S-OPT: A Points Selection Algorithm for Data-Driven Hyper-Reduction in Reduced Order Models

Siu Wun Cheung (cheung26@llnl.gov)

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   - Gresho vortex in compressible Euler equations

System of ordinary differential equations (ODE)

Consider a system of nonlinear ODEs with state dimension N:

$$\boldsymbol{M}(\boldsymbol{\mu})\dot{\boldsymbol{u}}(t;\boldsymbol{\mu}) = \boldsymbol{f}(\boldsymbol{u}(t;\boldsymbol{\mu}), t; \boldsymbol{\mu}), \quad \boldsymbol{u}(0;\boldsymbol{\mu}) = \boldsymbol{u}^0(\boldsymbol{\mu}).$$

- $t \in [0, T]$ denotes time,
- $\boldsymbol{\mu} \in \mathcal{D}$ denotes a vector of parameters,
- $\boldsymbol{M}(\boldsymbol{\mu}) \in \mathbb{R}^{N\times N}$ denotes the nonsingular system matrix,
- $\boldsymbol{f}\colon \mathbb{R}^N \times \mathbb{R} \times \mathcal{D} \rightarrow \mathbb{R}^N$ is a nonlinear function,
- $\boldsymbol{u}^0(\boldsymbol{\mu}) \in \mathbb{R}^N$ denotes the initial condition, and
- $\boldsymbol{u}(t;\boldsymbol{\mu}) \in \mathbb{R}^N$ denotes the state vector.

System of difference equations (OΔE)

$$\boldsymbol{M}(\boldsymbol{\mu})\dot{\boldsymbol{u}}(t;\boldsymbol{\mu}) = \boldsymbol{f}(\boldsymbol{u}(t;\boldsymbol{\mu}), t;\boldsymbol{\mu}), \quad \boldsymbol{u}(0;\boldsymbol{\mu}) = \boldsymbol{u}^0(\boldsymbol{\mu}).$$

- Partition the time domain into $0 = t_0 < t_1 < t_2 < \ldots < t_M = T$.
- Forward Euler discretization: $\dot{\boldsymbol{u}}(t_n) \approx \frac{\boldsymbol{u}(t_{n+1}) - \boldsymbol{u}(t_n)}{t_{n+1} - t_n} = \frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t_n}$.

$$\boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{u}^{n+1}(\boldsymbol{\mu}) = \boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{u}^n(\boldsymbol{\mu}) + \Delta t_n \boldsymbol{f}^n(\boldsymbol{u}^n(\boldsymbol{\mu});\boldsymbol{\mu}) \quad \text{(Explicit)}.$$

- Backward Euler discretization: $\dot{\boldsymbol{u}}(t_{n+1}) \approx \frac{\boldsymbol{u}(t_{n+1}) - \boldsymbol{u}(t_n)}{t_{n+1} - t_n} = \frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t_n}$.

$$\boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{u}^{n+1}(\boldsymbol{\mu}) - \Delta t_n \boldsymbol{f}^{n+1}(\boldsymbol{u}^{n+1}(\boldsymbol{\mu});\boldsymbol{\mu}) = \boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{u}^n(\boldsymbol{\mu}) \quad \text{(Implicit)}.$$

- High order discretization: linear multistep/Runge-Kutta methods.
- Requires to solve system of algebraic equations in $\mathbb{R}^N$.

Reduced order model (ROM)

- Objective: reduce complexity of numerical simulation.
- Low-dimensional solution representation by $\boldsymbol{y} \in \mathbb{R}^k$ $(k \ll N)$:

$$\boldsymbol{u} \approx \tilde{\boldsymbol{u}}(\boldsymbol{y}) = \boldsymbol{u}_{\text{ref}} + \boldsymbol{g}(\boldsymbol{y}).$$

- $\boldsymbol{u}_{\text{ref}} \in \mathbb{R}^N$ is a reference state.
- $\boldsymbol{g} : \mathbb{R}^k \to \mathbb{R}^N$ denotes a function.
- Linear subspace (LS)-ROM: $\boldsymbol{g}(\boldsymbol{y}) = \boldsymbol{\Phi}\boldsymbol{y}$, with $\boldsymbol{\Phi} \in \mathbb{R}^{N\times k}$ orthogonal.
- Galerkin projection – solve the reduced-dimensional ODE for $\boldsymbol{y} \in \mathbb{R}^k$:

$$\boldsymbol{\Phi}^\top \boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{\Phi}\dot{\boldsymbol{y}}(t;\boldsymbol{\mu}) = \boldsymbol{\Phi}^\top \boldsymbol{f}(\boldsymbol{u}_{\text{ref}} + \boldsymbol{\Phi}\boldsymbol{y}(t;\boldsymbol{\mu}), t; \boldsymbol{\mu}).$$

- Other ROM approaches:
  - Least-squares Petrov Galerkin ROM: full residual minimization.
  - Nonlinear manifold (NM)-ROM: $\boldsymbol{g}$ is a decoder neural network.

Proper orthogonal decomposition (POD)

- Snapshot data from direct numerical simulation or measurement

$$\mathbf{X} = \begin{bmatrix} \boldsymbol{u}^1(\boldsymbol{\mu}_{\text{train}}) - \boldsymbol{u}_{\text{ref}} & \cdots & \boldsymbol{u}^M(\boldsymbol{\mu}_{\text{train}}) - \boldsymbol{u}_{\text{ref}} \end{bmatrix} \in \mathbb{R}^{N \times M} \, (M \leq N).$$

- Snapshot singular value decomposition (SVD)

$$\mathbf{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T.$$

- Energy criteria: determine smallest integer $1 \leq k \leq N$ such that

$$\frac{\sum_{i=1}^{k} \sigma_i}{\sum_{i=1}^{M} \sigma_i} \geq \epsilon_\sigma.$$

- Solution basis $\boldsymbol{\Phi} = \boldsymbol{U} \begin{bmatrix} \mathbf{e}_1 & \cdots & \mathbf{e}_k \end{bmatrix} \in \mathbb{R}^{N \times k}$ is orthogonal.

POD modes of NACA0012 laminar airfoil

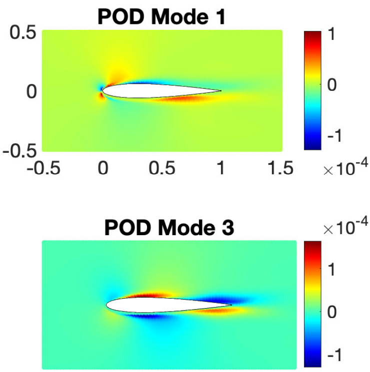


Figure: First four POD modes for the density variable for the laminar airfoil.

Hyper-reduction

- No speed-up due to evaluation of source term $\boldsymbol{f} \in \mathbb{R}^N$.

$$\boldsymbol{\Phi}^\top \boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{\Phi}\dot{\boldsymbol{y}}(t;\boldsymbol{\mu}) = \boldsymbol{\Phi}^\top \boldsymbol{f}(\boldsymbol{u}_{\text{ref}} + \boldsymbol{\Phi}\boldsymbol{y}(t;\boldsymbol{\mu}), t; \boldsymbol{\mu}).$$

- Low-dimensional source representation by $\widehat{\boldsymbol{f}} \in \mathbb{R}^{n_f}$ ($n_f \ll N$):

$$\boldsymbol{f} \approx \boldsymbol{\Phi}_{\boldsymbol{f}}\widehat{\boldsymbol{f}}, \quad \widehat{\boldsymbol{f}} = \underset{\mathbf{a}\in\mathbb{R}^{n_f}}{\operatorname{argmin}} \|\boldsymbol{Z}^\top(\boldsymbol{\Phi}_{\boldsymbol{f}}\mathbf{a} - \boldsymbol{f})\| = (\boldsymbol{Z}^\top\boldsymbol{\Phi}_{\boldsymbol{f}})^\dagger \boldsymbol{Z}^\top \boldsymbol{f},$$

  where $\boldsymbol{Z} = [\boldsymbol{e}_{i_1}, \cdots, \boldsymbol{e}_{i_n}] \in \mathbb{R}^{N\times n}$ ($n_f \leq n \ll N$) is a sampling matrix.
- Achievable speed-up due to evaluation of $\boldsymbol{Z}^\top \boldsymbol{f} \in \mathbb{R}^n$.

$$\boldsymbol{\Phi}^\top \boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{\Phi}\dot{\boldsymbol{y}}(t;\boldsymbol{\mu}) = \boldsymbol{\Phi}^\top \boldsymbol{\Phi}_{\boldsymbol{f}}(\boldsymbol{Z}^\top\boldsymbol{\Phi}_{\boldsymbol{f}})^\dagger \boldsymbol{Z}^\top \boldsymbol{f}(\boldsymbol{u}_{\text{ref}} + \boldsymbol{\Phi}\boldsymbol{y}(t;\boldsymbol{\mu}), t; \boldsymbol{\mu}).$$

- Keep the index set $\mathcal{Z} = \{i_1, \cdots i_n\}$ instead of full matrix $\boldsymbol{Z}$.
- $(\boldsymbol{Z}^\top\boldsymbol{\Phi}_{\boldsymbol{f}})^\dagger \in \mathbb{R}^{n_f\times n}$ is offline precomputed and stored.

Quasi-optimality of sampling matrix

Given $\boldsymbol{\Phi_f} \in \mathbb{R}^{N\times n_f}$ and $\boldsymbol{f} \in \mathbb{R}^N$, the optimal sampling matrix is

$$\boldsymbol{Z}^*(\boldsymbol{f}) = \underset{\boldsymbol{Z}=[\boldsymbol{e}_{i_1},\cdots,\boldsymbol{e}_{i_n}]\in\mathbb{R}^{N\times n}}{\operatorname{argmin}} \|(\mathbf{I} - \boldsymbol{\Phi_f}(\boldsymbol{Z}^\top\boldsymbol{\Phi_f})^\dagger\boldsymbol{Z}^\top)\boldsymbol{f}\|.$$

- The true optimum $\boldsymbol{Z}^*(\boldsymbol{f})$ depends on $\boldsymbol{f}$ and is impractical.
- Quasi-optimality: oblique projection error bound for generic $\boldsymbol{f}$.

Theorem

Let $\boldsymbol{\Phi_f} = \mathbf{QR}$ be the QR factorization of $\boldsymbol{\Phi_f}$.

$$\|(\mathbf{I} - \boldsymbol{\Phi_f}(\boldsymbol{Z}^\top\boldsymbol{\Phi_f})^\dagger\boldsymbol{Z}^\top)\boldsymbol{f}\| \leq \|(\boldsymbol{Z}^\top\mathbf{Q})^\dagger\|\|(\mathbf{I} - \mathbf{Q}\mathbf{Q}^\top)\mathbf{f}\|.$$

Discrete Empirical Interpolation Method (DEIM)

$$\boldsymbol{Z}^*_{\text{DEIM}} = \underset{\boldsymbol{Z}=[\boldsymbol{e}_{i_1},\cdots,\boldsymbol{e}_{i_n}]\in\mathbb{R}^{N\times n}}{\operatorname{argmin}} \|(\boldsymbol{Z}^\top \mathbf{Q})^\dagger\|.$$

Greedy sampling procedure to select the index with largest error.

1. Initialize $\mathcal{Z} = \{i^*\}$ where $i^* = \operatorname{argmax}_i |\mathbf{Q}_{i,1}|$
2. For $j = 1, \cdots, n_f$,
   1. Construct $\mathbf{A} = \mathbf{Q}\left[\mathbf{e}_1, \cdots, \mathbf{e}_j\right]$.
   2. For $k = 1, \cdots, K_j$,
      1. Construct $\boldsymbol{Z} = [\boldsymbol{e}_i]_{i\in\mathcal{Z}}$.
      2. Compute $\widetilde{\mathbf{q}} = \mathbf{A}(\boldsymbol{Z}^\top\mathbf{A})^\dagger\boldsymbol{Z}^\top\mathbf{Q}\mathbf{e}_j$.
      3. Find $i^* = \operatorname{argmax}_{i\notin\mathcal{Z}} |\mathbf{Q}_{i,j} - \widetilde{\mathbf{q}}_i|$.
      4. Enrich $\mathcal{Z} \leftarrow \mathcal{Z} \cup \{i^*\}$.
3. Set $n = |\mathcal{Z}|$ and output $\mathcal{Z}$.

$K_1 = 0$ and $K_j = 1$ for $j > 1 \implies$ original DEIM with $n = n_f$.

$K_1 > 0$ or $K_j > 1$ for $j > 1 \implies$ oversampling DEIM with $n > n_f$.

Another measure for quasi-optimality

Theorem

Let $\mathbf{\Phi_f} = \mathbf{QR}$ *be the QR factorization of* $\mathbf{\Phi_f}$.

$$\|(\mathbf{I} - \mathbf{\Phi_f}(\boldsymbol{Z}^\top \mathbf{\Phi_f})^\dagger \boldsymbol{Z}^\top)\boldsymbol{f}\|^2 = \|(\mathbf{I} - \mathbf{Q}\mathbf{Q}^\top)\mathbf{f}\|^2 + \|\epsilon(\boldsymbol{f}, \boldsymbol{Z})\|^2,$$

where $\epsilon(\boldsymbol{f}, \boldsymbol{Z}) = ((\boldsymbol{Z}^\top \mathbf{Q})^\top (\boldsymbol{Z}^\top \mathbf{Q}))^{-1} (\boldsymbol{Z}^\top \mathbf{Q})^\top \boldsymbol{Z}^\top (\mathbf{I} - \mathbf{Q}\mathbf{Q}^\top)\mathbf{f}$.

- Maximize the column orthogonality of $\boldsymbol{Z}^\top \mathbf{Q}$ to make residual small.
- Maximize the determinant of $(\boldsymbol{Z}^\top \mathbf{Q})^\top \boldsymbol{Z}^\top \mathbf{Q}$ for non-singularity.
- Define the measure $\mathcal{S} : \mathbb{R}^{m \times p} \to [0, 1]$ by:

$$\mathcal{S}(\mathbf{A}) = \left(\frac{\sqrt{\det \mathbf{A}^\top \mathbf{A}}}{\prod_{k=1}^{p} \|\mathbf{A}\mathbf{e}_k\|} \right)^{\frac{1}{p}} \quad \text{for all } \mathbf{A} \in \mathbb{R}^{m \times p}.$$

Another measure for quasi-optimality

Theorem

Let $\mathbf{A} \in \mathbb{R}^{m \times p}$ *with* $m < p$. *Then* $\mathcal{S}(\mathbf{A}) = 0$.

Theorem

Let $\mathbf{A} \in \mathbb{R}^{m \times m}$ *be full-rank,* $\mathbf{r}, \mathbf{c} \in \mathbb{R}^m$*, and* $\gamma \in \mathbb{R}$*. Define* $\widetilde{\mathbf{A}} = \begin{bmatrix} \mathbf{A} & \mathbf{c} \\ \mathbf{r}^\top & \gamma \end{bmatrix} \in \mathbb{R}^{(m+1)\times(m+1)}$*. Then*

$$(\mathcal{S}(\widetilde{\mathbf{A}}))^{2(m+1)} = (\det(\mathbf{A}^\top \mathbf{A})) \frac{1 + \mathbf{r}^\top \mathbf{b}}{\prod_{k=1}^{m}(\|\mathbf{A}\mathbf{e}_k\|^2 + r_k^2)} \frac{\mathbf{c}^\top \mathbf{c} + \gamma^2 - \alpha}{\mathbf{c}^\top \mathbf{c} + \gamma^2},$$

$$\mathbf{b} = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{r}, \quad \mathbf{g} = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{c},$$

$$\alpha = (\mathbf{c}^\top \mathbf{A} + \gamma \mathbf{r}^\top)(I - (1 + \mathbf{r}^\top \mathbf{b})^{-1} \mathbf{b}\mathbf{r}^\top)(\mathbf{g} + \gamma \mathbf{b}).$$

Another measure for quasi-optimality

Theorem

Let $\mathbf{A} \in \mathbb{R}^{m \times p}$ *with* $m \geq p$*. Then* $\mathcal{S}(\mathbf{A}) = 1 \iff \mathbf{A}^\top \mathbf{A} = \mathbf{I}$.

Theorem

Let $\mathbf{A} \in \mathbb{R}^{m \times p}$ *with* $m \geq p$ *be full-rank and* $\mathbf{r} \in \mathbb{R}^p$*. Define* $\widetilde{\mathbf{A}} = \begin{bmatrix} \mathbf{A} \\ \mathbf{r}^\top \end{bmatrix} \in \mathbb{R}^{(m+1) \times p}$*. Then*

$$(\mathcal{S}(\widetilde{\mathbf{A}}))^{2p} = (\det(\mathbf{A}^\top \mathbf{A})) \frac{1 + \mathbf{r}^\top (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{r}}{\prod_{k=1}^{p} (\|\mathbf{A}\mathbf{e}_k\|^2 + r_k^2)}.$$

S-OPT sampling algorithm

$$\boldsymbol{Z}^*_{\text{S-OPT}} = \underset{\boldsymbol{Z}=[\boldsymbol{e}_{i_1},\cdots,\boldsymbol{e}_{i_n}]\in\mathbb{R}^{N\times n}}{\text{argmax}} \mathcal{S}(\boldsymbol{Z}^\top \mathbf{Q}).$$

Greedy sampling procedure to select the index with largest measure $\mathcal{S}$.

1. Initialize $\mathcal{Z} = \{i^*\}$ where $i^* = \text{argmax}_i |\mathbf{Q}_{i,1}|$
2. For $j = 1, \cdots, n_f - 1$,
   1. Construct $\boldsymbol{Z} = [\boldsymbol{e}_i]_{i\in\mathcal{Z}}$, $\mathbf{A} = \boldsymbol{Z}^\top\mathbf{Q}\left[\mathbf{e}_1, \cdots, \mathbf{e}_j\right]$, $\mathbf{c} = \boldsymbol{Z}^\top\mathbf{Q}\mathbf{e}_{j+1}$, and $\mathbf{g} = (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{A}^\top\mathbf{c}$.
   2. Find $i^* = \underset{i\notin\mathcal{Z}}{\text{argmax}} \dfrac{1 + \mathbf{r}^\top\mathbf{b}}{\prod_{k=1}^{j}(\|\mathbf{A}\mathbf{e}_k\|^2 + r_k^2)} \dfrac{\mathbf{c}^\top\mathbf{c} + \gamma^2 - \alpha}{\mathbf{c}^\top\mathbf{c} + \gamma^2}$,
   $$\mathbf{r}^\top = \mathbf{e}_i^\top\mathbf{Q}\left[\mathbf{e}_1, \cdots, \mathbf{e}_j\right], \quad \mathbf{b} = (\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{r}, \quad \gamma = \mathbf{Q}_{i,j+1},$$
   3. Enrich $\mathcal{Z} \leftarrow \mathcal{Z} \cup \{i^*\}$.

S-OPT sampling algorithm

$$\boldsymbol{Z}^*_{\text{S-OPT}} = \underset{\boldsymbol{Z}=[\boldsymbol{e}_{i_1},\cdots,\boldsymbol{e}_{i_n}]\in\mathbb{R}^{N\times n}}{\operatorname{argmax}} \mathcal{S}(\boldsymbol{Z}^\top \mathbf{Q}).$$

Greedy sampling procedure to select the index with largest measure $\mathcal{S}$.

3 For $j = 1, \cdots, n - n_f$,
  1 Construct $\boldsymbol{Z} = [\boldsymbol{e}_i]_{i\in\mathcal{Z}}$ and $\mathbf{A} = \boldsymbol{Z}^\top\mathbf{Q}$.
  2 Find $i^* = \underset{i\notin\mathcal{Z}}{\operatorname{argmax}} \dfrac{1 + \mathbf{r}^\top(\mathbf{A}^\top\mathbf{A})^{-1}\mathbf{r}}{\prod_{k=1}^{n_f}(\|\mathbf{A}\mathbf{e}_k\|^2 + r_k^2)}$, with $\mathbf{r}^\top = \mathbf{e}_i^\top\mathbf{Q}$.
  3 Enrich $\mathcal{Z} \leftarrow \mathcal{Z} \cup \{i^*\}$.

4 Output $\mathcal{Z}$.

Perspective of optimal design

- Ordinary least squares with design matrix $\mathbf{X} = \boldsymbol{Z}^\top \mathbf{Q}$.
- Mean-unbiased estimator $\beta = \mathbf{R}\widehat{\boldsymbol{f}}$.
- Minimizing the variance $\iff$ Maximizing the Fisher information.
- Information matrix $(\boldsymbol{Z}^\top \mathbf{Q})^\top (\boldsymbol{Z}^\top \mathbf{Q})$.
- Optimal design $\iff$ optimization of certain statistical criteria.
- E-optimality: maximizing smallest eigenvalue of information matrix.

$$\boldsymbol{Z}^*_{\text{DEIM}} = \underset{\boldsymbol{Z}=[\boldsymbol{e}_{i_1},\cdots,\boldsymbol{e}_{i_n}]\in\mathbb{R}^{N\times n}}{\text{argmin}} \|(\boldsymbol{Z}^\top \mathbf{Q})^\dagger\|.$$

- S-optimality: maximizing column orthogonality of design matrix and determinant of information matrix.

$$\boldsymbol{Z}^*_{\text{S-OPT}} = \underset{\boldsymbol{Z}=[\boldsymbol{e}_{i_1},\cdots,\boldsymbol{e}_{i_n}]\in\mathbb{R}^{N\times n}}{\text{argmax}} \mathcal{S}(\boldsymbol{Z}^\top \mathbf{Q}).$$

NACA0012 airfoil in compressible Navier-Stokes flow

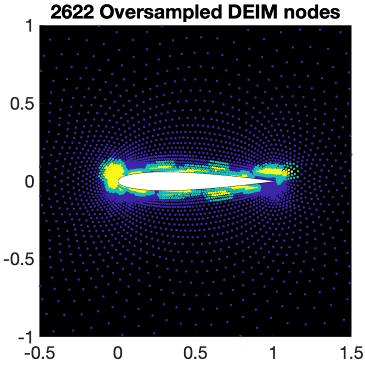


Figure: Partial domain near the airfoil. Selected nodes are in yellow. Neighboring nodes required for nonlinear term calculation are in cyan.

NACA0012 airfoil in compressible Navier-Stokes flow

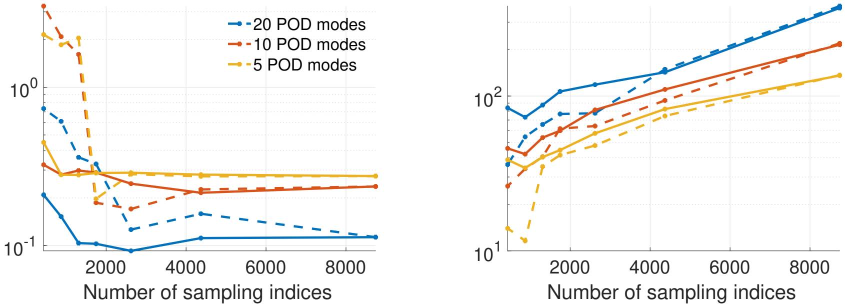


Figure: Comparison of oversampled DEIM (dashed) versus S-OPT (solid line) algorithms in maximum error (left) and simulation wall clock in seconds (right).

Gresho vortex in compressible Euler equations

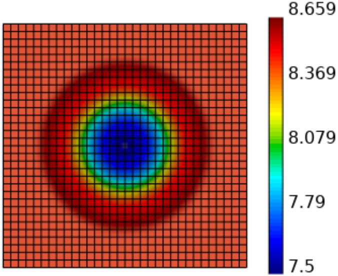


Figure: Initial condition (left) and final-time solution (right).

Gresho vortex in compressible Euler equations

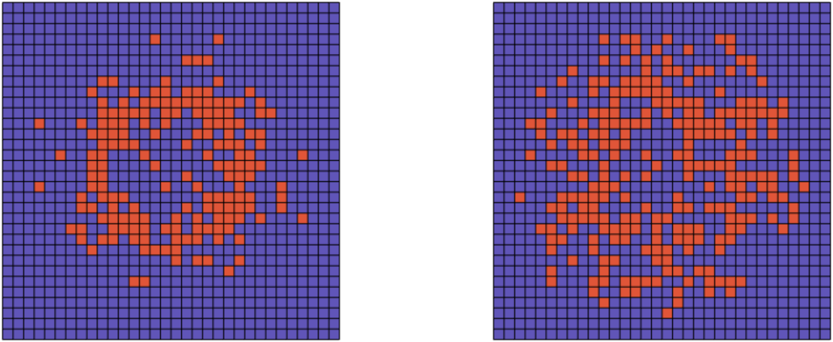
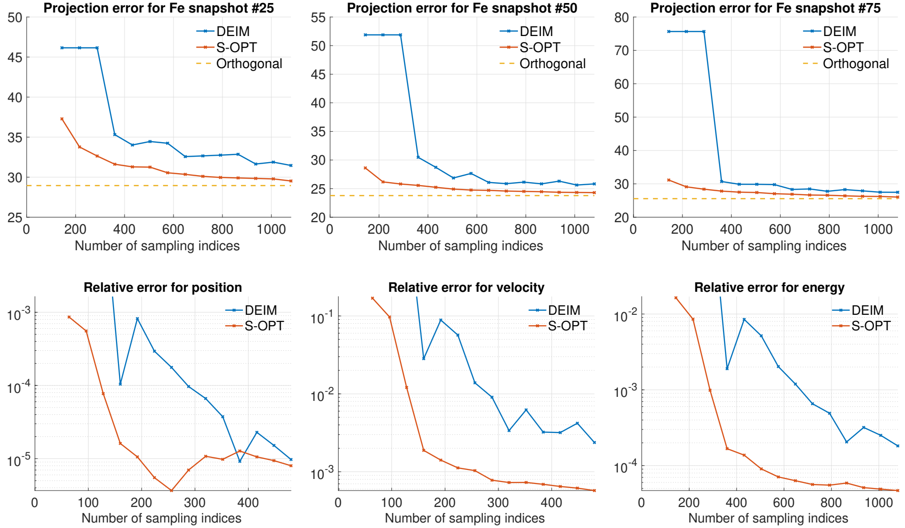


Figure: Nodes selected by DEIM (left) and S-OPT (right).

Gresho vortex in compressible Euler equations



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S-OPT: A Points Selection Algorithm for Hyper-Reduction in Reduced Order Models.
arXiv preprint arXiv:2203.16494.

libROM

GitHub repo: `https://github.com/LLNL/libROM`
Website: `https://www.librom.net`

Thank you for your attention. Any questions?

Siu Wun Cheung (cheung26@llnl.gov)

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