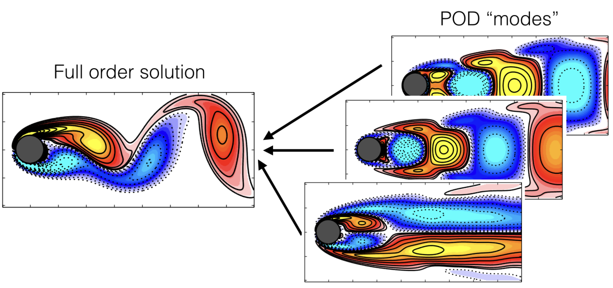
Entropy stable reduced order modeling of nonlinear conservation laws

Jesse Chan

Dept. of Computational and Applied Mathematics
Rice University

SIAM CSE minisymposium: reduced order model stabilizations and closures

Constructing stable projection-based reduced order models



- ROMs do not inherit FOM stability for nonlinear convection-dominated flows.
- Can lead to non-physical solution growth or blow-up, esp. for under-resolved features (e.g., shocks or turbulence).

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

Nonlinear conservation laws and entropy inequalities

- 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 w.r.t. convex entropy function $S(\boldsymbol{u})$, "entropy potential" $\psi(\boldsymbol{u})$, entropy variables $\boldsymbol{v}(\boldsymbol{u})$

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

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

- Goal: ensure ROM satisfies a discrete entropy inequality.

Nonlinear conservation laws and entropy inequalities

- 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 w.r.t. convex entropy function $S(\boldsymbol{u})$, "entropy potential" $\psi(\boldsymbol{u})$, entropy variables $\boldsymbol{v}(\boldsymbol{u})$

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

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

- Goal: ensure ROM satisfies a discrete entropy inequality.

FOM: entropy conservative finite volume methods

- Finite volume scheme:

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

- If $\boldsymbol{f}_S$ is an *entropy conservative* numerical flux

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

  then the 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.*

FOM: entropy stable finite volume methods

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

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

- If $\boldsymbol{f}_S$ is an *entropy conservative* numerical flux

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

then the numerical scheme dissipates entropy

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

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

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 a periodic finite volume scheme as

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

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 a periodic finite volume scheme as

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

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 a periodic finite volume scheme as

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

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 a periodic finite volume scheme as

$$\begin{bmatrix} \mathbf{F}_{1,2} - \mathbf{F}_{1,N} \\ \mathbf{F}_{2,3} - \mathbf{F}_{2,1} \\ \vdots \\ \mathbf{F}_{N,1} - \mathbf{F}_{N,N-1} \end{bmatrix} = 2(\mathbf{Q} \circ \mathbf{F})\mathbf{1}.$$

Interpretation using finite difference matrices

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

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

Key observation: generalizable beyond finite volumes

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

Note that $\mathbf{M}^{-1}\mathbf{Q}$ is a periodic differentiation matrix.

Interpretation using finite difference matrices

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

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

Key observation: generalizable beyond finite volumes

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

Note that $\mathbf{M}^{-1}\mathbf{Q}$ is a periodic differentiation matrix.

Reduced order modeling

Naive POD-Galerkin procedure

- Assume a POD basis s.t. $\mathbf{u} \approx \mathbf{V}\mathbf{u}_N$. Galerkin projection gives

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

- Test with projection of entropy variables for discrete entropy balance. Let $\mathbf{V}^\dagger =$ pseudoinverse, $\widetilde{\mathbf{v}} = \mathbf{V}\mathbf{V}^\dagger \boldsymbol{v}\left(\mathbf{V}\mathbf{u}_N\right)$

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

$$\implies \underbrace{\mathbf{1}^T \mathbf{M} \frac{\mathrm{d}S\left(\mathbf{V}\mathbf{u}_N\right)}{\mathrm{dt}}}_{\text{rate of change - avg. entropy}} + \widetilde{\mathbf{v}}^T 2\left(\mathbf{Q} \circ \mathbf{F}\right) \mathbf{1} = 0.$$

Naive POD-Galerkin procedure

- Assume a POD basis s.t. $\mathbf{u} \approx \mathbf{V}\mathbf{u}_N$. Galerkin projection gives

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

- Test with projection of entropy variables for discrete entropy balance. Let $\mathbf{V}^\dagger =$ pseudoinverse, $\widetilde{\mathbf{v}} = \mathbf{V}\mathbf{V}^\dagger \boldsymbol{v}\left(\mathbf{V}\mathbf{u}_N\right)$

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

$$\Longrightarrow \mathbf{1}^T\mathbf{M}\frac{\mathrm{d}S\left(\mathbf{V}\mathbf{u}_N\right)}{\mathrm{dt}} + \underbrace{\widetilde{\mathbf{v}}^T 2\left(\mathbf{Q}\circ\mathbf{F}\right)\mathbf{1}}_{\text{zero if entropy conservative}} = 0.$$

Entropy projection and discrete entropy stability

- Loss of entropy conservation: $\widetilde{\mathbf{v}} = \mathbf{V}\mathbf{V}^{\dagger}\boldsymbol{v}\left(\mathbf{V}\mathbf{u}_N\right) \neq \boldsymbol{v}(\mathbf{V}\mathbf{u}_N)$

$$\widetilde{\mathbf{v}}^T 2\left(\mathbf{Q}\circ\mathbf{F}\right)\mathbf{1} = \sum_{ij}\mathbf{Q}_{ij}\left(\widetilde{\mathbf{v}}_i - \widetilde{\mathbf{v}}_j\right)^T \boldsymbol{f}_S\left(\mathbf{u}_i,\mathbf{u}_j\right)$$
$$\neq \sum_{ij}\mathbf{Q}_{ij}\left(\psi(\mathbf{u}_i) - \psi(\mathbf{u}_j)\right) = 0.$$

- Restore entropy conservation by re-evaluating $\widetilde{\mathbf{u}} = \boldsymbol{u}\left(\widetilde{\mathbf{v}}\right)$.

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

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

- All results use Laplacian art. viscosity $\epsilon\mathbf{K}\mathbf{u}$ for entropy stability.

Entropy projection and discrete entropy stability

- Loss of entropy conservation: $\widetilde{\mathbf{v}} = \mathbf{V}\mathbf{V}^{\dagger}\boldsymbol{v}\left(\mathbf{V}\mathbf{u}_N\right) \neq \boldsymbol{v}(\mathbf{V}\mathbf{u}_N)$

$$\widetilde{\mathbf{v}}^T 2\left(\mathbf{Q} \circ \mathbf{F}\right)\mathbf{1} = \sum_{ij} \mathbf{Q}_{ij}\left(\widetilde{\mathbf{v}}_i - \widetilde{\mathbf{v}}_j\right)^T \boldsymbol{f}_S\left(\mathbf{u}_i, \mathbf{u}_j\right)$$
$$\neq \sum_{ij} \mathbf{Q}_{ij}\left(\psi(\mathbf{u}_i) - \psi(\mathbf{u}_j)\right) = 0.$$

- Restore entropy conservation by re-evaluating $\widetilde{\mathbf{u}} = \boldsymbol{u}\left(\widetilde{\mathbf{v}}\right)$.

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

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

- All results use Laplacian art. viscosity $\epsilon\mathbf{K}\mathbf{u}$ for entropy stability.

Evaluating nonlinear ROM terms dominates costs

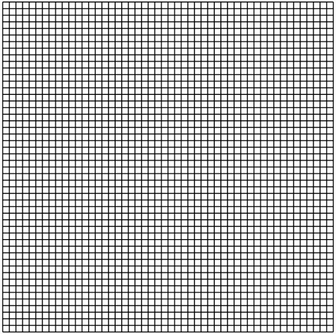
Cost of nonlinear terms still scales with FOM size.

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

- Hyper-reduction approximate 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, ...



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

Evaluating nonlinear ROM terms dominates costs

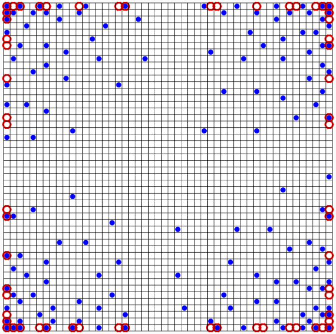
Cost of nonlinear terms still scales with FOM size.

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

- Hyper-reduction approximate 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, ...



Evaluating nonlinear ROM terms dominates costs

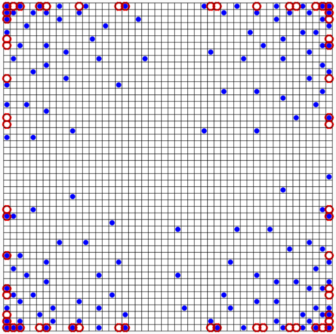
Cost of nonlinear terms still scales with FOM size.

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

- Hyper-reduction approximate nonlinear evaluations.

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

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



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

Two-step hyper-reduction: compress and project

$(\mathbf{Q} \circ \mathbf{F}) \approx (\mathbf{Q}_s \circ \mathbf{F})$. Must preserve $\mathbf{Q}_s = -\mathbf{Q}_s^T$ and $\mathbf{Q}_s\mathbf{1} = \mathbf{0}$!

1. Compress $\mathbf{Q}$ onto an expanded "test" basis $\mathbf{V}_t$

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

2. Hyper-reduced projection to determine test basis coefficients

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

3. Define hyper-reduced matrix $\mathbf{Q}_s$

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

$\Longrightarrow \mathbf{Q}_s$ is skew-symmetric, conservative, and accurate.

Hernandez et al. (2017). *Dimensional hyper-reduction of nonlinear FE models via empirical cubature.*

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

Two-step hyper-reduction: compress and project

$(\mathbf{Q} \circ \mathbf{F}) \approx (\mathbf{Q}_s \circ \mathbf{F})$. Must preserve $\mathbf{Q}_s = -\mathbf{Q}_s^T$ and $\mathbf{Q}_s \mathbf{1} = \mathbf{0}$!

1. Compress $\mathbf{Q}$ onto an expanded "test" basis $\mathbf{V}_t$

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

2. Hyper-reduced projection to determine test basis coefficients

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

3. Define hyper-reduced matrix $\mathbf{Q}_s$

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

$\Longrightarrow \mathbf{Q}_s$ is skew-symmetric, conservative, and accurate.

Hernandez et al. (2017). *Dimensional hyper-reduction of nonlinear FE models via empirical cubature.*

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

Two-step hyper-reduction: compress and project

$(\mathbf{Q} \circ \mathbf{F}) \approx (\mathbf{Q}_s \circ \mathbf{F})$. Must preserve $\mathbf{Q}_s = -\mathbf{Q}_s^T$ and $\mathbf{Q}_s \mathbf{1} = \mathbf{0}$!

1. Compress $\mathbf{Q}$ onto an expanded "test" basis $\mathbf{V}_t$

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

2. Hyper-reduced projection to determine test basis coefficients

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

3. Define hyper-reduced matrix $\mathbf{Q}_s$

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

$\Longrightarrow \mathbf{Q}_s$ is skew-symmetric, conservative, and accurate.

Hernandez et al. (2017). *Dimensional hyper-reduction of nonlinear FE models via empirical cubature.*

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

Two-step hyper-reduction: compress and project

$(\mathbf{Q} \circ \mathbf{F}) \approx (\mathbf{Q}_s \circ \mathbf{F})$. Must preserve $\mathbf{Q}_s = -\mathbf{Q}_s^T$ and $\mathbf{Q}_s \mathbf{1} = \mathbf{0}$!

1. Compress $\mathbf{Q}$ onto an expanded "test" basis $\mathbf{V}_t$

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

2. Hyper-reduced projection to determine test basis coefficients

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

3. Define hyper-reduced matrix $\mathbf{Q}_s$

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

$\Longrightarrow$ $\mathbf{Q}_s$ is skew-symmetric, conservative, and accurate.

Hernandez et al. (2017). *Dimensional hyper-reduction of nonlinear FE models via empirical cubature.*
Carlberg, Barone, Antil (2017). *Galerkin v. LSPG projection in nonlinear model reduction.*

A hyper-reduced entropy conservative ROM

- Approx. integrals of target space of inner products of POD basis (most accurate + smallest number of points in practice)

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

- Add "stabilizing" points to avoid singular test mass matrix $\boldsymbol{M}_t$.

- Entropy stable reduced order model with hyper-reduction:

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

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

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

Hernandez et al. (2017). *Dimensional hyper-reduction of nonlinear FE models via empirical cubature.*

A hyper-reduced entropy conservative ROM

- Approx. integrals of target space of inner products of POD basis (most accurate + smallest number of points in practice)

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

- Add "stabilizing" points to avoid singular test mass matrix $\boldsymbol{M}_t$.

- 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.

Hernandez et al. (2017). *Dimensional hyper-reduction of nonlinear FE models via empirical cubature.*

Non-periodic boundary conditions

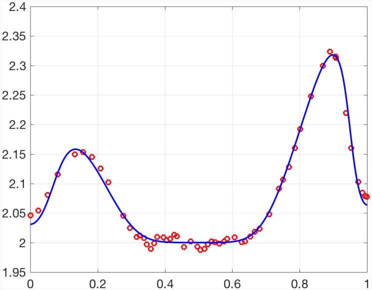
- Impose BCs via FV fluxes + summation-by-parts operators.
- In 2D and 3D, entropy stability requires a discrete integration-by-parts property involving surface interpolation matrix $\mathbf{V}_f$ + hyper-reduced surface weights $\mathbf{w}_f$.

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

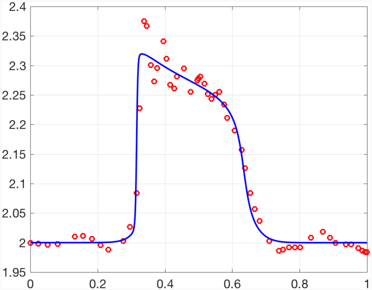
Enforce conditions using constrained hyper-reduction + LP.

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, $T = .25$

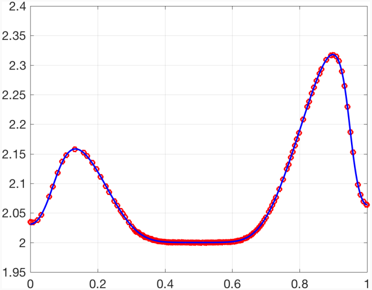


(b) 25 modes, $T = .75$

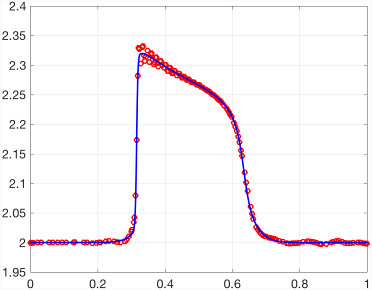
FOM with 2500 points, viscosity $\epsilon = 2 \times 10^{-4}$, ROM with 25, 75, 125 modes.

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

1D Euler with reflective BCs + shock



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

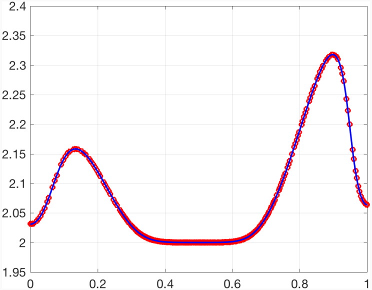


(b) 75 modes, $T = .75$

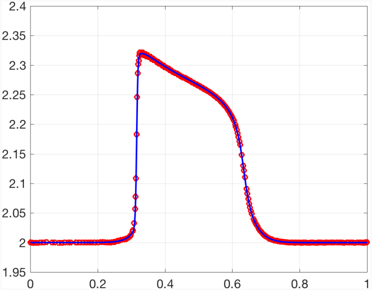
FOM with 2500 points, viscosity $\epsilon = 2 \times 10^{-4}$, ROM with 25, 75, 125 modes.

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

1D Euler with reflective BCs + shock



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

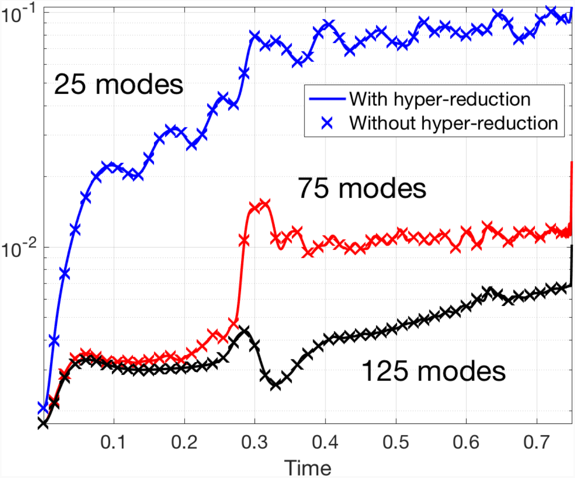


(b) 125 modes, $T = .75$

FOM with 2500 points, viscosity $\epsilon = 2 \times 10^{-4}$, ROM with 25, 75, 125 modes.

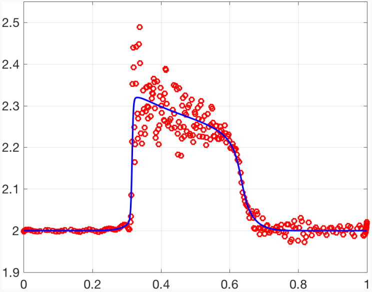
Number of modes N	25	75	125	175
Number of empirical cubature points	54	158	259	355
Number of stabilizing points	3	21	36	28

Error with and without hyper-reduction

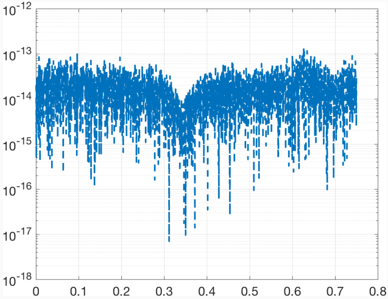


Error over time for a $K = 2500$ FOM and ROM with $25, 75, 125$ modes.

Entropy conservation test



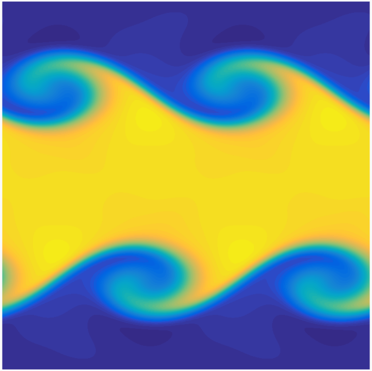
(a) Density ρ (125 modes, no viscosity)



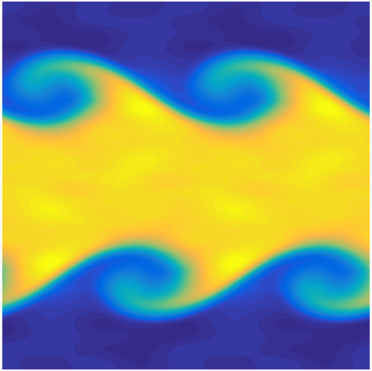
(b) Convective entropy contribution

Figure 1: Reduced order solution and discrete entropy production $\left|\widetilde{\mathbf{v}}^T \mathbf{V}(\mathcal{I},:)^T (2\mathbf{Q}_s \circ \mathbf{F}) \mathbf{1}\right|$ when setting $\epsilon = 0$ (zero viscosity).

2D Kelvin-Helmholtz instability



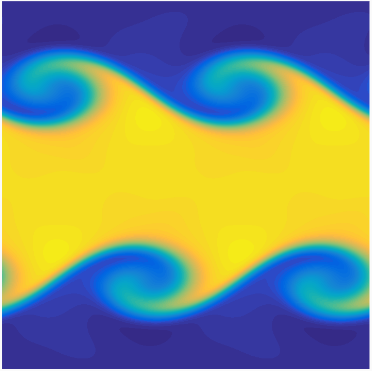
(a) Density, full order model



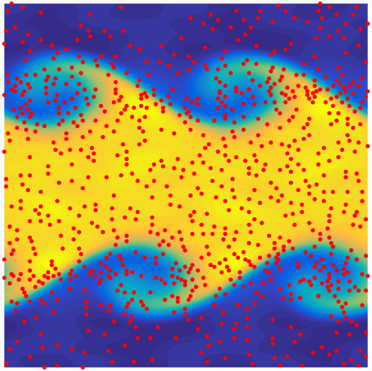
(b) Reduced order model

FOM with 200×200 points, viscosity $\epsilon = 10^{-3}$. ROM with 75 modes, 884 reduced points (no stabilizing points), 1.02% rel. L^2 error at $T = 3$.

2D Kelvin-Helmholtz instability



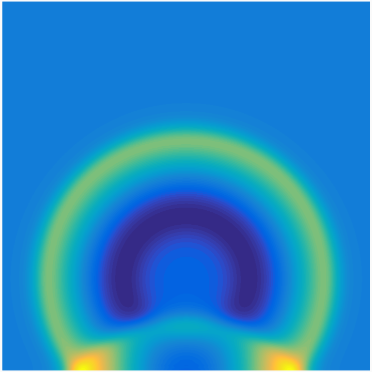
(c) Density, full order model



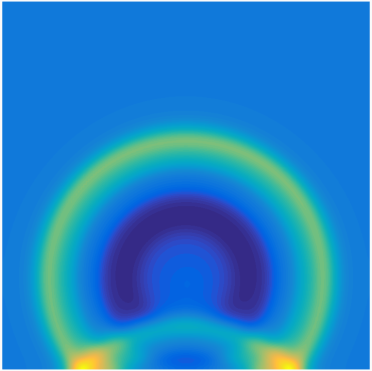
(d) ROM w/reduced quad. points

FOM with 200×200 points, viscosity $\epsilon = 10^{-3}$. ROM with 75 modes, 884 reduced points (no stabilizing points), 1.02% rel. L^2 error at $T = 3$.

2D Gaussian pulse with reflective wall



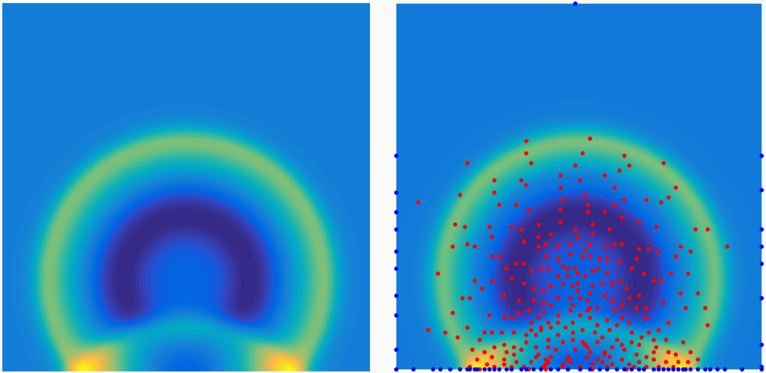
(a) Density, full order model



(b) Reduced order model

FOM with 100×100 grid points, viscosity $\epsilon = 10^{-3}$. ROM with 25 modes, 306 volume points (one stabilizing point), 82 surface points, $.57\%$ relative error at $T = .25$.

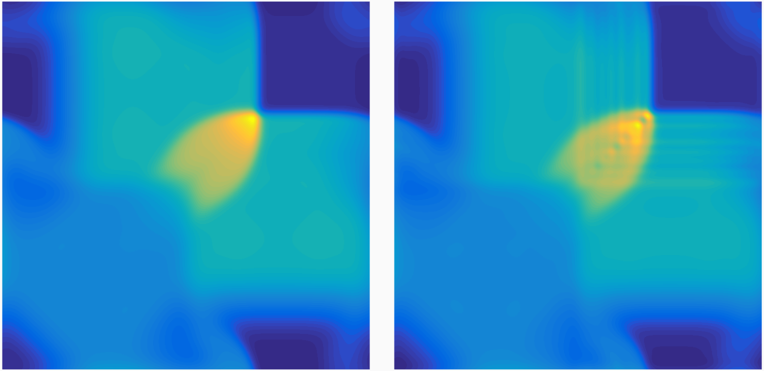
2D Gaussian pulse with reflective wall



(c) Density, full order model **(d)** ROM w/reduced quad. points

FOM with 100×100 grid points, viscosity $\epsilon = 10^{-3}$. ROM with 25 modes, 306 volume points (one stabilizing point), 82 surface points, $.57\%$ relative error at $T = .25$.

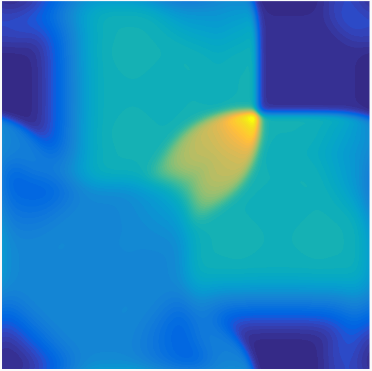
2D Riemann problem on periodic domain



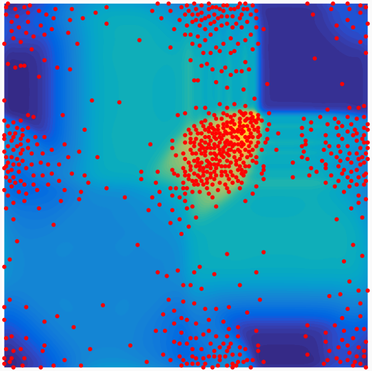
(a) Full order model **(b)** Reduced order model, 50 modes

FOM with 200×200 points, viscosity $\epsilon = 5 \times 10^{-3}$, $T = .25$. ROM with 50 modes, 812 reduced quadrature points (no stabilizing points), 3.278% relative L^2 error.

2D Riemann problem on periodic domain



(c) Full order model

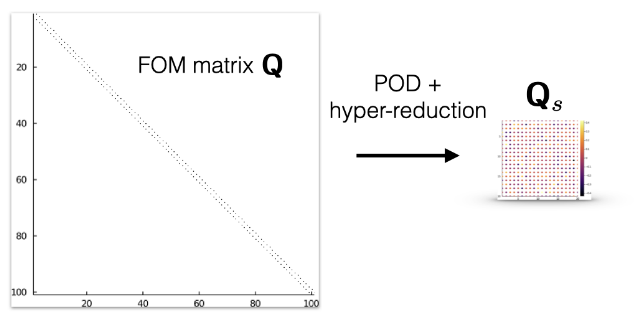


(d) ROM w/reduced quad. points

FOM with 200×200 points, viscosity $\epsilon = 5 \times 10^{-3}$, $T = .25$. ROM with 50 modes, 812 reduced quadrature points (no stabilizing points), 3.278% relative L^2 error.

Time-explicit entropy stable ROMs can be more expensive

Explicit-in-time: compute $(\mathbf{Q} \circ \mathbf{F})\,\mathbf{1} \Rightarrow \sum_j \mathbf{Q}_{ij} \boldsymbol{f}_S(\mathbf{u}_i, \mathbf{u}_j)$ on the fly.



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

Current directions: implicit time-stepping (leverage recent work on efficient computation of entropy stable Jacobian matrices).

Computational timings for Jacobians

Jacobian timings for Burgers' equation and 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
One explicit RHS eval. (reference)	.120	.623	2.403

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

Summary and future work

- Entropy stable modal formulations and reduced order modeling improve robustness while retaining accuracy.
- Current work: implicit time-stepping.

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

Example of EC fluxes (compressible Euler equations)

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

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

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

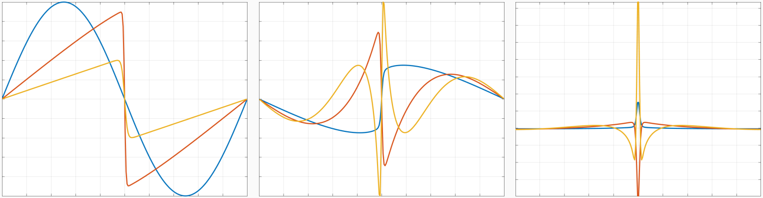
- Non-standard logarithmic mean, "inverse temperature" β

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

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

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 ($\mathbf{V}$ columns) **(c)** Mode derivatives $\mathbf{QV}$

- 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.*

Current methods for computing Jacobian matrices

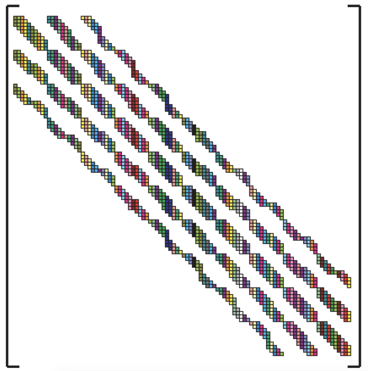


Figure from Gebremedhin, Manne, Pothen (2005), *What color is your Jacobian? Graph coloring for computing derivatives.*

- 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*

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

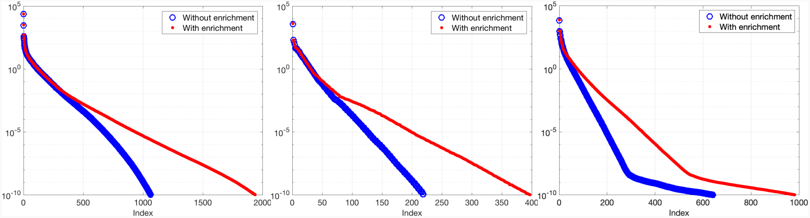
The Jacobian matrix is then

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

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

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

Singular value decay with entropy variable enrichment



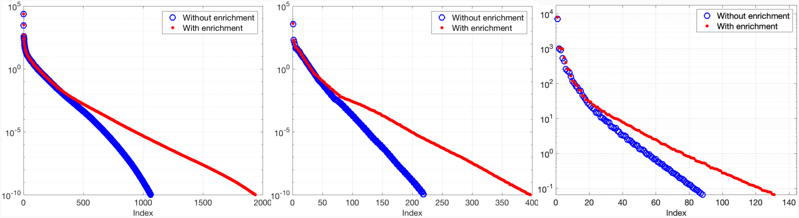
(d) KH instability
(75 modes used)

(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.

Singular value decay with entropy variable enrichment



(g) KH instability (75 modes used)

(h) Gaussian pulse (25 modes used)

(i) Riemann problem (50 modes used)

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