Entropy stable reduced order modeling of nonlinear conservation laws using high order DG methods

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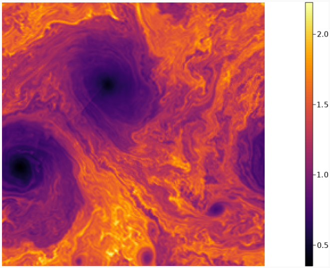
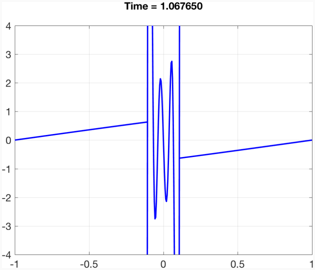
Motivation - entropy stable ROM



(a) Kelvin–Helmholtz instability



(b) 1D Burgers'

- High-fidelity simulations require extreme-scale evaluations.
- Reduced order models (ROMs) enable efficient many-query contexts.
- Both full order models (FOMs) and ROMs tend to blow up around shocks and turbulence.

Chan et al. (2022) *On the entropy projection and the robustness of high order entropy stable discontinuous Galerkin schemes for under-resolved flows.*

Talk outline

1. Nonlinear conservation laws
2. Full order model (FOM) construction
3. Reduced order model (ROM) construction
4. Numerical Experiments

Nonlinear conservation laws

Nonlinear conservation laws and entropy stability

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

$$\frac{\partial \mathbf{u}}{\partial t} + \sum_{i}^{d} \frac{\partial \mathbf{f}^i(\mathbf{u})}{\partial \boldsymbol{x}^i} = 0. \tag{1}$$

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

$$\begin{aligned} &\int_\Omega \mathbf{v}^T \left(\frac{\partial \mathbf{u}}{\partial t} + \sum_i^d \frac{\partial \mathbf{f}^i(\mathbf{u})}{\partial \boldsymbol{x}^i} \right) = 0, \qquad \boxed{\mathbf{v}(\mathbf{u}) = \frac{\partial S}{\partial \mathbf{u}}} \\ \Longrightarrow &\int_\Omega \frac{\partial S(\mathbf{u})}{\partial t} + \sum_i^d \left(\mathbf{v}^T \mathbf{f}^i(\mathbf{u}) - \psi^i(\mathbf{u}) \right)\Big|_{-1}^{1} = 0. \end{aligned} \tag{2}$$

Nonlinear conservation laws and entropy stability

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Entropy conservative flux

- The entropy stability is a generalization of energy stability principle for nonlinear conservation laws.
- The entropy stable schemes that we utilize rely on special numerical fluxes. Denote $\mathbf{u}_L, \mathbf{u}_R$ the left and right solution states. The two-point flux $\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R)$ is entropy-conservative if

$$\mathbf{f}_S(\mathbf{u}, \mathbf{u}) = \mathbf{f}(\mathbf{u}), \text{ (consistency)}$$
$$\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R) = \mathbf{f}_S(\mathbf{u}_R, \mathbf{u}_L), \text{ (symmetry)}$$
$$(\mathbf{v}_L - \mathbf{v}_R)^T \mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R) = \psi(\mathbf{u}_L) - \psi(\mathbf{u}_R). \text{ (conservation)}$$

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

Tadmor. (2003) *Entropy stability theory for difference approximations of nonlinear conservation laws and related time-dependent problems.*

Full order model (FOM) construction

Entropy stable high order DG formulation

- A global DG formulation of (1) is

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + \sum_{i=1}^{d}\left(2\left(\mathbf{Q}^i \circ \mathbf{F}^i\right)\mathbf{1} + \mathbf{E}^T\mathbf{B}^i\left(\mathbf{f}^{i,*} - \mathbf{f}^i(\mathbf{u})\right)\right) = \text{dissipation},$$

where $(\mathbf{F}^i)_{j,k} = \mathbf{f}^i(\mathbf{u}_j, \mathbf{u}_k)$ is a matrix of nonlinear flux evaluations, $\mathbf{E}$ is a boundary extraction matrix, and $\mathbf{Q}^i$ is a global summation-by-parts (SBP) operator with zero row sum

$$\mathbf{Q}^i + (\mathbf{Q}^i)^T = \mathbf{E}^T\mathbf{B}^i\mathbf{E}, \qquad \mathbf{Q}^i\mathbf{1} = \mathbf{0}.$$

- We can prove a semi-discrete entropy stability condition

$$\mathbf{1}^T\mathbf{M}\frac{\mathrm{d}S(\mathbf{u})}{\mathrm{dt}} \leq 0.$$

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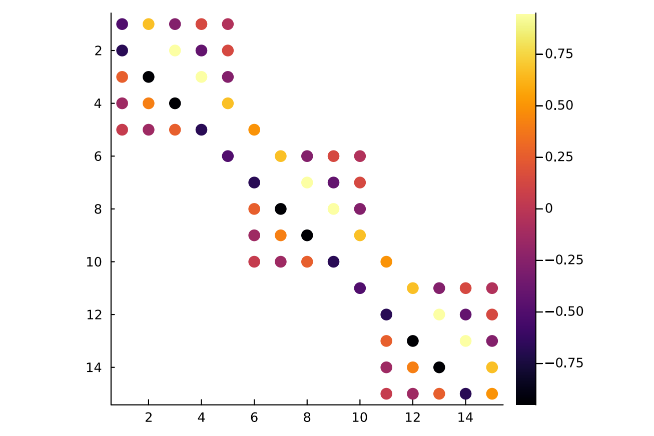
An example of a global SBP operator



Spy plot of $\mathbf{Q}^1$ (1D domain, 3 elements with 5 nodes in each)

Reduced order model (ROM) construction

Galerkin projection ROM

- Galerkin projection ROM ($\mathbf{V}_N$ is the POD basis):

$$\mathbf{M}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + \sum_{i=1}^{d} (2\mathbf{V}_N^T(\mathbf{Q}^i \circ \mathbf{F}^i)\mathbf{1} + \mathbf{V}_b^T \mathbf{B}^i(\mathbf{f}^{i,\star} + \mathbf{f}^i)) = \mathbf{0},$$

  $\mathbf{u} \approx \mathbf{V}_N \mathbf{u}_N$, $\mathbf{M}_N = \mathbf{V}_N^T \mathbf{M} \mathbf{V}_N$, and $\mathbf{V}_b = \mathbf{E}\mathbf{V}_N$.

- To achieve entropy stability, use entropy projection

$$\widetilde{\mathbf{u}} = \mathbf{u}(\mathbf{V}_N \mathbf{V}_N^\dagger \mathbf{v}(\mathbf{V}_N \mathbf{u}_N)) = \mathbf{u}(\widetilde{\mathbf{v}}), \qquad (\mathbf{F}^i)_{j,k} = \mathbf{f}^i(\widetilde{\mathbf{u}}_j, \widetilde{\mathbf{u}}_k).$$

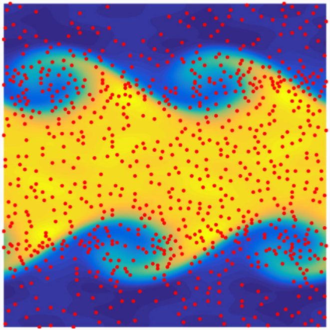
- Still has high computational cost! Needs hyper-reduction. Hyper-reduction of volume and boundary terms are independent.

Hyper-reduction of volume terms

Main idea: find a set of volume nodes and positive weights $(\mathcal{I}, \mathbf{w})$

$$\mathbf{V}_N^T g(\mathbf{V}_N \mathbf{u}_N) \approx \mathbf{V}_N(\mathcal{I}, :)^T \mathrm{diag}(\mathbf{w}) g(\mathbf{V}_N(\mathcal{I}, :)\mathbf{u}_N).$$

We use the greedy algorithm for empirical cubature.



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

Hernádez et al. (2017) *Dimensional hyper-reduction of nonlinear finite element models via empirical cubature.*

Two-step hyper-reduction

Motivation: need to preserve previous properties (SBP and zero row sum) for hyper-reduced differential operator $\overline{\mathbf{Q}}$ for entropy stability.

(Step 1) Compression: expanded basis approach with intermediate reduced operator

$$\widehat{\mathbf{Q}}_t = \mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t,$$

where $\mathbf{V}_t$ is some test basis at least spans $\mathcal{R}(\mathbf{V}_N)$.

(Step 2) Projection ($\mathbf{W} = \operatorname{diag}(\mathbf{w})$ orthogonal):

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

Finally, hyper-reduced differential matrix

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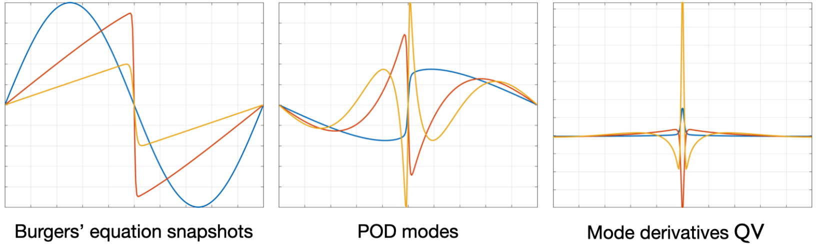
Choice of test basis



- For shocks, POD basis $\mathbf{V}_N$ poorly samples derivative matrix (e.g. $\mathbf{V}_N^T \mathbf{Q} \mathbf{V}_N \approx \mathbf{0}$).
- Additionally, the error $\mathbf{Q} - \overline{\mathbf{Q}}$ should be orthogonal to $\mathbf{V}_N$ if we use all nodes for hyper-reduction.
- Choice of test basis for DG methods: $\mathbf{V}_N$ augmented with $\boxed{\mathbf{M}^{-1}\mathbf{Q}^T\mathbf{V}_N}$.

Theorem of zero "ideal" hyper-reduction error

Theorem

If $\mathcal{R}(\mathbf{V}_N)$, $\mathcal{R}(\mathbf{M}^{-1}\mathbf{Q}^T\mathbf{V}_N) \subset \mathcal{R}(\mathbf{V}_t)$, *then* $\mathbf{V}_N^T(\mathbf{Q} - \overline{\mathbf{Q}}) = \mathbf{0}$ *under "ideal" hyper-reduction (using all nodes).*

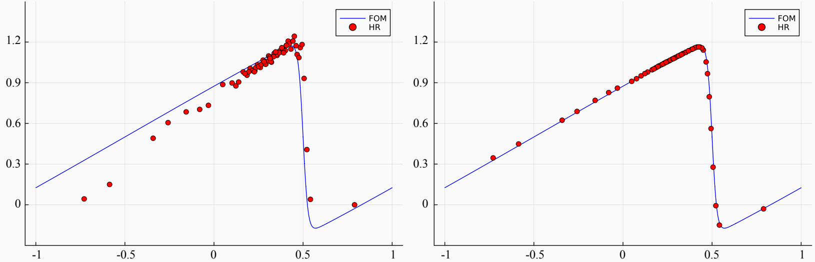


Figure 1: Comparison of including $\mathcal{R}(\mathbf{QV}_N)$ or $\mathcal{R}(\mathbf{M}^{-1}\mathbf{QV}_N)$ in test basis for 1D Burgers' equation using DG methods (25 modes).

Hyper-reduction of boundary terms

Assume hyper-reduction on boundary $(\mathcal{I}_b, \mathbf{w}_b)$ and denote

$$\overline{\mathbf{B}}^i = \text{diag}(\mathbf{n}^i)\text{diag}(\mathbf{w}_b).$$

Suppose $\mathbf{V}^i$ is some ROM boundary test basis matrix for the ith coordinate,

$$\mathbf{1}^T\mathbf{Q}^i\mathbf{V}^i = \mathbf{1}^T\overline{\mathbf{B}}^i\mathbf{V}^i(\mathcal{I}_b,:),$$

is a matrix form of the fundamental theorem of calculus, and we need to enforce this equality to preserve entropy stability.

A natural way to do this: Carathéodory pruning.

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Carathéodory's pruning

Carathéodory's theorem states that, for any M-point positive quadrature rule exact on space $\mathbf{V}$ with $\dim(\mathbf{V}) = N$, we can always generate a new N-point positive rule to preserve all moments.

In our case,

$$\mathbf{1}^T \mathbf{B}^i \mathbf{V}^i = \int \phi_j^i(\mathbf{x}_k)\mathbf{n}^i = \sum_{k=1}^{M} \mathbf{w}_{b,j} \mathbf{n}_j^i \phi_j(\mathbf{x}_k).$$

In practice, we concatenate all dimensions

$$\begin{bmatrix} \text{diag}(\mathbf{n}^1)\mathbf{V}^1 & \cdots & \text{diag}(\mathbf{n}^d)\mathbf{V}^d \end{bmatrix}$$

which yields $\mathcal{O}(dN)$ hyper-reduced positive boundary weights $\mathbf{w}_b$ and node indices $\mathcal{I}_b$.

Van Den Bos, Sanderse, Bierbooms, Van Bussel (2020). *Generating nested quadrature rules with positive weights based on arbitrary sample sets.*

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Numerical Experiments

DG ROM Example 1 - 1D reflective wall boundary conditions

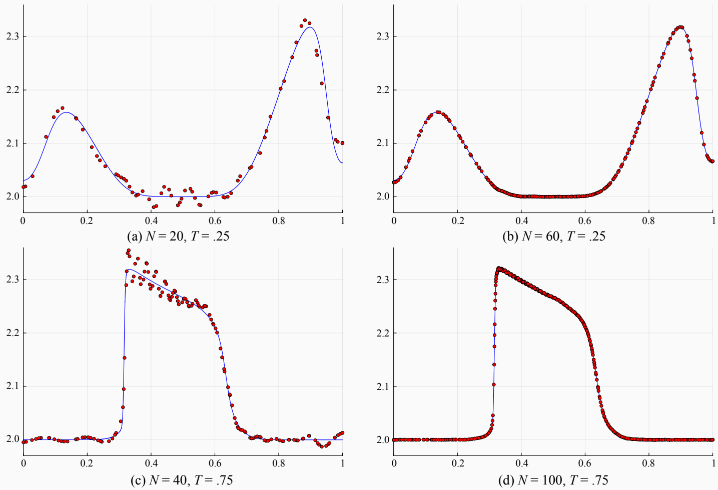
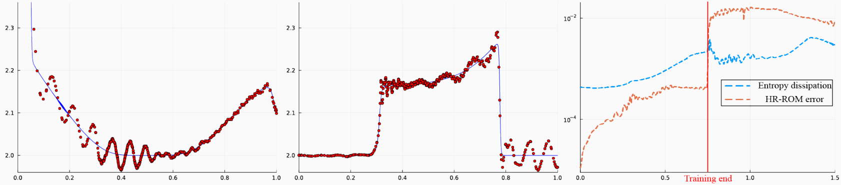


Figure 2: 1D Compressible Euler (reflective wall). FOM dim: 2048. Viscosity: 2×10^{-4}. Runtime $T = .75$.

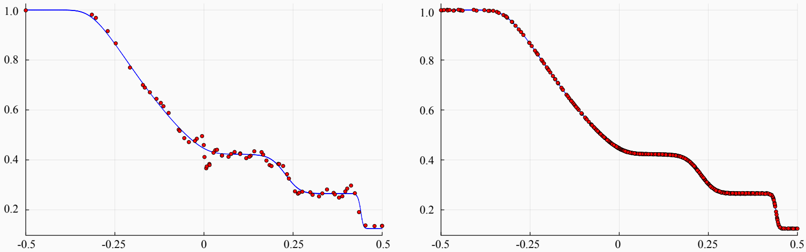
DG ROM Example 1 - 1D reflective wall boundary conditions



(a) 100 modes, $T = 1.0$ (b) 100 modes, $T = 1.5$ (c) Error and entropy dissipation

Figure 3: Snapshot runtime $T = .75$. Prediction at $T = 1.0$ and $T = 1.5$.

DG ROM Example 2 - Sod shock tube

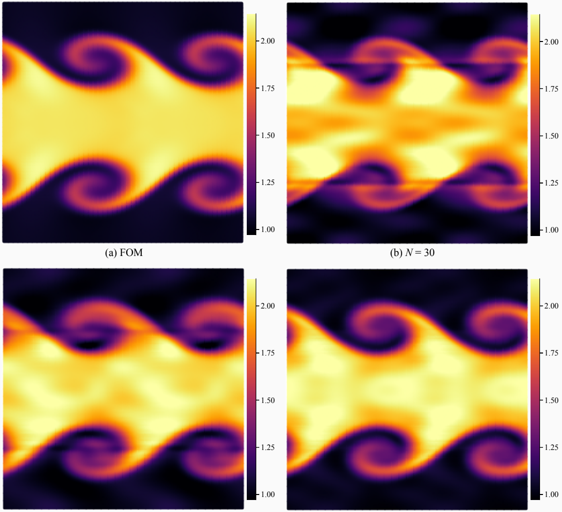


(a) $N = 20$, $T = .25$

(b) $N = 100$, $T = .25$

Figure 4: FOM dim: 2048. Viscosity: 5×10^{-4}. Runtime T = $.25$.

DG ROM Example 3 - Kelvin-Helmholtz instability



(a) FOM (b) $N = 30$ (c) $N = 40$ (d) $N = 50$

Figure 5: FOM dim: 25,600. Viscosity: 1×10^{-3}. Runtime $T = 3.0$.

DG ROM Example 4 - 2D reflective wall boundary conditions

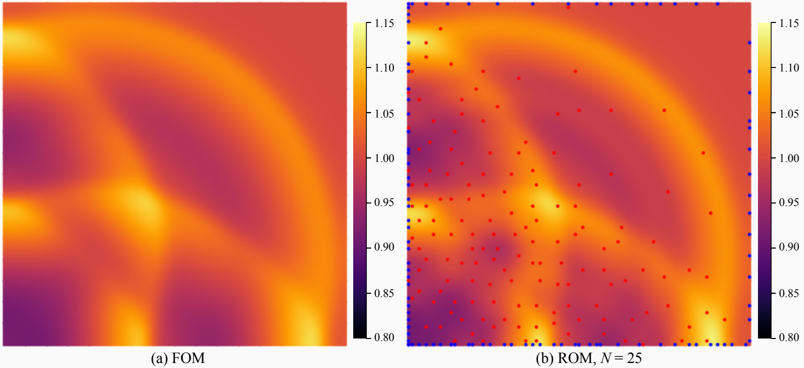


Figure 6: 2D compressible Euler (reflective wall). FOM dim: 6400. Viscosity: 1×10^{-3}. Run time $T = 1.0$. Boundary hyper-reduced by Carathéodory pruning (blue nodes).

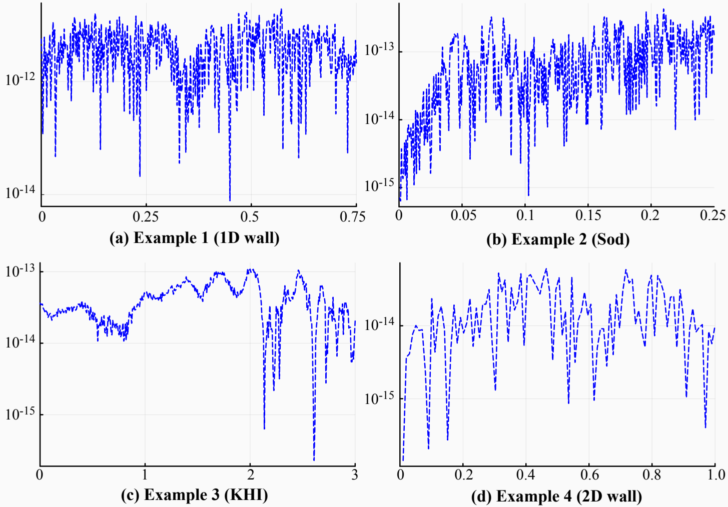


Figure 7: Convective entropy of DG ROM examples.

Summary and acknowledgement

In this work, we

- present an entropy stable reduced order modeling of nonlinear conservation laws based on high order DG methods.
- develop structure-preserving hyper-reduction techniques (weighted test basis and Carathéodory pruning) which preserve entropy stability.

This work was supported by NSF grant DMS-1943186.