\right) \\ &= \sum_{ij} (\boldsymbol{Q}_{ij} - \boldsymbol{Q}_{ji}) \boldsymbol{v}_i^T \boldsymbol{f}_S\left(\boldsymbol{u}_i, \boldsymbol{u}_j\right) \\ &= \sum_{ij} \boldsymbol{Q}_{ij} (\psi(\boldsymbol{u}_i) - \psi(\boldsymbol{u}_j)) = \underbrace{\psi^T \boldsymbol{Q}\mathbf{1} - \mathbf{1}^T \boldsymbol{Q}\psi}_{=0} \end{aligned}$$

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

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- Use $\boldsymbol{Q} = -\boldsymbol{Q}^T$ and $\boldsymbol{Q1} = \boldsymbol{0}$ to show $\boldsymbol{v}^T (\boldsymbol{Q} \circ \boldsymbol{F})\boldsymbol{1} = 0$.

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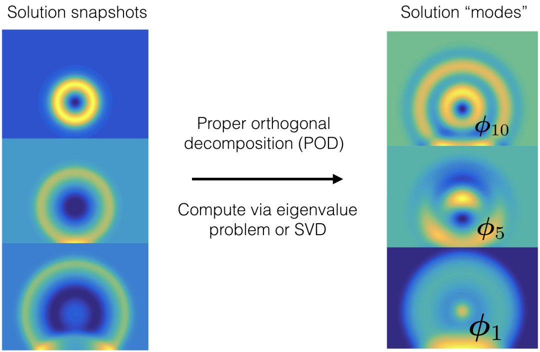
3 Entropy stable hyper-reduction
- Non-periodic boundary conditions

4 Numerical experiments

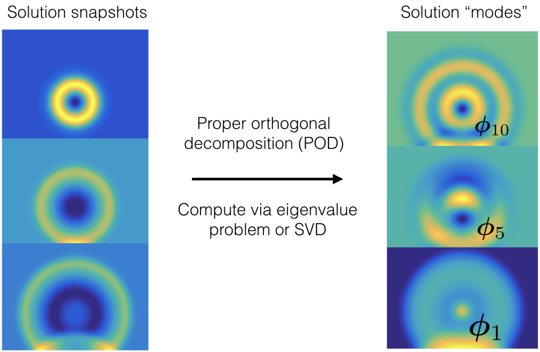
Naive POD-Galerkin procedure



Step 1 (offline): compute "modes" from solution component snapshots.

$$\boldsymbol{V} = \begin{bmatrix} | & & | \\ \phi_1 & \cdots & \phi_N \\ | & & | \end{bmatrix}, \qquad \boldsymbol{u} \approx \boldsymbol{V}\boldsymbol{u}_N.$$

Naive POD-Galerkin procedure



Step 2 (online): Galerkin projection - does not conserve entropy!

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

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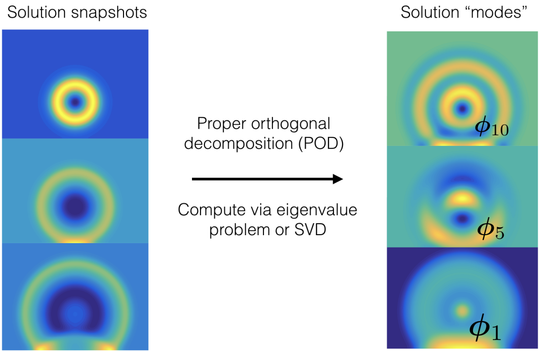

Step 2 (online): Galerkin projection - does not conserve entropy!

$$\Delta x \boldsymbol{V}^T \boldsymbol{V} \frac{\mathrm{d}\boldsymbol{u}_N}{\mathrm{dt}} + 2\boldsymbol{V}^T (\boldsymbol{Q} \circ \boldsymbol{F}) \boldsymbol{1} = 0.$$

Deriving a discrete entropy balance

- Entropy variables are not in ROM *test space*. Solution: test with coefficients of the projection (pseudoinverse) of the entropy variables

$$\left(\boldsymbol{V}^{\dagger}\boldsymbol{v}\left(\boldsymbol{V}\boldsymbol{u}_N\right)\right)^T\left(\Delta x\boldsymbol{V}^T\boldsymbol{V}\frac{\mathrm{d}\boldsymbol{u}_N}{\mathrm{dt}}+2\boldsymbol{V}^T\left(\boldsymbol{Q}\circ\boldsymbol{F}\right)\boldsymbol{1}\right)=0$$

- Recovers time derivative of discrete entropy

$$\left(\boldsymbol{V}^{\dagger}\boldsymbol{v}\left(\boldsymbol{V}\boldsymbol{u}_N\right)\right)^T\boldsymbol{V}^T\boldsymbol{V}\frac{\mathrm{d}\boldsymbol{u}_N}{\mathrm{dt}}=\boldsymbol{v}\left(\boldsymbol{V}\boldsymbol{u}_N\right)^T\underbrace{\left(\boldsymbol{V}^T\boldsymbol{V}\boldsymbol{V}^{\dagger}\right)^T}_{\boldsymbol{V}}\frac{\mathrm{d}\boldsymbol{u}_N}{\mathrm{dt}}$$

$$=\left.\frac{\partial S}{\partial \boldsymbol{u}}\right|_{\left(\boldsymbol{V}\boldsymbol{u}_N\right)}^T\frac{\mathrm{d}\left(\boldsymbol{V}\boldsymbol{u}_N\right)}{\mathrm{dt}}=\boldsymbol{1}^T\frac{\mathrm{d}S\left(\boldsymbol{V}\boldsymbol{u}_N\right)}{\mathrm{dt}}$$

Evaluating fluxes using entropy projection

- Projected entropy variables are no longer mappings of the conservative variables! Let $\widetilde{\boldsymbol{v}} = \boldsymbol{V}\boldsymbol{V}^{\dagger}\boldsymbol{v}\left(\boldsymbol{V}\boldsymbol{u}_N\right)$, then

$$\boxed{\widetilde{\boldsymbol{v}}_i \neq \boldsymbol{v}\left(\boldsymbol{u}_i\right)} \Longleftrightarrow \boxed{\left(\widetilde{\boldsymbol{v}}_i - \widetilde{\boldsymbol{v}}_j\right)^T \boldsymbol{f}_S\left(\boldsymbol{u}_i, \boldsymbol{u}_j\right) \neq \psi(\boldsymbol{u}_i) - \psi(\boldsymbol{u}_j)}$$

- Fix: evaluate flux using projected entropy variables, enrich snapshots with entropy variables to ensure accuracy.

$$\widetilde{\boldsymbol{u}} = \boldsymbol{u}\left(\boldsymbol{V}\boldsymbol{V}^{\dagger}\boldsymbol{v}\left(\boldsymbol{V}\boldsymbol{u}_N\right)\right).$$

- Modified Galerkin projection ROM is discretely entropy stable

$$\Delta x \boldsymbol{V}^T\boldsymbol{V}\frac{\mathrm{d}\boldsymbol{u}_N}{\mathrm{dt}} + 2\boldsymbol{V}^T\left(\boldsymbol{Q}\circ\boldsymbol{F}\right)\boldsymbol{1} = 0, \qquad \boldsymbol{F}_{ij} = \boldsymbol{f}_S\left(\widetilde{\boldsymbol{u}}_i, \widetilde{\boldsymbol{u}}_j\right).$$

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Evaluating nonlinear ROM terms dominates costs

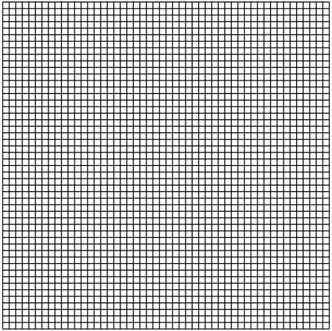
Problem: cost of evaluating ROM nonlinear terms scales with number of grid points! Cost still scales with size of full order model.

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

- Hyper-reduction reduces costs by approximating nonlinear evaluations.

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

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



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

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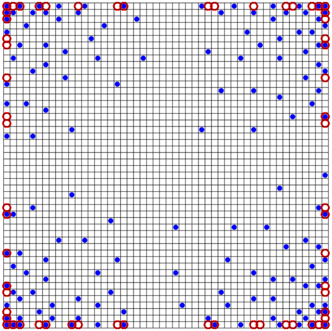

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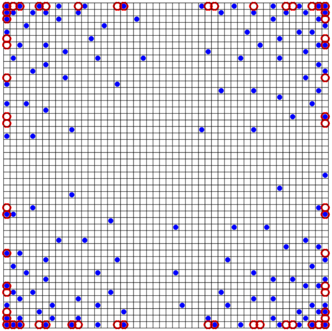

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Entropy stability and standard hyper-reduction

- How to hyper-reduce $(\boldsymbol{Q} \circ \boldsymbol{F})$? Sample the full order matrix $\boldsymbol{Q}$ to construct a hyper-reduced nodal differentiation matrix $\boldsymbol{Q}_s$.

- Options: sub-sample rows and columns of full matrix $\boldsymbol{Q}$ or approximate $\boldsymbol{Q}$ by weighted sum of local skew matrices $\boldsymbol{Q}_e$.

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

Problems: either $\boldsymbol{Q}_s \neq \boldsymbol{Q}_s^T$ or $\boldsymbol{Q}_s \boldsymbol{1} \neq \boldsymbol{0}$.

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

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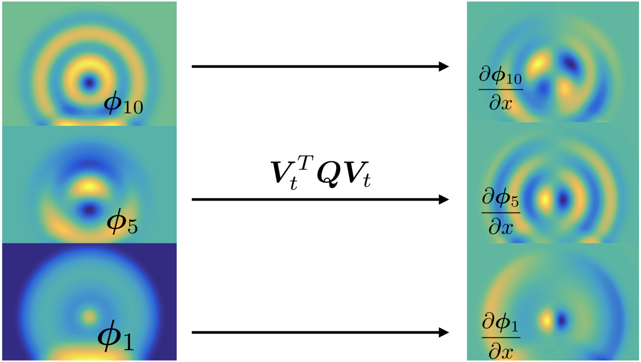
Two-step hyper-reduction: compress and project

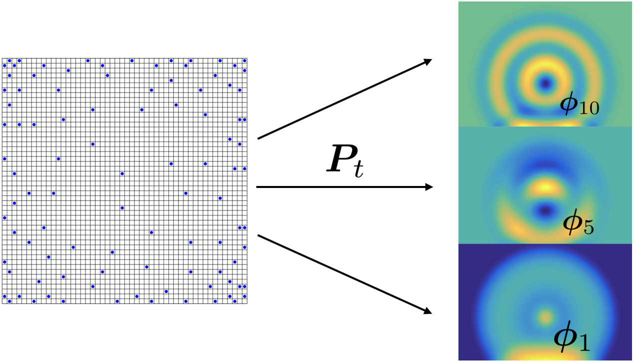


Step 1: compress $\boldsymbol{Q}$ using an expanded "test" basis $\boldsymbol{V}_t$

$$\boldsymbol{V}_t^T \boldsymbol{Q} \boldsymbol{V}_t, \qquad \boldsymbol{V}_t^T \boldsymbol{Q} \boldsymbol{u} \approx \boldsymbol{V}_t^T \boldsymbol{Q} \boldsymbol{V}_t \boldsymbol{u}_N \quad \text{if } \boldsymbol{u} \approx \boldsymbol{V}_t \boldsymbol{u}_N$$

Exactly differentiates constants if $\mathbf{1} \in \mathcal{R}(\boldsymbol{V}_t)$!

Two-step hyper-reduction: compress and project

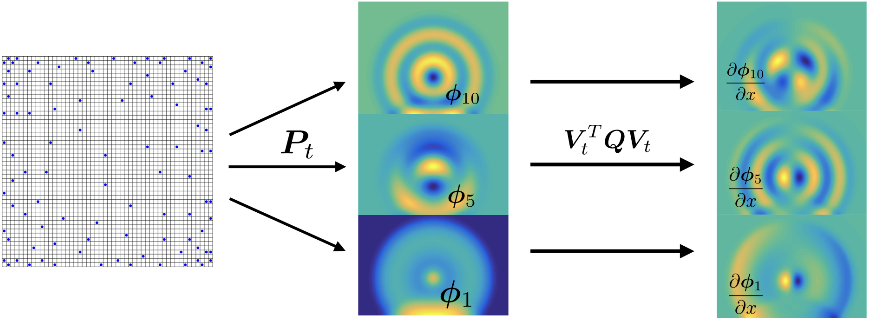


Step 2: determine test basis coefficients using hyper-reduced points.

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

$\boldsymbol{P}_t$ is a weighted projection onto the test basis, reproduces $\mathcal{R}\left(\boldsymbol{V}_t\right)$ exactly.

Two-step hyper-reduction: compress and project



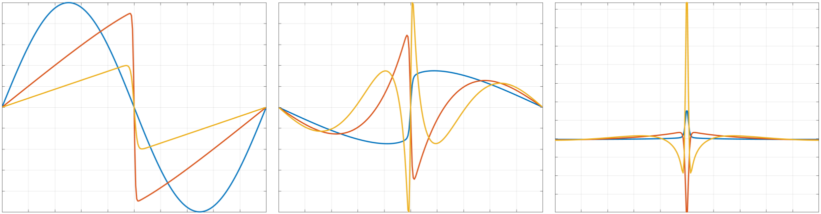
Step 3: combine Steps 1 and 2 by defining

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

Then, $\boldsymbol{Q}_s = -\boldsymbol{Q}_s^T$ and $\boldsymbol{Q}_s \mathbf{1} = \mathbf{0}$!

Choosing the test basis

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



(a) Shock snapshots (b) Modes (columns of $\boldsymbol{V}$) (c) Mode derivatives $\boldsymbol{QV}$

- Fix: sample $\boldsymbol{Q}$ using an expanded "test" basis $\boldsymbol{V}_t$

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

$\boldsymbol{Q}_s = \boldsymbol{P}_t^T\left(\boldsymbol{V}_t^T\boldsymbol{QV}_t\right)\boldsymbol{P}_t$ is accurate, $\boldsymbol{Q}_s = -\boldsymbol{Q}_s^T$, and $\boldsymbol{Q}_s\boldsymbol{1} = \boldsymbol{0}$.

Carlberg, Barone, Antil (2017). *Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction.*

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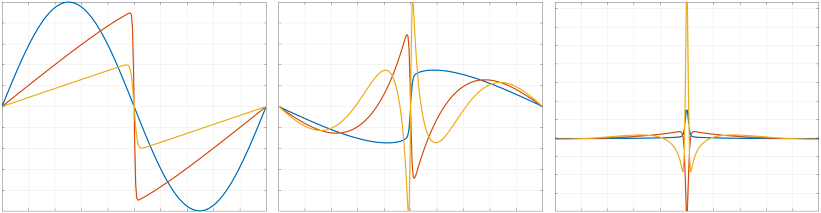

(a) Shock snapshots (b) Modes (columns of $\boldsymbol{V}$) (c) Mode derivatives $\boldsymbol{QV}$

- Fix: sample $\boldsymbol{Q}$ using an expanded "test" basis $\boldsymbol{V}_t$

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

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

Carlberg, Barone, Antil (2017). *Galerkin v. least-squares Petrov–Galerkin projection in nonlinear model reduction.*

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 constrained least squares for positive quadrature weights.
- Target basis: products of modes

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

Reduce costs by substituting leading POD modes.

Hernandez, Caicedo, Ferrer (2017). *Dimensional hyper-reduction of nonlinear finite element models via empirical cubature.*

Hyper-reduction: empirical cubature

- Approximate inner products of POD basis: most accurate + smallest number of points in practice

$$\boldsymbol{V}^T\boldsymbol{V} \approx \boldsymbol{V}(\mathcal{I},:)^T\boldsymbol{W}\boldsymbol{V}(\mathcal{I},:).$$

- Problem: target space focuses on $\boldsymbol{V}$, ignores rest of test basis

$$\boldsymbol{V}_t = \operatorname{orth}\left(\begin{bmatrix}\boldsymbol{V} & \mathbf{1} & \boldsymbol{Q}\boldsymbol{V}\end{bmatrix}\right)$$

  Reduced test mass matrix $\boldsymbol{M}_t = \boldsymbol{V}_t(\mathcal{I},:)^T\boldsymbol{W}\boldsymbol{V}_t(\mathcal{I},:)$ may be singular $\Longrightarrow$ projection matrix $\boldsymbol{P}_t$ undefined!

- Fix: add "stabilizing" points to integrate the near null space of $\boldsymbol{M}_t$.

An, Kim, James (2009). *Optimizing cubature for efficient integration of subspace deformations.*

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Hyper-reduction of viscous terms

- The diffusion matrix $\boldsymbol{K}$ can be decomposed as

$$\boldsymbol{K} = \boldsymbol{D}^T\boldsymbol{D}, \qquad \boldsymbol{D} = \frac{1}{\Delta x}\begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{bmatrix}$$

- Rewrite derivatives in terms of entropy variables

$$-\frac{\partial^2 \boldsymbol{u}}{\partial \boldsymbol{x}^2} = -\frac{\partial}{\partial x}\left(\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{v}}\frac{\partial \boldsymbol{v}}{\partial x}\right), \qquad \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{v}} \text{ is SPD if entropy is convex}$$

- Hyper-reduce $\boldsymbol{K}$ by sampling and weighting rows of $\boldsymbol{D}$

$$\boxed{\boldsymbol{v}^T\boldsymbol{K}\boldsymbol{u}} \Longleftrightarrow \boxed{\boldsymbol{v}_N^T\boldsymbol{D}\left(\mathcal{I}_D,:\right)^T\boldsymbol{W}_D\boldsymbol{H}\boldsymbol{D}\left(\mathcal{I}_D,:\right)\boldsymbol{v}_N} \qquad \boldsymbol{H}_{ii} = \left.\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{v}}\right|_{x_i}$$

Summary: entropy stable ROMs on periodic domains

- Two-step hyper-reduction of $(\boldsymbol{Q} \circ \boldsymbol{F})$: compress and project
  - Test basis $\boldsymbol{V}_t$ spans $\mathbf{1}$, $\boldsymbol{V}$, and $\boldsymbol{QV}$.
  - Project sampled values onto modes of test basis

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

- Entropy stable reduced order model with hyper-reduction:

$$\boldsymbol{V}(\mathcal{I},:)^T \boldsymbol{W} \boldsymbol{V}(\mathcal{I},:) \frac{\mathrm{d}\boldsymbol{u}_N}{\mathrm{dt}} + 2\boldsymbol{V}(\mathcal{I},:)^T (\boldsymbol{Q}_s \circ \boldsymbol{F}) \mathbf{1} = \text{viscous terms},$$
$$\boldsymbol{F}_{ij} = \boldsymbol{f}_S(\widetilde{\boldsymbol{u}}_i, \widetilde{\boldsymbol{u}}_j), \quad \widetilde{\boldsymbol{u}} = \boldsymbol{u}(\boldsymbol{V}(\mathcal{I},:)\boldsymbol{P}\boldsymbol{v}(\boldsymbol{V}\boldsymbol{u}_N)),$$

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

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

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Talk outline

1 An entropy stable full order model

2 Entropy stable reduced order modeling

3 Entropy stable hyper-reduction
- Non-periodic boundary conditions

4 Numerical experiments

Non-periodic domains and summation by parts

- Full order matrix $\boldsymbol{Q}$ mimics integration by parts

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

- Enforce boundary conditions *weakly* using numerical flux $\boldsymbol{f}_S(\boldsymbol{u}, \boldsymbol{u}^+)$

$$\boxed{2\left(\boldsymbol{Q} \circ \boldsymbol{F}\right)} \Longrightarrow \boxed{\left(\left(\boldsymbol{Q} - \boldsymbol{Q}^T\right) \circ \boldsymbol{F}\right) + \boldsymbol{B}\boldsymbol{f}(\boldsymbol{u}).}$$

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Reduced bases and summation by parts

- No summation by parts property for reduced $\boldsymbol{Q}_s$!

$$\boldsymbol{Q}_s = \boldsymbol{P}_t^T \left(\boldsymbol{V}_t^T \boldsymbol{Q} \boldsymbol{V}_t \right) \boldsymbol{P}_t, \qquad \boldsymbol{Q}_s \neq -\boldsymbol{Q}_s^T + \boldsymbol{B}.$$

- Augmented "hybridized" matrix satisfies $\boldsymbol{Q}_h \mathbf{1} = \mathbf{0}$ in 1D

$$\boldsymbol{Q}_h = \frac{1}{2} \begin{bmatrix} \boldsymbol{Q}_s - \boldsymbol{Q}_s^T & \boldsymbol{E}^T \boldsymbol{B} \\ -\boldsymbol{B}\boldsymbol{E} & \boldsymbol{B} \end{bmatrix}, \qquad \boldsymbol{Q}_h = -\boldsymbol{Q}_h^T + \begin{bmatrix} \mathbf{0} & \\ & \boldsymbol{B} \end{bmatrix}$$

$\boldsymbol{E}$ extrapolates from sampled volume points to sampled surface points.

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

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

Surface hyper-reduction

- In 2D/3D, entropy stability requires surface weights $\boldsymbol{w}_f$ to satisfy a constraints involving surface interpolation matrix $\boldsymbol{V}_f$.

- Enforce conditions using dual simplex method with constraints

$$
\begin{gathered}
\min \mathbf{1}^T \boldsymbol{w}_f \quad s.t. \\
\boldsymbol{w}_f \geq \mathbf{0}, \\
\boldsymbol{V}_f^T \operatorname{diag}(\boldsymbol{w}_f)\, \boldsymbol{V}_f \approx \Delta x \boldsymbol{V}_f^T \boldsymbol{V}_f, \\
\boldsymbol{V}_t^T \boldsymbol{Q}_x^T \mathbf{1} = \boldsymbol{V}_f^T (\boldsymbol{n}_x \circ \boldsymbol{w}_f), \\
\boldsymbol{V}_t^T \boldsymbol{Q}_y^T \mathbf{1} = \boldsymbol{V}_f^T (\boldsymbol{n}_y \circ \boldsymbol{w}_f).
\end{gathered}
$$

Dual simplex method seeks a *sparse* solution $\boldsymbol{w}_f$.

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

Talk outline

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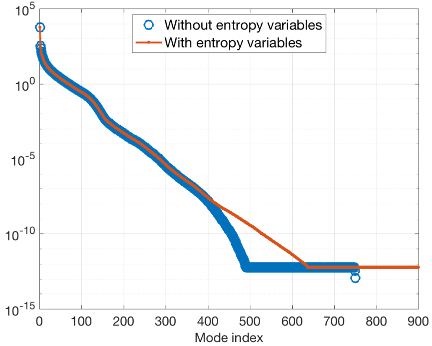
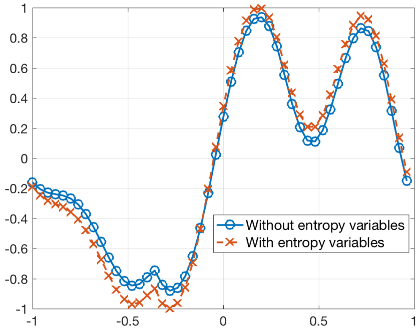
Enriching snapshots with entropy variables



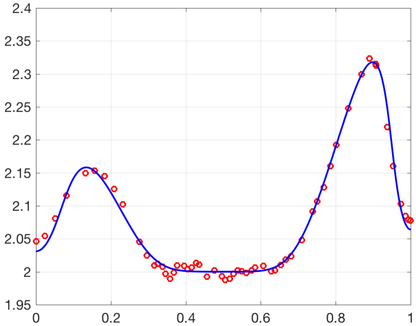
(a) Singular values



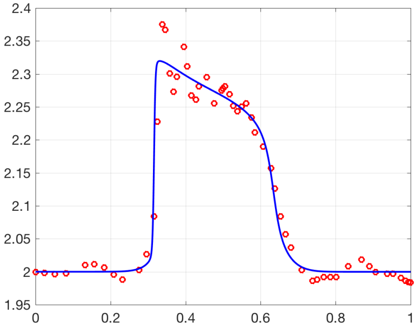
(b) Fifth singular vector

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

1D Euler with reflective BCs + shock



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

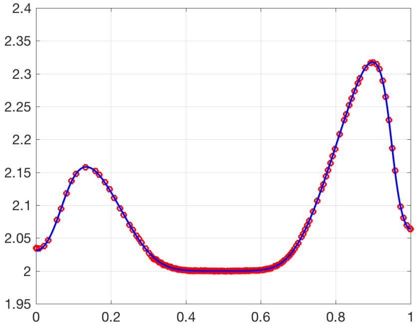


(b) 25 modes, $T = .75$

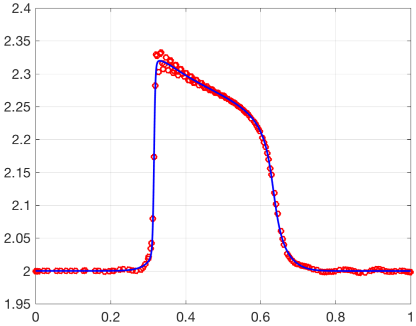
FOM with 2500 grid points, viscosity coefficient $\epsilon = 2e-4$, ROM with 25 modes.

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, $T = .75$

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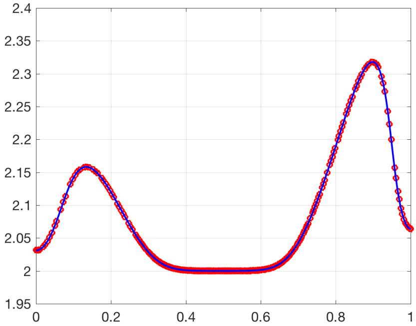
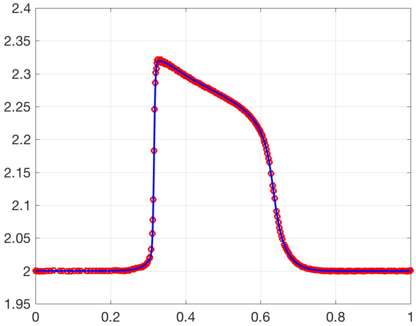


(a) 125 modes, $T = .25$



(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
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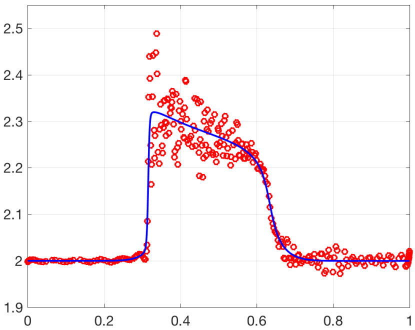
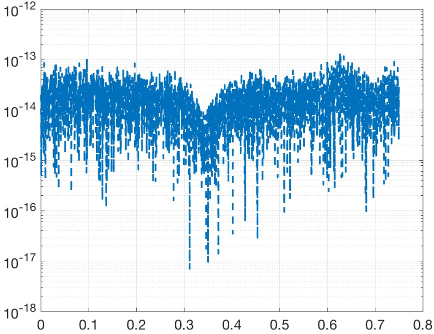
Entropy conservation test



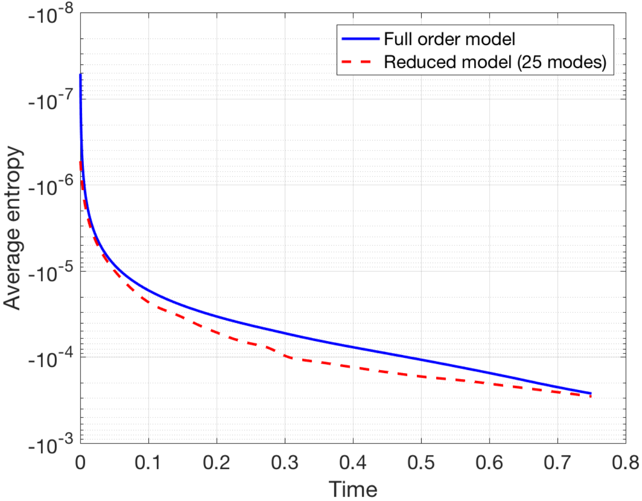
(a) Density ρ (125 modes, no viscosity)



(b) Convective entropy contribution

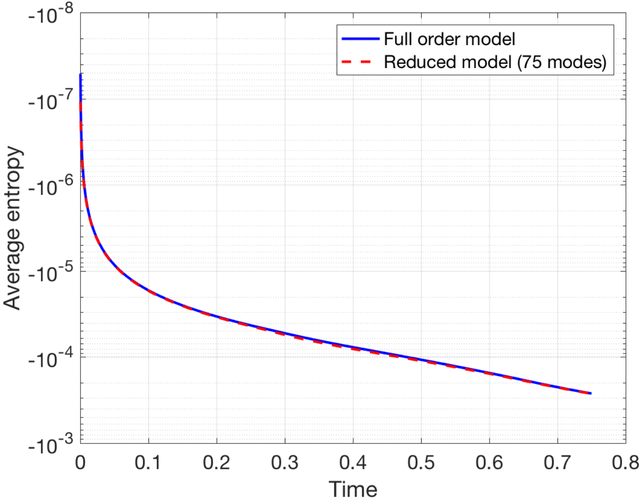
Figure: Reduced order solution and convective entropy RHS contribution $\left|\boldsymbol{v}_N^T \boldsymbol{V}_h^T \left(\boldsymbol{Q}_h \circ \boldsymbol{F}\right) \mathbf{1}\right|$ for the case of zero viscosity.

Evolution of average entropy



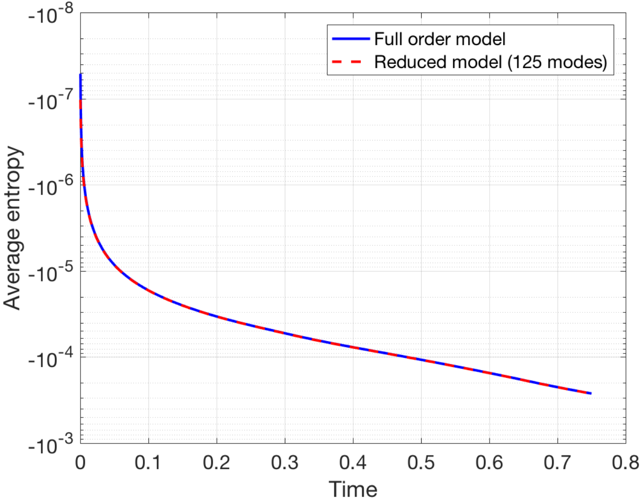
Average entropy over time (25 modes).

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

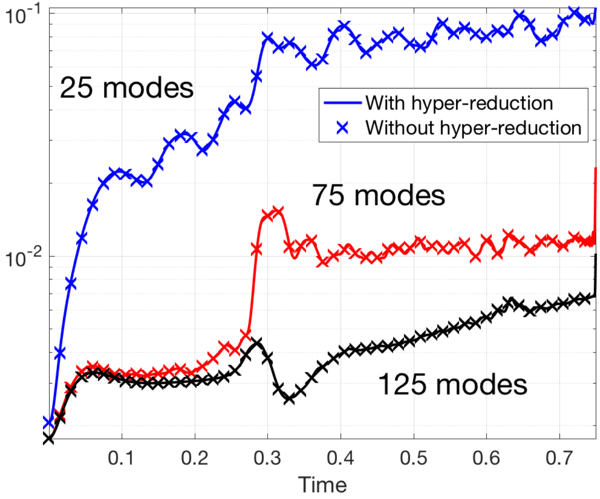
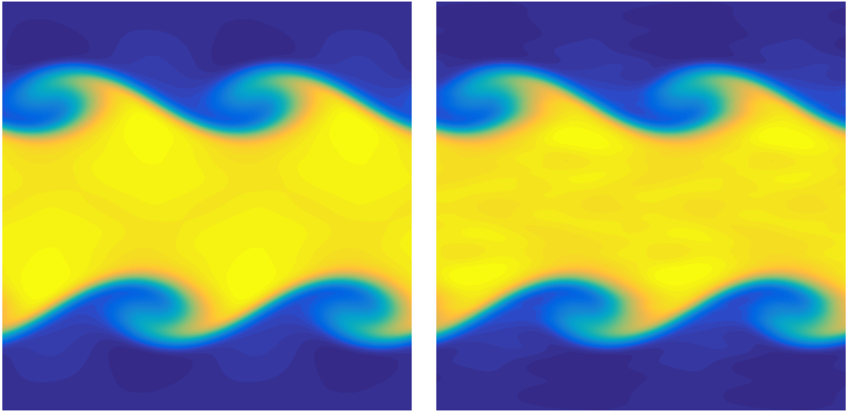


Figure: Error over time for a $K = 2500$ FOM and ROM with $25, 75, 125$ modes.

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 $T = 2.5$.

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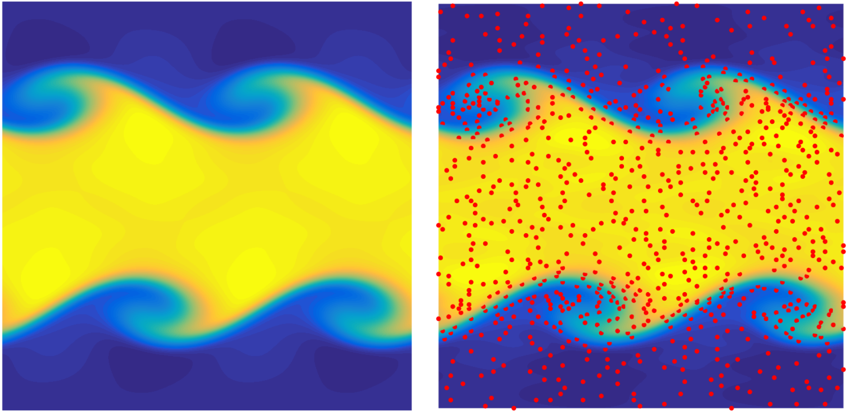

(a) Density, full order model (b) ROM w/reduced quad. points

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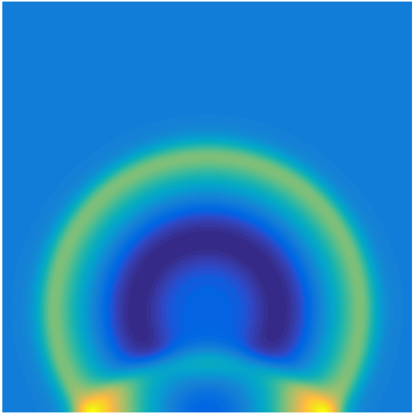
2D Gaussian pulse with reflective wall



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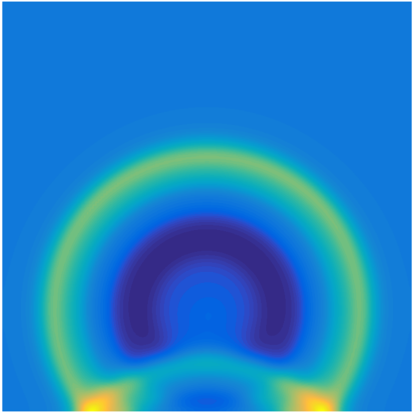
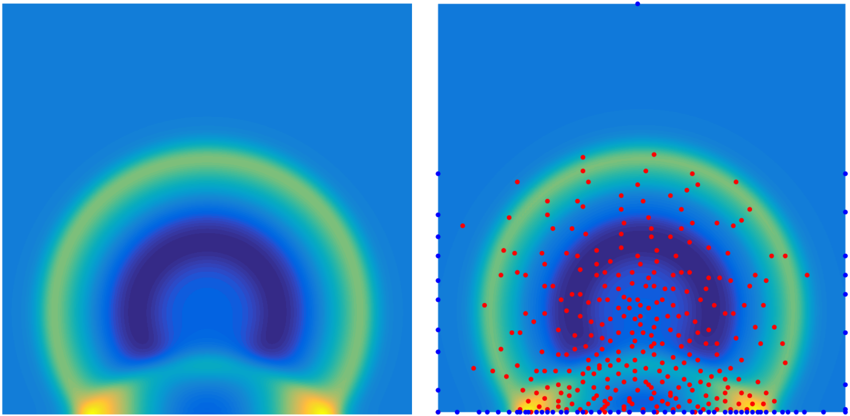


(b) Reduced order model

Figure: FOM with 22500 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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Summary and future work

- Entropy stable ROMs reproduce a semi-discrete entropy inequality.
- Current work: implicit solvers, approximation of transport and shocks.

- This work is supported by DMS-1719818 and DMS-1712639.

Thank you! Questions?

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

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

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

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

Additional slides