A Local POD-HROM framework for fast and accurate numerical simulations

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Presenting ourselves

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Kratos github site
Objetives of the talk

- Presenting a Local POD framework implemented on a powerful open source FEM software.

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- POD
  \[ u \approx \Phi \, q \]

- Local POD
  \[ u_{\text{new}} \approx u_{\text{old}} + \Phi^i \, q \]
Proper Orthogonal Decomposition

Full Order Model (FOM)

Solution manifold: \( M = \{ u(t; \mu) \mid t \in (0, T), \mu \in \mathcal{P} \} \subset \mathbb{R}^n \)

Reduced Order Model (ROM)

A MUCH SMALLER SYSTEM! \( A^* q = b^* \)
Proper Orthogonal Decomposition

Solve the FOM using Finite Elements

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\[ \mu = (T_D, q_1, q_2, q_{SB}) \in \mathcal{P} \]
Proper Orthogonal Decomposition

Store the nodal solution $u$ the Snapshots matrix $S = [ u_1 \ u_2 \ \ldots \ u_p ]$

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Each column collects the temperature on all the nodes in the mesh, for a given choice of the fluxes $q_1 \ q_2 \ q_{sb}$
Proper Orthogonal Decomposition

Take the SVD of $S = UΣV^T \approx U_k Σ_k V_k^T$
Proper Orthogonal Decomposition

Take the SVD of $S = U \Sigma V^T \approx U_k \Sigma_k V_k^T$.

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Proper Orthogonal Decomposition

\[ S = U\Sigma V^T \approx U_k \Sigma_k V_k^T \]

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Example in CFD

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Proper Orthogonal Decomposition

Full Order Model (FOM)

\[ \begin{align*}
A & \quad u \\
\hline
\end{align*} \quad = \quad \begin{align*}
b \\
\end{align*} \]

Solution manifold: \( \mathcal{M} = \{ u(t; \mu) | t \in (0, T], \mu \in \mathcal{P} \} \subset \mathbb{R}^n \)

Let \( u \approx \Phi q \)

Reduced Order Model (ROM)

\[ \begin{align*}
\Phi^T & \quad A \\
\hline
\Phi & \quad q \\
\hline
\end{align*} \quad = \quad \begin{align*}
\Phi^T & \quad b \\
\hline
\end{align*} \]

A MUCH SMALLER SYSTEM!

\[ \begin{align*}
A^* & \quad q \\
\hline
\end{align*} \quad = \quad \begin{align*}
b^* \\
\end{align*} \]

PROBLEM: STILL EXPENSIVE TO MOUNT THE SYSTEM
Hyper-reduction

The goal is to find a **subset of elements and corresponding weights** by solving an optimization problem

\[
(E, W) = \arg \min \| \zeta \|_0 \quad \text{s.t.} \quad \| G_1 - G \zeta \|_2 \leq \epsilon \| G_1 \|_2 \\
\zeta_i \geq 0
\]

Where \( G = G(\Phi, R) \)

NP-HARD. Solving via greedy procedure

\[
(E, W) = \arg \min \left\| \sum_{i=1}^{n} g_i - \sum_{i \in E} g_i \omega_i \right\|_2^2 \\
\text{s.t.} \quad \omega_i > 0
\]

Hyper-reduction

Assembly comparison FOM vs HROM:

\[
\left( \prod_{e=1}^{n\ elem} A_e \right) \mathbf{u} = \prod_{e=1}^{n\ elem} b_e \\
\xrightarrow{\text{HROM}} \left( \sum_{e \in E} \Phi_e^T A_e \Phi_e \omega_e \right) q = \sum_{e \in E} \Phi_e^T b_e \omega_e
\]
Link to the external world

Kratos provides an interface to retrieve data from sensors placed in situ.
Kratos ROM on a Raspberry Pi
POD weaknesses and strengths

- Straightforward procedure for training and inference

- Not ideal for certain problems (convection dominated, highly nonlinear)
Local POD

Full Order Model (FOM)

\[ A \begin{bmatrix} u \\ \end{bmatrix} = b \]

Solution manifold: \( \mathcal{M} = \{ \mathbf{u}(t; \mu) \mid t \in (0, T], \mu \in \mathcal{P} \} \subset \mathbb{R}^n \)

Let \( u_{new} \approx u_{old} + \Phi^i q \)
Local POD

Full Order Model (FOM)

\[
A \vec{u} = \vec{b}
\]

Reduced Order Model (ROM)

\[
\Phi^2 \Phi^T \vec{q} = \Phi^2 \Phi^T \vec{b}
\]

Let \( \vec{u}_{new} \approx \vec{u}_{old} + \Phi^i \vec{q} \)

Solution manifold: \( \mathcal{M} = \{ \vec{u}(t; \mu) | t \in (0,T], \mu \in \mathcal{P} \} \subset \mathbb{R}^n \)
Local POD. K-means

Given: \( \{x_j\}_{j=1}^N \)

Find centroids: \( \{c_i\}_{i=1}^n \) and assignments: \( s_{ij} \)

\[
\min \sum_{j=1}^n \sum_{i=1}^N s_{ij} \| x_j - c_i \|_2^2
\]

s.t. \( \sum_{i} s_{ij} = 1, \quad s_{ij} \in \{0,1\} \)

Solve via alternating minimization:

\[
s_{ij} = \begin{cases} 
1 & \text{nearest centroid} \\
0 & \text{otherwise}
\end{cases}
\]

\[
c_i = \frac{\sum_{j=1}^N s_{ij} x_j}{\sum_{j=1}^N s_{ij}}
\]
Local POD. Building multiple bases

Use an unsupervised learning method to build clusters

1. Get Non-overlapping clusters \( S_i = \text{kmeans}(S) \)
Local POD. Building multiple bases

Use an unsupervised learning method to build clusters

1. Get Non-overlapping clusters \( S_i = \text{kmeans}(S) \)
2. Add fixed overlapping \( S_i^+ = \text{overlap}(S_i) \)  (Farhat, 2012): doi.org/10.2514/6.2012-2686
Local POD. Overlapping proposal

**Locally Linear Embedding (LLE):**

\[
\min_c \sum_{j=1}^{N} \| x_j - \sum c_{ij} x_i \|^2_2 \\
\text{s.t.} \quad c_{ij} = 0 \quad \text{if } x_i \text{ not } k-\text{NN to } x_j \\
\sum_{i=1}^{N} c_{ij} = 1
\]

(Roweis, 2000): doi.org/10.1126/science.290.5500.2323

1. Get Non-overlapping clusters \( S_i = \text{kmeans}(S) \)
2. Add necessary overlapping \( S_i^+ = \text{overlap}(S_i) \)

Each cluster \( S_i^+ \) should consist of its snapshots, and the neighbours of its snapshots
Local POD. Overlapping comparison

\[ \mathcal{M} \subset \mathbb{R}^3, \quad \dim(\mathcal{M}) = 2 \]
Local POD. Overlapping comparison

Synthetic 2-Manifold
Local POD. Overlapping comparison

Synthetic 2-Manifold
Local POD. Overlapping comparison
Local POD. Overlapping comparison

Synthetic 2-Manifold
Local POD. Overlapping comparison

Synthetic 2-Manifold
Local POD. Overlapping comparison

Synthetic 2-Manifold
Local POD. Overlapping comparison
Local POD. Example 1
Local POD. Hyper-reduction

Reduced Order Model (ROM)

\[ \Phi^2 \begin{bmatrix} A \\ \Phi^2 \end{bmatrix} q = \Phi^2 b \]

\[ G = G(\Phi, R) \]

\[(E, W) = \arg \min \left\| \sum_{i=1}^{n} g_i - \sum_{i \in E}^{n} g_i \omega_i \right\|_2^2 \]

s.t. \( \omega_i > 0 \)

(Grinberg, 2020): doi.org/10.1002/nme.6603
Local POD. Improved hyper-reduction

Reduced Order Model (ROM)

\[ \Phi^T A \Phi = \Phi^T b \]

\[ G = G(\Phi, R) \]

\[ (E, \tilde{W}) = \arg \min \left\| \sum_{i=1}^{n} g_i^k - \sum_{i \in E} g_i^k \tilde{\omega}_i \right\|_2^2 \]

subject to \[ \tilde{\omega}_i \geq 0 \]

*Find a single set of elements and as many sets of weights as bases.*
Local POD. Example 2
Local POD. Example 2
Local POD. Example 2

32 trajectories
50 snapshots per trajectory
1600 snapshots
Local POD. Example 2

32 trajectories
50 snapshots per cluster
1600 snapshots
Local POD. Example 2

- 32 trajectories
- 50 snapshots per cluster
- **1600 snapshots**
Local POD. Example 2

32 trajectories
50 snapshots per cluster
1600 snapshots
Local POD. Example 2

32 trajectories
50 snapshots per cluster
1600 snapshots
Local POD. Example 2

- 32 trajectories
- 50 snapshots per cluster
- 1600 snapshots
Local POD. Example 2

FOM

HROM
Local POD. Example 2

10X less elements required compared with a single basis

5X less modes required compared with a single basis
Local POD. Strengths and weaknesses

• Reasonable overhead in training and negligible in inference
• Smaller bases and elements sets, therefore faster ROMs

• Easy to overfit to training trajectories
General conclusions

• The capabilities of the Local POD - HROM framework
• Promising results and exciting challenges
THANK YOU

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[EdgeTwins logo]

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[QR code link to Kratos github site]
References:


