Entropy stable reduced order modeling of nonlinear conservation laws using discontinuous Galerkin methods

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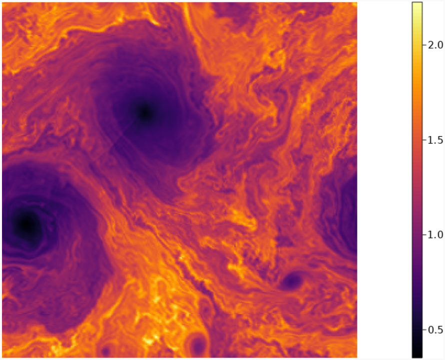
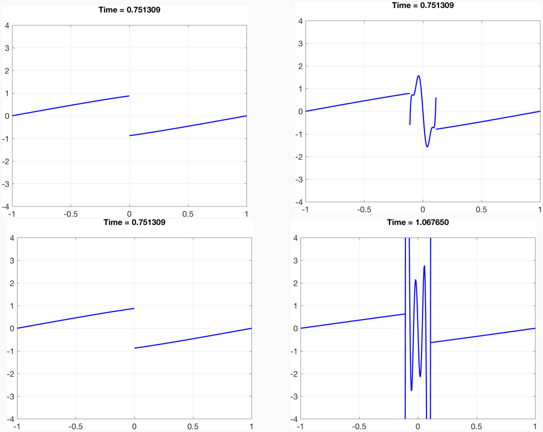
Why reduced order modeling?



- High-fidelity simulations are nice, but often involves extreme-scale nonlinear evaluations (Example).
- Reduced order modeling (ROM) enables real-time simulation and analysis as well as the exploration of parameter spaces in many-query contexts.

Why entropy stability?



(a) Exact solution **(b)** High order DG

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

Entropy stability for nonlinear problems

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

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

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

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

$$\Longrightarrow \int_{\Omega} \frac{\partial S(\mathbf{u})}{\partial \mathrm{t}} + \sum_{i}^{d} \left(\mathbf{v}^T \mathbf{f}_i(\mathbf{u}) - \psi_i(\mathbf{u}) \right) \Big|_{-1}^{1} \leq 0.$$

Talk outline

1. Mode construction for 1D periodic domain

2. Model construction for 1D domain with weakly imposed boundary conditions

3. Extension to domain with higher dimensions (with Carathéodory pruning)

4. Numerical experiments

Mode construction for 1D periodic domain

Local formulation

- Domain Ω (1D) is decomposed into k elements, each with N_p (Gauss-Lobatto) interpolation degree.

- A local DG formulation on element D^k is

$$J_k \mathbf{M}_{\text{loc}} \frac{\mathrm{d}\mathbf{u}_k}{\mathrm{dt}} + ((\mathbf{Q}_{\text{loc}} - \mathbf{Q}_{\text{loc}}^T) \circ \mathbf{F}^k)\mathbf{1} + \mathbf{B}_{\text{loc}} \mathbf{f}^* = \mathbf{0},$$

$$\mathbf{f}^* = \begin{bmatrix} \mathbf{f}_S(\mathbf{u}_{1,k}^+, \mathbf{u}_{1,k}) & 0 & \cdots & 0 & \mathbf{f}_S(\mathbf{u}_{N_p,k}^+, \mathbf{u}_{N_p,k}) \end{bmatrix}^T.$$

  For periodic boundary condition,

$$\mathbf{u}_{1,1}^+ = \mathbf{u}_{N_p,K}, \qquad \mathbf{u}_{N_p,K}^+ = \mathbf{u}_{1,1}.$$

- Summation-by-parts (SBP) property: $\mathbf{Q}_{\text{loc}} + \mathbf{Q}_{\text{loc}}^T = \mathbf{B}_{\text{loc}}$.

Global formulation

- ROM necessitates global formulation. Denote global solution vector $\mathbf{u} = [\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_K]^T$. A global formulation is

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + 2(\mathbf{Q} \circ \mathbf{F})\mathbf{1} = \mathbf{0},$$

$$\mathbf{M} = \mathbf{I} \bigotimes \mathbf{M}_{\mathsf{loc}}, \quad \mathbf{F} = \begin{bmatrix} \mathbf{F}_{11} & \cdots & \mathbf{F}_{1K} \\ \vdots & \ddots & \vdots \\ \mathbf{F}_{K1} & \cdots & \mathbf{F}_{KK} \end{bmatrix},$$

$$\mathbf{Q} = \frac{1}{2}\begin{bmatrix} \mathbf{S} & \mathbf{B}_R & & -\mathbf{B}_L \\ -\mathbf{B}_L & \mathbf{S} & \mathbf{B}_R & \\ & -\mathbf{B}_L & \ddots & \mathbf{B}_R \\ \mathbf{B}_R & & -\mathbf{B}_L & \mathbf{S} \end{bmatrix}, \quad \mathbf{S} = (\mathbf{Q}_{\mathsf{loc}} - \mathbf{Q}_{\mathsf{loc}}^T),$$

$$\mathbf{B}_L = \begin{bmatrix} & & 1 \\ & \iddots & \\ 0 & & \end{bmatrix}, \qquad \mathbf{B}_R = \mathbf{B}_L^T = \begin{bmatrix} & & 0 \\ & \iddots & \\ 1 & & \end{bmatrix}.$$

Entropy stability

- The two-point flux $\mathbf{f}_S(\mathbf{u}_L, \mathbf{u}_R)$ is entropy-conservative if it satisfies

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

- We can prove a semi-discrete entropy conservation condition

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

using the fact that $\mathbf{Q}$ is skew-symmetric ($\mathbf{Q} = -\mathbf{Q}^T$) and has zero row sums ($\mathbf{Q}\mathbf{1} = \mathbf{0}$).

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

Entropy stability - proof

Testing global formulation with entropy variable $\mathbf{v} = \mathbf{v}(\mathbf{u})$,

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

Assuming time continuity, then

$$\begin{aligned}
\mathbf{v}^T \mathbf{M} \frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} &= \sum_i \mathbf{M}_{i,i} \mathbf{v}_i^T \frac{\mathrm{d}\mathbf{u}_i}{\mathrm{dt}} \\
&= \sum_i \mathbf{M}_{i,i} (\frac{\mathrm{d}S(\mathbf{u})}{\mathrm{d}\mathbf{u}})_i^T \frac{\mathrm{d}\mathbf{u}_i}{\mathrm{dt}} \\
&= \sum_i \mathbf{M}_{i,i} \frac{\mathrm{d}S(\mathbf{u}_i)}{\mathrm{dt}} \\
&= \mathbf{1}^T \mathbf{M} \frac{\mathrm{d}S(\mathbf{u})}{\mathrm{dt}},
\end{aligned}$$

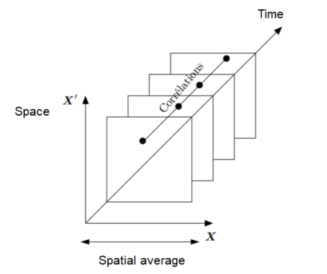
Entropy stability - proof

It is left to show the flux term goes to 0 (with entropy conservative flux).

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

Reduced order model - POD method

- Denote $\{\phi_j(\mathbf{x}_i)\}_{j=1}^N$ as our reduced basis, $\mathbf{V}_N$ as the general Vandermonde matrix $(\mathbf{V}_N)_{ij} = \phi_j(\mathbf{x}_i)$.
- Various techniques to construct $\mathbf{V}_N$ - we use proper orthogonal decomposition (POD).
- $\mathbf{V}_{\text{snap}} = U\Sigma V^T$, $\mathbf{V}_N = U[:, 1:N]$.



Liang et al. (2000) *Proper orthogonal decomposition and its applications-Part I: Theory.*

Reduced order model - Galerkin projection

Galerkin projection ROM ($\mathbf{u} \approx \mathbf{V}_N \mathbf{u}_N$):

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

Two issues:

- Not entropy stable.
- No necessarily less computational cost.

Rowley et al. (2004) *Model reduction for compressible flows using POD and Galerkin projection.*

Reduced order model - entopy stability

Testing (1) with $\mathbf{v}_N$ and following same steps in prior proof, we can get to a point that

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

where $\widetilde{\mathbf{v}} = \mathbf{V}_N \mathbf{v}_N$.

Why: $\widetilde{\mathbf{v}}(\cdot)$ and $\mathbf{u}(\cdot)$ are no longer coupled mappings.

Solution: new mapping

$$\widetilde{\mathbf{u}} = \mathbf{u}(\mathbf{V}_N \mathbf{V}_N^{\dagger} \mathbf{v}(\mathbf{V}_N \mathbf{u}_N)) = \mathbf{u}(\widetilde{\mathbf{v}}).$$

Entropy stable reduced order model

The final entropy stable ROM is

$$
\begin{aligned}
&\mathbf{M}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + 2\mathbf{V}_N^T(\mathbf{Q} \circ \mathbf{F})\mathbf{1} = \mathbf{0}, \\
&\mathbf{M}_N = \mathbf{V}_N^T \mathbf{M} \mathbf{V}_N, \qquad \mathbf{F}_{ij} = \mathbf{f}_S(\widetilde{\mathbf{u}}_i, \widetilde{\mathbf{u}}_j), \\
&\widetilde{\mathbf{u}} = \mathbf{u}(\mathbf{V}_N \mathbf{V}_N^\dagger \mathbf{v}(\mathbf{V}_N \mathbf{u}_N)).
\end{aligned} \tag{2}
$$

Still has high computational cost! Hyper-reduction on flux term is necessary to reduce computational cost.

Hyper-reduction - main idea

- Main idea: weighting and sampling strategy

$$\mathbf{V}_N^T g(\mathbf{V}_N \mathbf{u}_N) \approx \bar{\mathbf{V}}_N^T \mathbf{W} g(\bar{\mathbf{V}}_N \mathbf{u}_N), \ \bar{\mathbf{V}}_N = \mathbf{V}_N(I,:)$$
$$\implies \mathbf{V}_N^T(\mathbf{Q} \circ \mathbf{F}) \approx \bar{\mathbf{V}}_N^T \mathbf{W}(\bar{\mathbf{Q}} \circ \bar{\mathbf{F}}).$$

  Still entropy stable if $\bar{\mathbf{Q}}$ is skew-symmetric and has zero row sums.

- To maintain these properties of $\bar{\mathbf{Q}}$, we must apply a two-step hyper-reduction.

Farhat et al. (2015) *Structure-preserving, stability, and accu- racy properties of the energy-conserving sampling and weighting method for the hyper reduction of nonlinear finite element dynamic models.*

Chapman et al. (2017) *Accelerated mesh sampling for the hyper reduction of nonlinear computational models.*

Two-step hyper-reduction: compress and project

Compression: Galerkin projection with expanded basis approach.

$\mathbf{V}_t$: a test basis such that $R(\mathbf{V}_N) \subset R(\mathbf{V}_t)$.
The intermediate reduced operator is defined as

$$\mathbf{Q}_t = \mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t.$$

By construction, $\mathbf{Q}_t$ is skew-symmetric.

One can show, if $\mathbf{1}$ lies in the span of the test basis ($\mathbf{1} = \mathbf{V}_t \mathbf{e}$ for some coefficient vector $\mathbf{e}$) then

$$\mathbf{Q}_t \mathbf{e} = \mathbf{0}.$$

Two-step hyper-reduction: compress and project

Projection: construct test mass matrix

$$\mathbf{M}_t = \bar{\mathbf{V}}_t \mathbf{W} \bar{\mathbf{V}}_t, \qquad \bar{\mathbf{V}}_t = \mathbf{V}_t(I,:).$$

Then we can construct a projection matrix

$$\mathbf{P}_t = \mathbf{M}_t^{-1} \bar{\mathbf{V}}_t^T \mathbf{W}.$$

Suppose $\mathbf{f} = \bar{\mathbf{V}}_t \mathbf{c}$ for some coefficients $\mathbf{c}$, then

$$\mathbf{P}_t \mathbf{f} = \mathbf{M}_t^{-1} \mathbf{M}_t \mathbf{c} = \mathbf{c}.$$

Finally, hyper-reduced differential matrix

$$\bar{\mathbf{Q}} = \mathbf{P}_t^T \mathbf{Q}_t \mathbf{P}_t = (\mathbf{M}_t^{-1} \bar{\mathbf{V}}_t^T \mathbf{W})^T (\mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t) \mathbf{M}_t^{-1} \bar{\mathbf{V}}_t^T \mathbf{W}.$$

Entropy stability and choice of test basis

$\bar{\mathbf{Q}}$ is skew-symmetric by construction. If $\mathbf{1}$ lies in the span of test basis, $\mathbf{1} = \bar{\mathbf{V}}_t\mathbf{e}$ and $\mathbf{Q}_t\mathbf{e} = \mathbf{0}$ for some coefficient $\mathbf{e}$. Then,

$$\bar{\mathbf{Q}}\mathbf{1} = \mathbf{P}_t^T\mathbf{Q}_t\mathbf{e} = \mathbf{0}.$$

Thus, the test basis must span $\mathbf{1}$ and $\mathbf{V}_N$. We also enhance it with $\mathbf{Q}\mathbf{V}_N$ to accurately evaluate derivatives. In the absence of hyper-reduction, this projector ensures that:

$$\mathbf{P}_t = \mathbf{V}_t^\dagger \quad \Longrightarrow \quad \bar{\mathbf{Q}}\mathbf{V}_N = (\mathbf{V}_t\mathbf{V}_t^\dagger)^T\mathbf{Q}\mathbf{V}_t\mathbf{V}_t^\dagger\mathbf{V}_N = \mathbf{Q}\mathbf{V}_N.$$

Algorithm and target space

Numerous methods to select hyper-reduced nodes. We developed greedy algorithm from empirical cubature. The algorithm produces an index set and corresponding new weights such that:

$$\mathbf{V}_{\text{target}}^T \mathbf{w}_{\text{target}} \approx \mathbf{V}_{\text{target}}(I,:)^T \mathbf{w}.$$

This algorithm selects the row index that positively aligned with the residual and subsequently computes the weight vector that minimizes the residual using a non-negative least squares solver. It terminates when the norm of the residual falls below

$$tol = \sqrt{(\sum_{j=N+1}^{M} \sigma_j^2)/(\sum_{j=1}^{M} \sigma_j^2)}.$$

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

Stabilization points

- Three options for $\mathbf{V}_{\text{target}}$: $\mathbf{V}_N \circ \mathbf{V}_N$, $\mathbf{V}_N \circ \mathbf{V}_t$, and $\mathbf{V}_t \circ \mathbf{V}_t$.
- If singular test mass matrix $\bar{\mathbf{V}}_t^T \mathbf{W} \bar{\mathbf{V}}_t$: add "stabilization" points.

  Construct matrix $\mathbf{Z}$ from the eigenvectors

$$\mathbf{Z} = \begin{bmatrix} \mathbf{V}_t \mathbf{z}_1 & \cdots & \mathbf{V}_t \mathbf{z}_{N_z} \end{bmatrix},$$

  Approximating $\mathbf{Z}^T \mathbf{W} \mathbf{Z}$ ensures non-singularity. Set

$$\mathbf{Z}_{\text{target}} = \mathbf{Z}(:, i) \circ \mathbf{Z}(:, j).$$

  We then obtain an additional set of nodes, and then recalculate weights from

$$\mathbf{w} = \arg\min_{\mathbf{c} \geq 0} \frac{1}{2} (\|\mathbf{V}_{\text{target}}(I, :)^T \mathbf{c} - \mathbf{b}\|^2 + \alpha_Z \|\mathbf{Z}_{\text{target}}(I, :)^T \mathbf{c} - \mathbf{d}\|^2),$$

  where $\mathbf{d} = \mathbf{Z}_{\text{target}}^T \mathbf{w}_{\text{target}}$.

Summary of offline hyper-reduction

1. Compute a $N-$mode reduced basis matrix $\mathbf{V}_N$ from solution snapshots of both conservative and entropy variables in full order model.
2. Compute a test basis matrix $\mathbf{V}_t$ such that $R(\mathbf{V}_t) = R(\mathbf{1}, \mathbf{V}_N, \mathbf{Q}\mathbf{V}_N)$, and compute test matrix $\mathbf{Q}_t = \mathbf{V}_t^T \mathbf{Q} \mathbf{V}_t$.
3. Compute a hyper-reduced quadrature using greedy algorithm to obtain a set of hyper-reduced nodes I and new quadrature weights $\mathbf{w}$, with stabilizing points if necessary to ensure that the test mass matrix $\mathbf{M}_t = \bar{\mathbf{V}}_t \mathbf{W} \bar{\mathbf{V}}_t$ is non-singular.
4. Construct the hyper-reduced nodal differentiation matrix $\bar{\mathbf{Q}} = \mathbf{P}_t^T \mathbf{Q}_t \mathbf{P}_t$ using the projection $\mathbf{P}_t = \mathbf{M}_t^{-1} \bar{\mathbf{V}}_t^T \mathbf{W}$ onto the test basis.

Hyper-reduced ROM

The final ROM with hyper-reduction

$$\begin{aligned}
&\bar{\mathbf{M}}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + 2\bar{\mathbf{V}}_N^T(\bar{\mathbf{Q}} \circ \mathbf{F})\mathbf{1} = \mathbf{0} \\
&\bar{\mathbf{V}}_N = \mathbf{V}_N(I,:), \qquad \bar{\mathbf{M}}_N = \bar{\mathbf{V}}_N^T \mathbf{W} \bar{\mathbf{V}}_N, \\
&\mathbf{P} = \bar{\mathbf{M}}_N^{-1} \bar{\mathbf{V}}_N^T \mathbf{W}, \qquad \mathbf{v}_N = \mathbf{P}\mathbf{v}(\bar{\mathbf{V}}_N \mathbf{u}_N), \\
&\widetilde{\mathbf{v}} = \bar{\mathbf{V}}_N \mathbf{v}_N, \qquad \widetilde{\mathbf{u}} = \mathbf{u}(\widetilde{\mathbf{v}}), \qquad \mathbf{F}_{ij} = \mathbf{f}_S(\widetilde{\mathbf{u}}_i, \widetilde{\mathbf{u}}_j),
\end{aligned} \tag{3}$$

which semi-discretely conserves the sampled and weighted average entropy

$$\mathbf{1}^T \mathbf{W} \frac{\mathrm{d}S(\bar{\mathbf{V}}_N \mathbf{u}_N)}{\mathrm{dt}} = 0.$$

Model construction for 1D domain with weakly imposed boundary conditions

Global formulation

From local formulation,

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + 2(\mathbf{Q} \circ \mathbf{F})\mathbf{1} + \mathbf{B}(\mathbf{f}^* - \mathbf{f}(\mathbf{u})) = \mathbf{0}, \tag{4}$$

where $\mathbf{Q}$ is now

$$\mathbf{Q} = \frac{1}{2}\begin{bmatrix} \mathbf{S} & \mathbf{B}_R & & \\ -\mathbf{B}_L & \mathbf{S} & \mathbf{B}_R & \\ & -\mathbf{B}_L & \ddots & \mathbf{B}_R \\ & & -\mathbf{B}_L & \mathbf{S} \end{bmatrix} + \frac{1}{2}\mathbf{B},$$

satisfying SBP property $\mathbf{Q} + \mathbf{Q}^T = \mathbf{B}$.

The formulation is entropy conservative if we use entropy conservative boundary flux.

Chen and Shu. (2017) *Entropy stable high order discontinuous galerkin meth- ods with suitable quadrature rules for hyperbolic conservation laws.*

Hybridized operator

$\bar{\mathbf{Q}}$ does not satisfy SBP property. Instead,

$$\bar{\mathbf{Q}} + \bar{\mathbf{Q}}^T = \mathbf{E}^T\mathbf{B}_w\mathbf{E}, \qquad \bar{\mathbf{Q}} = \mathbf{P}_t^T\mathbf{V}_t^T\mathbf{Q}\mathbf{V}_t\mathbf{P}_t,$$

where in 1D

$$\mathbf{B}_w = \begin{bmatrix} -1 & \\ & 1 \end{bmatrix}, \qquad \mathbf{E} = \mathbf{V}_{bt}\mathbf{P}_t, \qquad \mathbf{V}_{bt} = \begin{bmatrix} \mathbf{V}_t(1,:) \\ \mathbf{V}_t(N,:) \end{bmatrix}.$$

To impose nonlinear boundary conditions, we employ a hybridzed SBP operator

$$\mathbf{Q}_h = \frac{1}{2}\begin{bmatrix} \bar{\mathbf{Q}} - \bar{\mathbf{Q}}^T & \mathbf{E}^T\mathbf{B} \\ -\mathbf{B}\mathbf{E} & \mathbf{B} \end{bmatrix},$$

satisfying a block SBP property

$$\mathbf{Q}_h + \mathbf{Q}_h^T = \begin{bmatrix} \mathbf{0} & \\ & \mathbf{B} \end{bmatrix} = \mathbf{B}_h.$$

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

Hyper-reduced ROM

One can show

$$\mathbf{Q}_h \mathbf{1} = \frac{1}{2} \begin{bmatrix} \bar{\mathbf{Q}}\mathbf{1} - \bar{\mathbf{Q}}^T \mathbf{1} + \mathbf{E}^T \mathbf{B} \mathbf{1} \\ -\mathbf{B}\mathbf{E}\mathbf{1} + \mathbf{B}\mathbf{1} \end{bmatrix} = \mathbf{0}.$$

Denote

$$\mathbf{V}_b = \begin{bmatrix} \mathbf{V}_N(1,:) \\ \mathbf{V}_N(N_p,:) \end{bmatrix}, \qquad \mathbf{V}_h = \begin{bmatrix} \bar{\mathbf{V}}_N \\ \mathbf{V}_b \end{bmatrix}.$$

Then we can build the following hyper-reduced ROM

$$\begin{aligned} &\bar{\mathbf{M}}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + 2\mathbf{V}_h^T (\mathbf{Q}_h \circ \mathbf{F})\mathbf{1} + \mathbf{V}_b^T \mathbf{B}(\mathbf{f}^* - \mathbf{f}(\widetilde{\mathbf{u}}_b)) = \mathbf{0} \\ &\bar{\mathbf{V}}_N = \mathbf{V}_N(I,:), \qquad \bar{\mathbf{M}}_N = \bar{\mathbf{V}}_N^T \mathbf{W} \bar{\mathbf{V}}_N,, \qquad \mathbf{P} = \bar{\mathbf{M}}_N^{-1} \bar{\mathbf{V}}_N^T \mathbf{W}, \\ &\mathbf{v}_N = \mathbf{P}\mathbf{v}(\bar{\mathbf{V}}_N \mathbf{u}_N), \qquad \widetilde{\mathbf{v}} = \mathbf{V}_h \mathbf{v}_N, \qquad \widetilde{\mathbf{v}}_b = \mathbf{V}_b \mathbf{v}_N, \\ &\widetilde{\mathbf{u}} = \mathbf{u}(\widetilde{\mathbf{v}}), \qquad \widetilde{\mathbf{u}}_b = \mathbf{u}(\widetilde{\mathbf{v}}_b), \qquad \mathbf{F}_{ij} = \mathbf{f}_S(\widetilde{\mathbf{u}}_i, \widetilde{\mathbf{u}}_j). \end{aligned} \tag{5}$$

Hyper-reduced ROM - entropy stability

By the block SBP property of $\mathbf{Q}_h$, formulation (5) is equivalent to

$$\bar{\mathbf{M}}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + \mathbf{V}_h^T((\mathbf{Q}_h - \mathbf{Q}_h^T) \circ \mathbf{F})\mathbf{1} + \mathbf{V}_b^T \mathbf{B}\mathbf{f}^* = \mathbf{0}, \tag{6}$$

which admits entropy conservation for boundary entropy conservative flux

$$\mathbf{1}^T \mathbf{W} \frac{\mathrm{d}S(\mathbf{V}_N \mathbf{u}_N)}{\mathrm{dt}} = 0.$$

Proof: Testing (6) with $\mathbf{v}_N$,

$$\mathbf{1}^T \mathbf{W} \frac{\mathrm{d}S(\mathbf{V}_N \mathbf{u}_N)}{\mathrm{dt}} + \widetilde{\mathbf{v}}^T((\mathbf{Q}_h - \mathbf{Q}_h^T) \circ \mathbf{F})\mathbf{1} + \widetilde{\mathbf{v}}_b^T \mathbf{B}\mathbf{f}^* = \mathbf{0}.$$

Hyper-reduced ROM - entropy stability

$$
\begin{aligned}
&\widetilde{\mathbf{v}}^T((\mathbf{Q}_h - \mathbf{Q}_h^T) \circ \mathbf{F})\mathbf{1} \\
&= \frac{1}{2}\sum_{ij}(\mathbf{Q}_h - \mathbf{Q}_h^T)_{ij}(\widetilde{\mathbf{v}}_i - \widetilde{\mathbf{v}}_j)^T \mathbf{f}_S(\widetilde{\mathbf{u}}_i, \widetilde{\mathbf{u}}_j) \\
&= \frac{1}{2}\sum_{ij}(\mathbf{Q}_h - \mathbf{Q}_h^T)_{ij}(\psi(\widetilde{\mathbf{u}}_i)) - \psi(\widetilde{\mathbf{u}}_j)) \\
&= \psi(\widetilde{\mathbf{u}})^T \mathbf{Q}_h \mathbf{1} - \mathbf{1}^T \mathbf{Q}_h \psi(\widetilde{\mathbf{u}}) \\
&= -\mathbf{1}^T \mathbf{B}_h \psi(\widetilde{\mathbf{u}}) \\
&= -\mathbf{1}^T \mathbf{B} \psi(\widetilde{\mathbf{u}}_b),
\end{aligned}
$$

$$
\Longrightarrow \mathbf{1}^T \mathbf{W} \frac{\mathrm{d}S(\mathbf{V}_N \mathbf{u}_N)}{\mathrm{dt}} - \mathbf{1}^T \mathbf{B}(\psi(\widetilde{\mathbf{u}}_b) - \widetilde{\mathbf{v}}_b^T \mathbf{f}^*) = \mathbf{0}.
$$

With an entropy conservative boundary flux, $\psi(\widetilde{\mathbf{u}}_b) = \widetilde{\mathbf{v}}_b^T \mathbf{f}^*$

$$
\mathbf{1}^T \mathbf{W} \frac{\mathrm{d}S(\mathbf{V}_N \mathbf{u}_N)}{\mathrm{dt}} = 0.
$$

Extension to domain with higher dimensions (with Carathéodory pruning)

Periodic domain - FOM

For a periodic domain with dimension d,

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + \sum_{i=1}^{d} 2(\mathbf{Q}^i \circ \mathbf{F}^i)\mathbf{1} = \mathbf{0}, \tag{7}$$

Complicated explicit form, but (for vectors $\mathbf{u}$, $\mathbf{v}$) satisfies

$$\mathbf{v}^T\mathbf{Q}^i\mathbf{u} = \sum_k \left(\int_{D^k} \frac{\partial \mathbf{u}}{\partial \mathbf{x}_i}\mathbf{v} + \int_{\partial D^k} \frac{1}{2}[\![\mathbf{u}]\!]\mathbf{n}^i\mathbf{v} \right). \tag{8}$$

To prove entropy stability, one can show that $\mathbf{Q}^i$ is skew-symmetric and has zero row sums.

Periodic domain - ROM

Applying hyper-reduction on each dimension to construct

$$\bar{\mathbf{Q}}^i = (\mathbf{P}_t^i)^T (\mathbf{V}_t^i)^T \mathbf{Q}^i \mathbf{V}_t^i \mathbf{P}_t^i,$$

we get the entropy conservative hyper-reduced ROM

$$\begin{aligned}
&\bar{\mathbf{M}}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + \sum_{i=1}^{d} (2\bar{\mathbf{V}}_N^T (\bar{\mathbf{Q}}^i \circ \mathbf{F}^i)\mathbf{1}) = \mathbf{0} \\
&\bar{\mathbf{V}}_N = \mathbf{V}_N(I,:), \qquad \bar{\mathbf{M}}_N = \bar{\mathbf{V}}_N^T \mathbf{W} \bar{\mathbf{V}}_N, \\
&\mathbf{P} = \bar{\mathbf{M}}_N^{-1} \bar{\mathbf{V}}_N^T \mathbf{W}, \qquad \mathbf{v}_N = \mathbf{P}\mathbf{v}(\bar{\mathbf{V}}_N \mathbf{u}_N), \\
&\widetilde{\mathbf{v}} = \bar{\mathbf{V}}_N \mathbf{v}_N, \qquad \widetilde{\mathbf{u}} = \mathbf{u}(\widetilde{\mathbf{v}}), \qquad \mathbf{F}_{jk}^i = \mathbf{f}_S^i(\widetilde{\mathbf{u}}_j, \widetilde{\mathbf{u}}_k).
\end{aligned} \tag{9}$$

Domain with weak BC - FOM

We can extend (4) to higher dimensions

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{dt}} + \sum_{i=1}^{d}(2(\mathbf{Q} \circ \mathbf{F})\mathbf{1} + \mathbf{B}(\mathbf{f}^* - \mathbf{f}(\mathbf{u}))) = \mathbf{0}, \tag{10}$$

where $\mathbf{Q}^i + (\mathbf{Q}^i)^T = \mathbf{B}$.

Domain with weak BC - ROM

Suppose we have similar hyper-reduction on boundary nodes $(I_b, \mathbf{w}_b)$, and denote

$$\bar{\mathbf{B}}^i = \text{diag}(\mathbf{n}^i)\mathbf{W}_b, \qquad \bar{\mathbf{E}}^i = \bar{\mathbf{V}}_{bt}^i \mathbf{P}_t^i, \qquad \bar{\mathbf{V}}_{bt} = \mathbf{V}_{bt}(I_b, :).$$

The hybridized SBP operator for differentiation along the ith coordinate is then

$$\mathbf{Q}_h^i = \begin{bmatrix} \bar{\mathbf{Q}}^i - (\bar{\mathbf{Q}}^i)^T & (\bar{\mathbf{E}}^i)^T \bar{\mathbf{B}}^i \\ -\bar{\mathbf{B}}^i \bar{\mathbf{E}}^i & \bar{\mathbf{B}}^i \end{bmatrix}.$$

Hyper-reduced ROM:

$$\bar{\mathbf{M}}_N \frac{\mathrm{d}\mathbf{u}_N}{\mathrm{dt}} + \sum_{i=1}^{d} (\mathbf{V}_h^T ((\mathbf{Q}_h^i - (\mathbf{Q}_h^i)^T) \circ \mathbf{F}^i) \mathbf{1} + \bar{\mathbf{V}}_b^T \bar{\mathbf{B}}^i \mathbf{f}^{i,*}) = \mathbf{0}. \quad (11)$$

Hyper-reduction on boundary

In general,

$$\mathbf{Q}_h^i \mathbf{1} = \begin{bmatrix} \bar{\mathbf{Q}}^i \mathbf{1} - (\bar{\mathbf{Q}}^i)^T \mathbf{1} + (\bar{\mathbf{E}}^i)^T \bar{\mathbf{B}}^i \mathbf{1} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} -(\bar{\mathbf{Q}}^i)^T \mathbf{1} + (\bar{\mathbf{E}}^i)^T \bar{\mathbf{B}}^i \mathbf{1} \\ \mathbf{0} \end{bmatrix} \neq \mathbf{0}.$$

Note

$$(\bar{\mathbf{Q}}^i)^T \mathbf{1} = (\bar{\mathbf{E}}^i)^T \bar{\mathbf{B}}^i \mathbf{1} \iff \mathbf{1}^T \mathbf{Q}^i \mathbf{V}_t^i = \mathbf{1}^T \bar{\mathbf{B}}^i \bar{\mathbf{V}}_{bt}^i,$$

We need to enforce this equality to preserve entropy conservation.

Hyper-reduction on boundary

Approach 1: linear programming

$$
\begin{aligned}
\text{minimize} \quad & \sum_{j=1} (\mathbf{w}_b)_j \\
\text{subject to} \quad & \bar{\mathbf{V}}_{bt}^T \text{diag}(\mathbf{n}^i) \mathbf{w}_b = \mathbf{V}_t^T (\mathbf{Q}^i)^T \mathbf{1}, \qquad i = 1, ..., d \\
& \mathbf{w}_b \geq \mathbf{0}.
\end{aligned}
$$

Then use certain types of LP solvers (e.g. dual simplex).

Carathéodory's theorem

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 interpolatory positive rule to preserve all moments. In detail, suppose $M \geq N$ and for all $n = 1, ..., N$:

$$m_n := \int v_n(x)dx = \sum_{m=1}^{M} w_m v_n(x_m), \qquad \mathbf{V} = \text{span}\{v_1, ..., v_N\}.$$

This is equivalent to

$$\mathbf{A}\mathbf{w} = \begin{bmatrix} v_1(x_1) & v_1(x_2) & \cdots & v_1(x_M) \\ v_2(x_1) & v_2(x_2) & \cdots & v_2(x_M) \\ \vdots & \vdots & \ddots & \vdots \\ v_N(x_1) & v_N(x_2) & \cdots & v_N(x_M) \end{bmatrix} \begin{bmatrix} w_1 \\ w_1 \\ \vdots \\ w_M \end{bmatrix} = \mathbf{m},$$

with $\mathbf{w} \geq 0$, m is in the convex hull of $\mathbf{0}$ and the M columns of $\mathbf{A}$. Carathéodory's theorem then states that $\mathbf{m}$ lies in the convex hull of a subset of N columns of $\mathbf{A}$.

Hyper-reduction on boundary - Carathéodory pruning

Approach 2: Carathéodory pruning

Given $\mathbf{A} \in \mathbb{R}^{M \times N}$ and $\mathbf{w}$, we use pivoted QR update for pruning through iterations $1 : M - N$

- Determine null vector $\mathbf{c}$ using pivoted QR decomposition.
- Find indices for all positive components in $\mathbf{c}$.
- Select α such that $\mathbf{w} - \alpha\mathbf{c} \geq 0$ and $\mathbf{w}(k_0) = \alpha\mathbf{c}(k_0)$.
- Execute pruning: remove k_0-th entry in $\mathbf{w}$ and I and remove k_0-th row in $\mathbf{A}$.

Hyper-reduction on boundary - Carathéodory pruning

In our case,

$$\mathbf{1}^T\mathbf{B}^i\mathbf{V}_{bt}^i = \int \phi_{bt,j}^i(\mathbf{x}_k)\mathbf{n}^i = \sum_{k=1}^{M\leq 2N+1} \mathbf{w}_{b,j}\mathbf{n}_j^i\phi_{bt,j}(\mathbf{x}_k).$$

In practice, if we only want a single set, we construct the input $\mathbf{A}$ to concatenate all dimensions

$$\mathbf{A} = \begin{bmatrix}\text{diag}(\mathbf{n}^1)\mathbf{V}_{bt}^1 & \cdots & \text{diag}(\mathbf{n}^d)\mathbf{V}_{bt}^d\end{bmatrix}.$$

Following the pruning process, we acquire the hyper-reduced boundary weights $\mathbf{w}_b$ along with node indices I_b.

Numerical experiments

Example 1 - 1D Euler

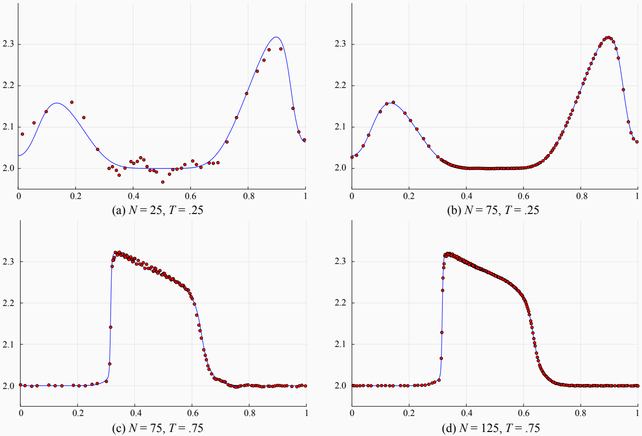


Figure 1: 1D Compressible Euler. DoF 1280. Runtime $T = 0.75$. 400 snapshots.

Example 1 - entropy condition

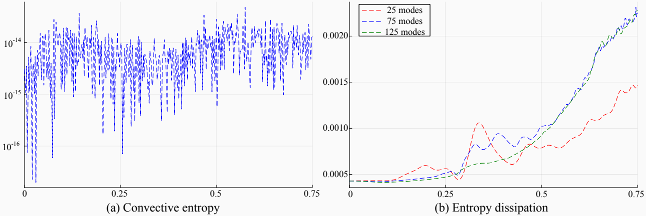
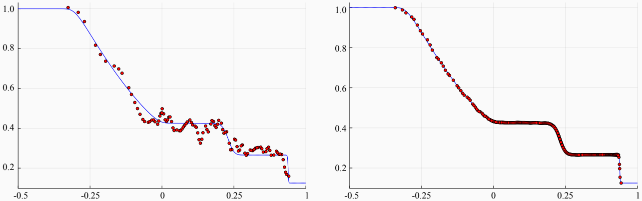


Figure 2: Convective entropy contribution $|\mathbf{v}_N^T \mathbf{V}_h^T (\mathbf{Q}_h \circ \mathbf{F})\mathbf{1}|$ and viscous entropy dissipation over time.

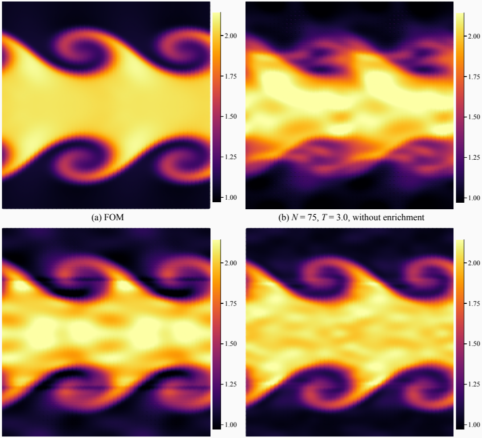
Example 2 - sod shock tube



(a) $N = 50$, $T = .25$ (b) $N = 250$, $T = .25$

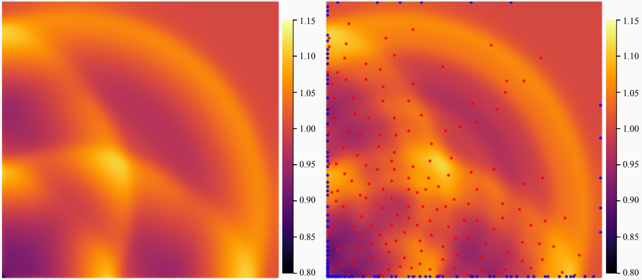
Figure 3: 1D sod shock tube. DoF 1280. Runtime $T = 0.25$. 400 snapshots.

Example 3 - Kelvin-Helmholtz



(a) FOM (b) $N = 75$, $T = 3.0$, without enrichment (c) $N = 75$, $T = 3.0$, with enrichment (d) $N = 125$, $T = 3.0$, with enrichment

Figure 4: 200x200 elements with $N_p = 4$. 200 snapshots with entropy enrichment.



(a) FOM (b) $N = 25$, $T = 1.0$, with enrichment

Figure 5: 2D compressible Euler. Run time $T = 1.0$. 400 snapshots. Boundary hyper-reduced by Catatheodory pruning.

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 (Carathéodory pruning) which preserve entropy stability.

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