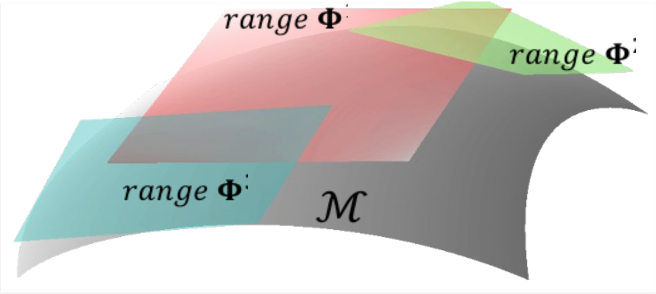
fast and accurate numerical simulations



Mr. Raul Bravo

Prof. Riccardo Rossi

Prof. Joaquin Hernandez

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

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.

FOM: $\boldsymbol{u} \in \mathbb{R}^n$ **ROM**: $\boldsymbol{q} \in \mathbb{R}^k$

- POD $\boxed{\boldsymbol{u} \approx \boldsymbol{\Phi}\,\mathbf{q}}$

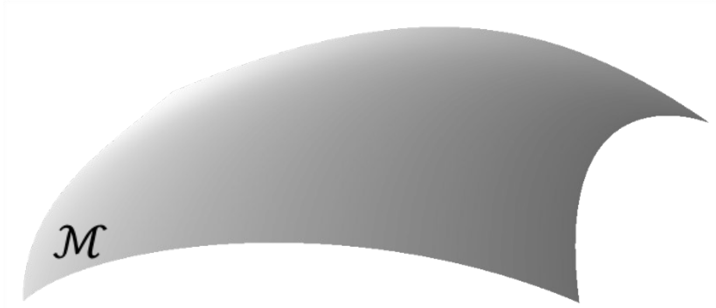
- Local POD $\boxed{\boldsymbol{u}_{new} \approx \boldsymbol{u}_{old} + \boldsymbol{\Phi}^{\mathbf{i}}\,\mathbf{q}}$

Proper Orthogonal Decomposition

Full Order Model (FOM)

$$A \; u = b$$

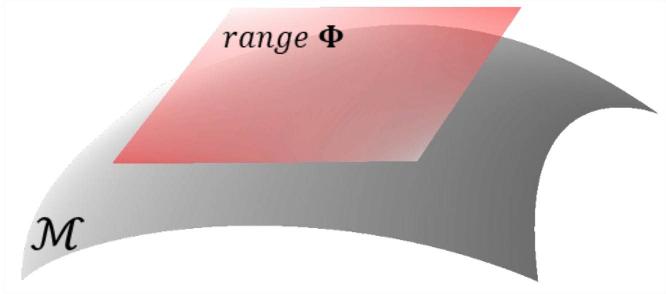
Solution manifold: $\mathcal{M} = \{\, \boldsymbol{u}(t;\boldsymbol{\mu}) \mid t \in (0,T], \boldsymbol{\mu} \in \mathcal{P} \,\} \subset \mathbb{R}^n$



$\boxed{\text{Let } \boldsymbol{u} \approx \boldsymbol{\Phi}\, \mathbf{q}}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^T \; A \; \boldsymbol{\Phi} \; q = \boldsymbol{\Phi}^T \; b$$



A MUCH SMALLER SYSTEM! $A^* \; q = b^*$

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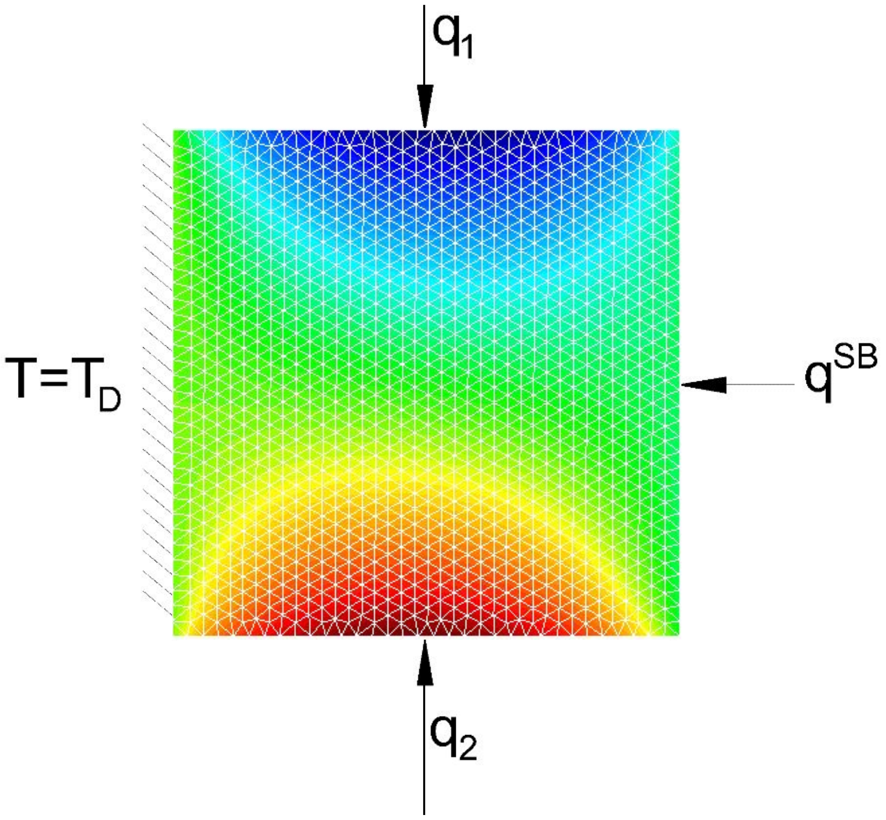
Proper Orthogonal Decomposition

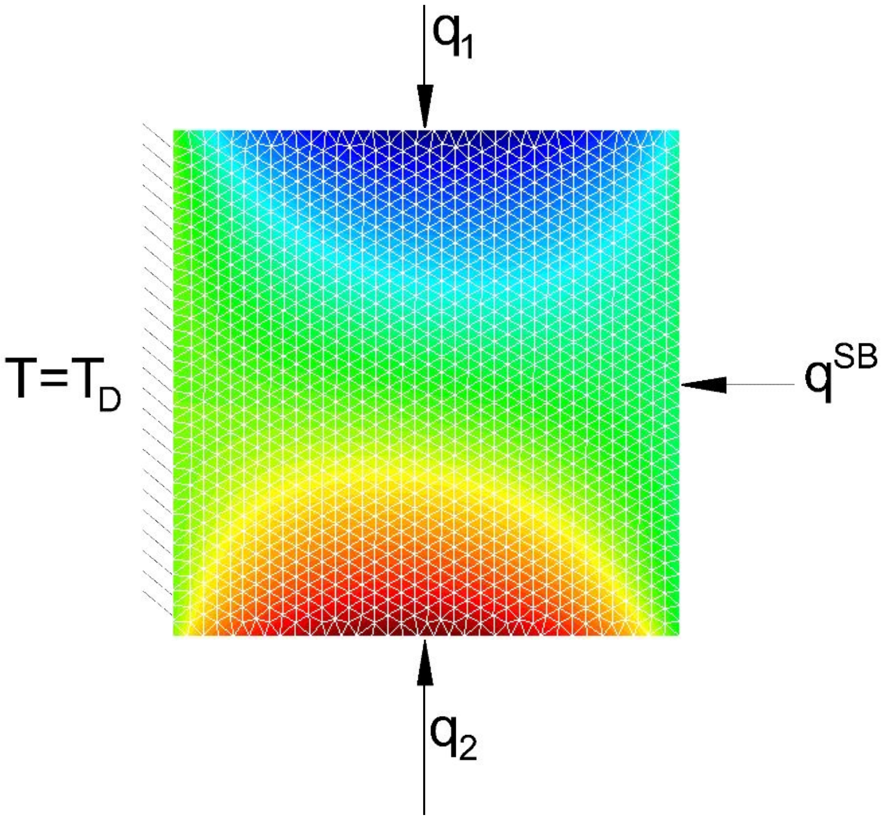
Solve the FOM using Finite Elements

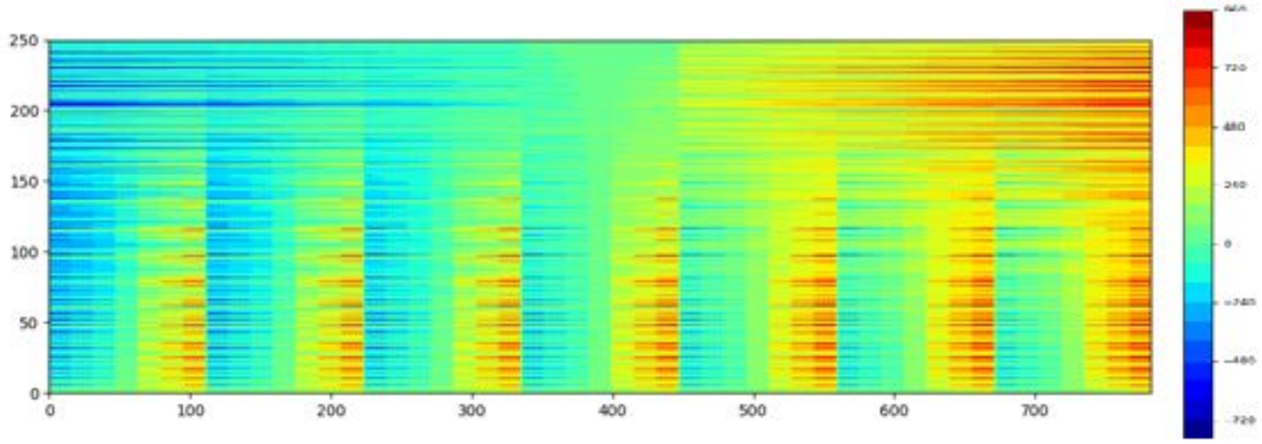


$$\boldsymbol{\mu} = (T_D, q_1, q_2, q_{SB}) \in \mathcal{P}$$

Proper Orthogonal Decomposition

- Store the nodal solution $\boldsymbol{u}$ the Snapshots matrix $\boldsymbol{S} = [\, \boldsymbol{u}_1 \boldsymbol{u}_2 \ldots \, \boldsymbol{u}_p \,]$

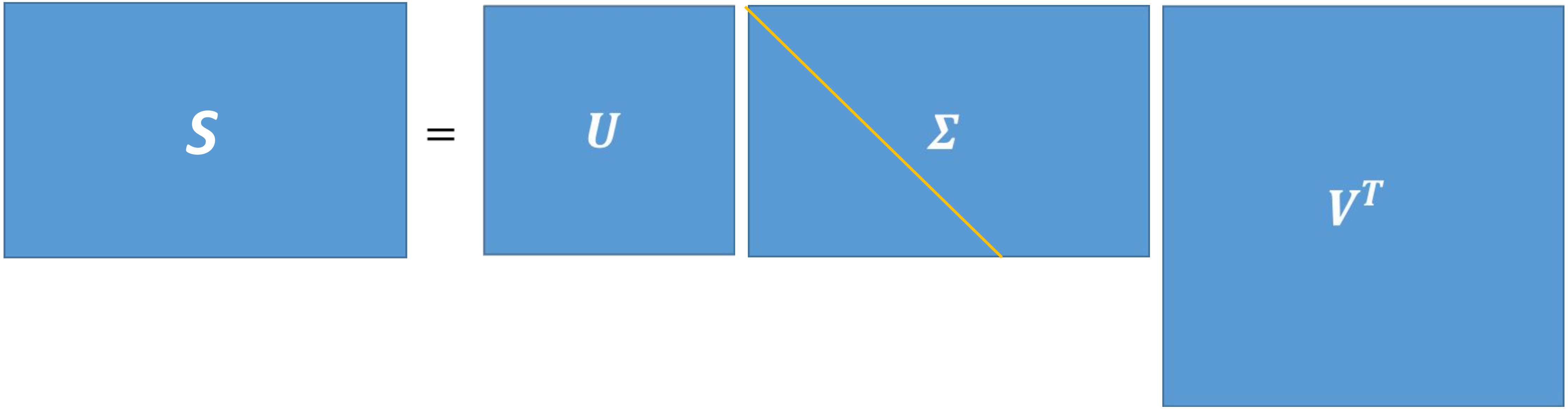




Each column collects the temperature on all the nodes in the mesh, for a given choice of the fluxes $q_1 \; q_2 \; q_{sb}$

Proper Orthogonal Decomposition

- Take the SVD of $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathrm{T}} \approx \boldsymbol{U}_k\boldsymbol{\Sigma}_{\mathbf{k}}\mathbf{V}_{\mathbf{k}}^{\mathrm{T}}$



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Proper Orthogonal Decomposition

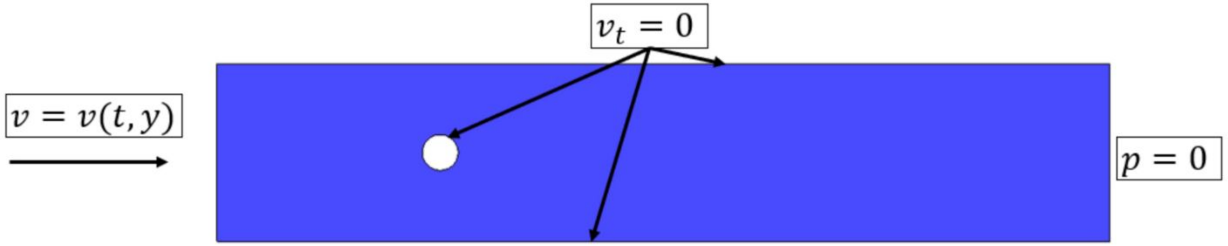
- Take the SVD of $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathrm{T}} \approx \boldsymbol{U}_k\boldsymbol{\Sigma}_{\mathbf{k}}\mathbf{V}_{\mathbf{k}}^{\mathrm{T}}$

Proper Orthogonal Decomposition

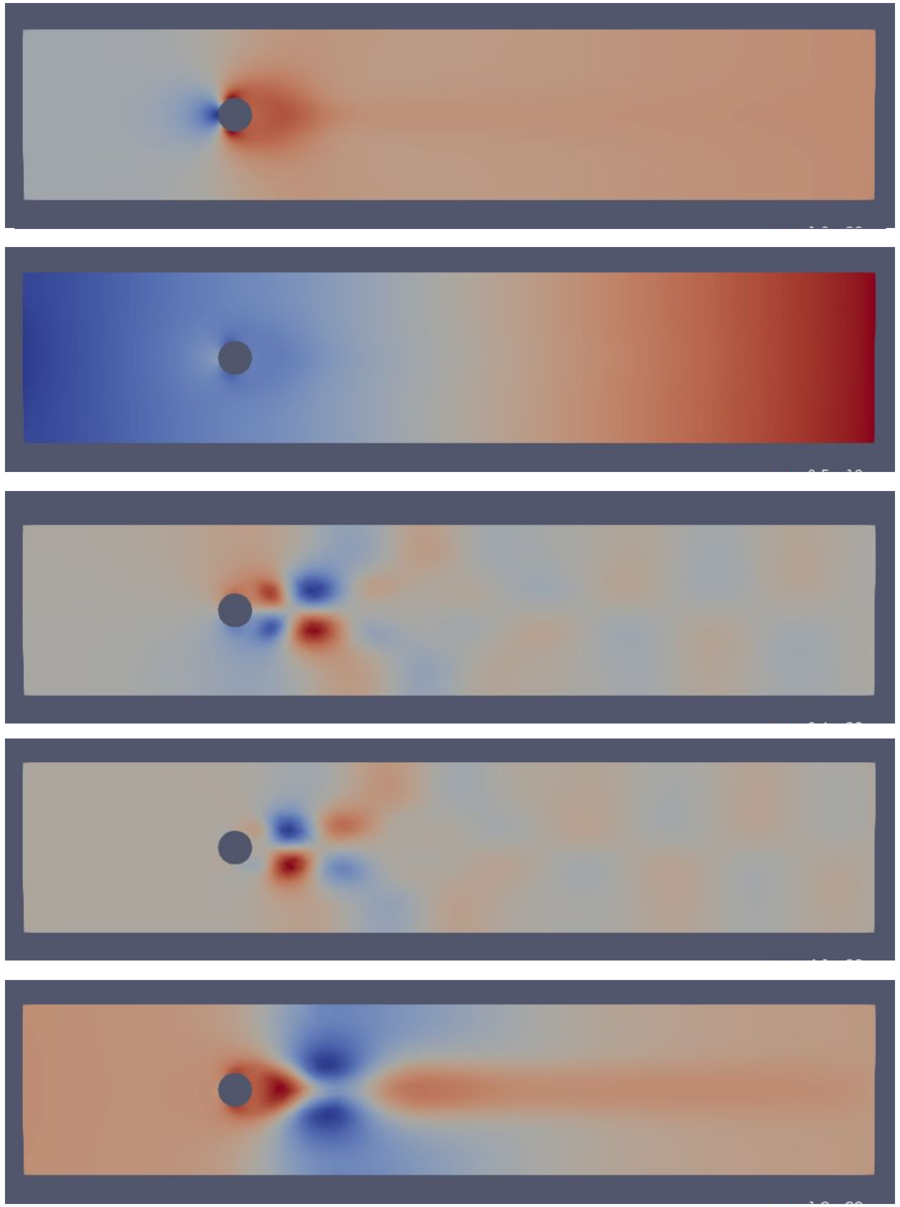
- Take the SVD of $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathrm{T}} \approx \boldsymbol{U}_k\boldsymbol{\Sigma}_{\mathbf{k}}\mathbf{V}_{\mathbf{k}}^{\mathrm{T}}$

$$\boldsymbol{\Phi} := \boldsymbol{U}_k$$

Example in CFD



$\Phi =$

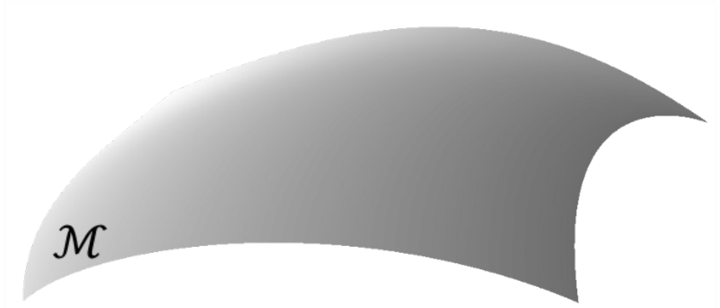


Proper Orthogonal Decomposition

Full Order Model (FOM)

$$A \quad u \quad = \quad b$$

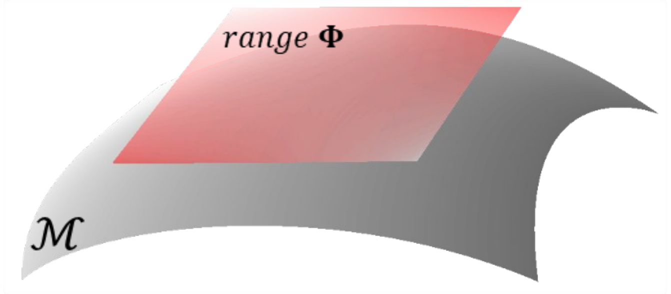
Solution manifold: $\mathcal{M} = \{\, \boldsymbol{u}(t;\boldsymbol{\mu}) \mid t \in (0,T], \boldsymbol{\mu} \in \mathcal{P} \,\} \subset \mathbb{R}^n$



$\boxed{\text{Let } \boldsymbol{u} \approx \boldsymbol{\Phi}\,\mathbf{q}}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^T \quad A \quad \boldsymbol{\Phi} \quad q \quad = \quad \boldsymbol{\Phi}^T \quad b$$



A MUCH SMALLER SYSTEM! $A^* \quad q \quad = \quad b^*$

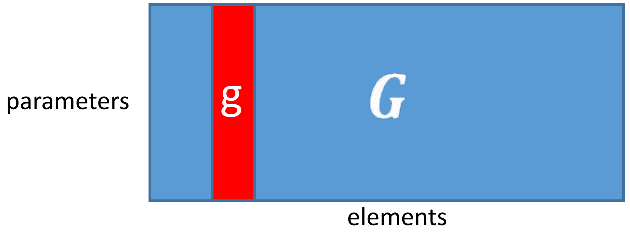
PROBLEM: **STILL EXPENSIVE TO MOUNT THE SYSTEM**

Hyper-reduction

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

$$\begin{aligned}(\boldsymbol{E},\boldsymbol{W}) &= \arg\min \|\boldsymbol{\zeta}\|_0 \\ s.t. \quad & \left\|\boldsymbol{G}\mathbf{1} - \boldsymbol{G}\boldsymbol{\zeta}\right\|_2^2 \leq \epsilon \left\|\boldsymbol{G}\mathbf{1}\right\|_2^2 \\ & \zeta_i \geq 0\end{aligned}$$

Where $\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi},\boldsymbol{R})$



NP-HARD. Solving via greedy procedure

$$(\boldsymbol{E},\boldsymbol{W}) = \arg\min \left\| \sum_{i=1}^{n} \boldsymbol{g}_i - \sum_{i\in E} \boldsymbol{g}_i \boldsymbol{\omega}_i \right\|_2^2$$

$$s.t. \quad \omega_i > 0$$

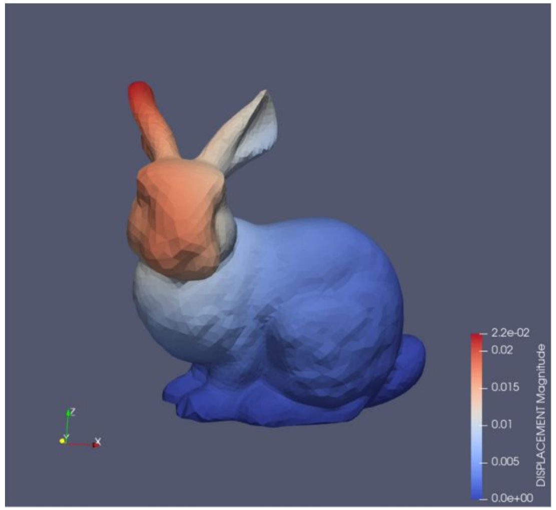
(Hernández, 2020): doi.org/10.1016/j.cma.2020.113192

Hyper-reduction

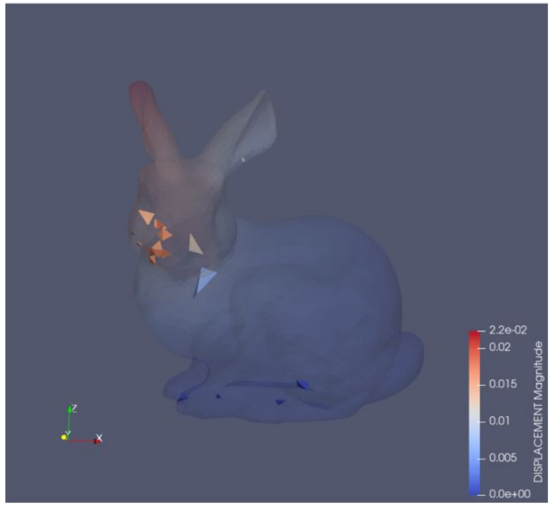
Assembly comparison FOM vs HROM:

$$\left(\prod_{e=1}^{n\,elem} A_e\right)\boldsymbol{u} = \prod_{e=1}^{n\,elem} b_e \quad\longrightarrow\quad \left(\sum_{e\in E} \boldsymbol{\Phi}_e^T \boldsymbol{A}_e \boldsymbol{\Phi}_\mathbf{e}\, \omega_e\right)\boldsymbol{q} = \sum_{e\in E} \boldsymbol{\Phi}_\mathbf{e}^T \boldsymbol{b}_e \omega_e$$

FOM Simulation



HROM Simulation



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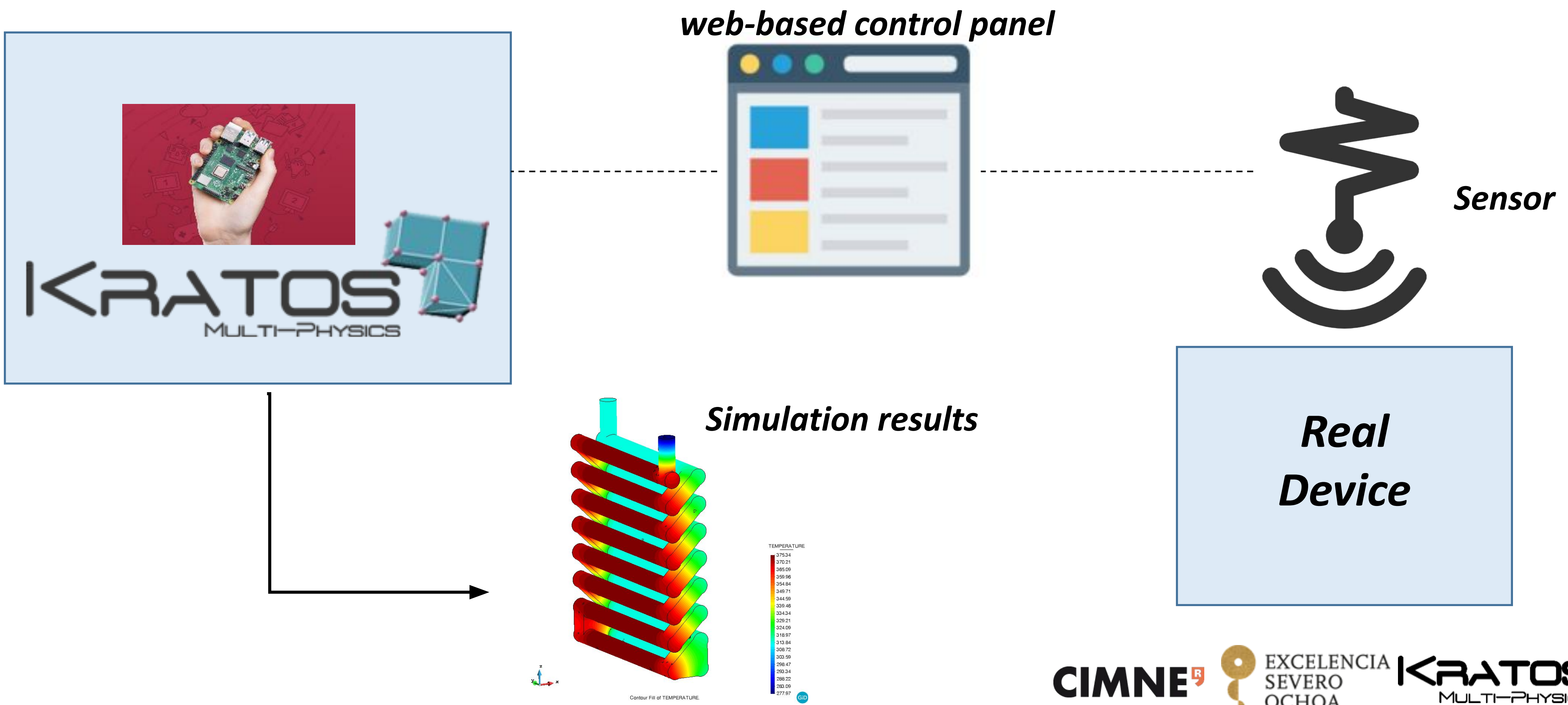
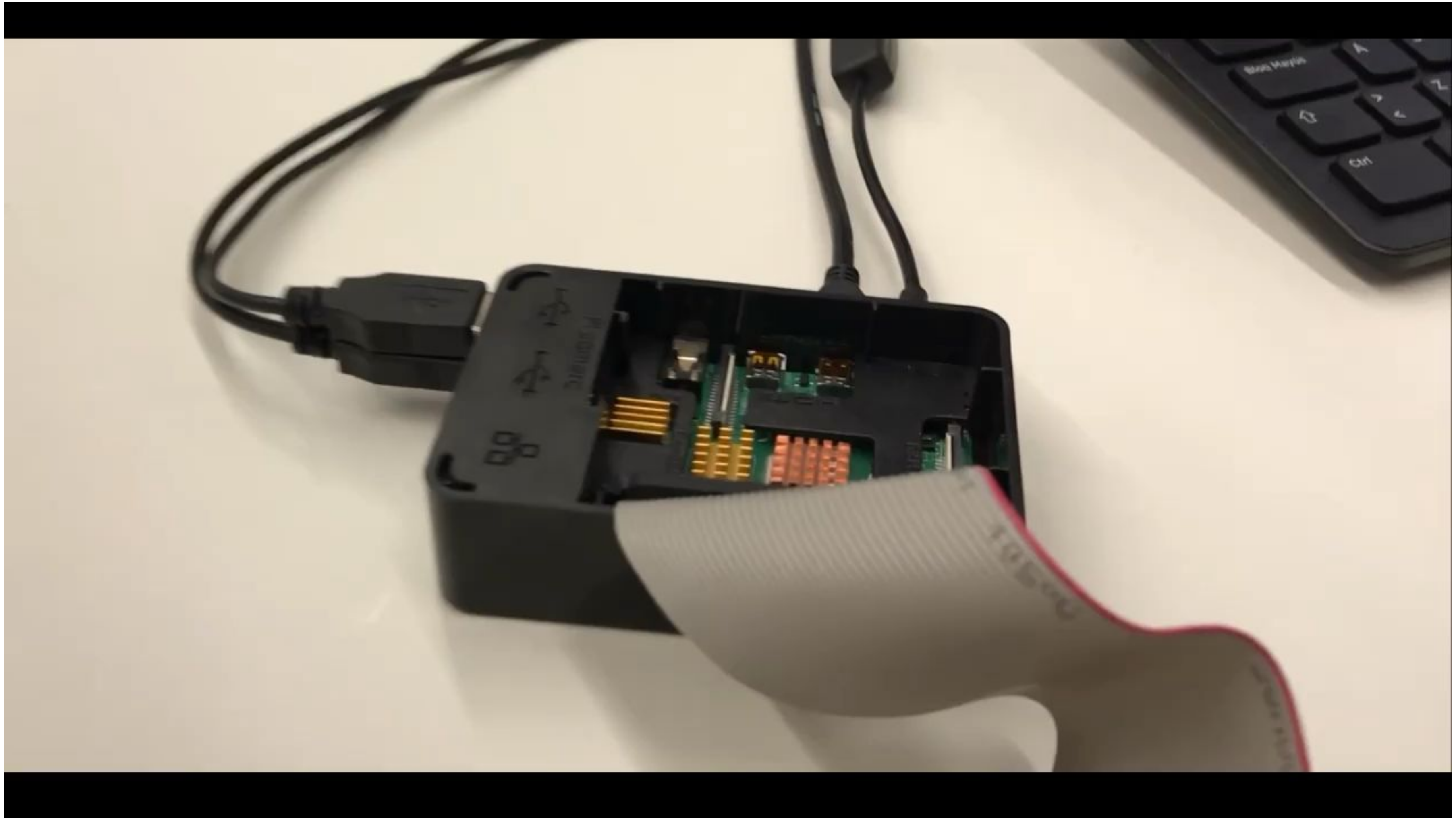
Link to the external world

Kratos provides an interface to retrieve data from sensors placed in situ.



Kratos ROM on a Raspberry Pi



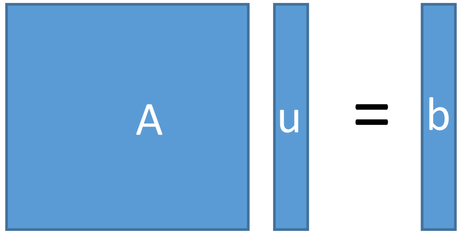
POD weaknesses and strengths

- Straightforward procedure for training and inference

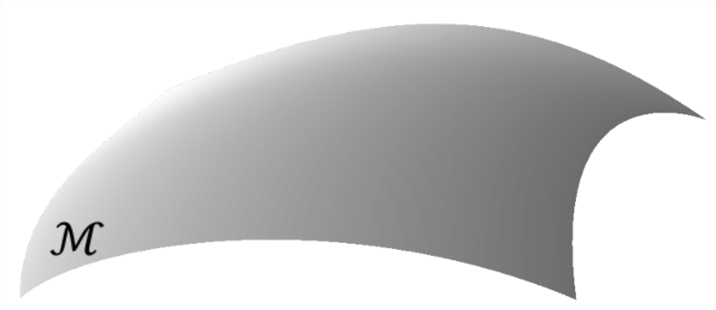
- Not ideal for certain problems(convection dominated, highly nonlinear)

Local POD

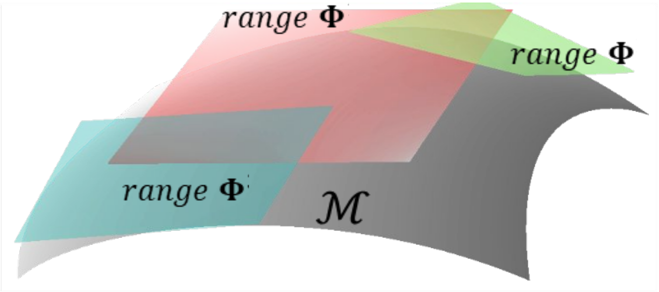
Full Order Model (FOM)



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



$\boxed{\text{Let } \boldsymbol{u}_{new} \approx \boldsymbol{u}_{old} + \boldsymbol{\Phi}^{\mathbf{i}}\,\mathbf{q}}$



Local POD

Full Order Model (FOM)

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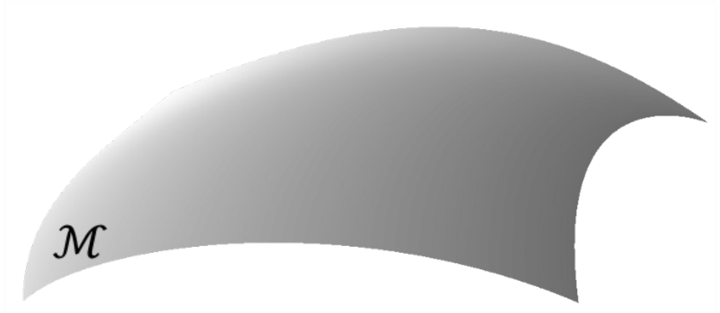
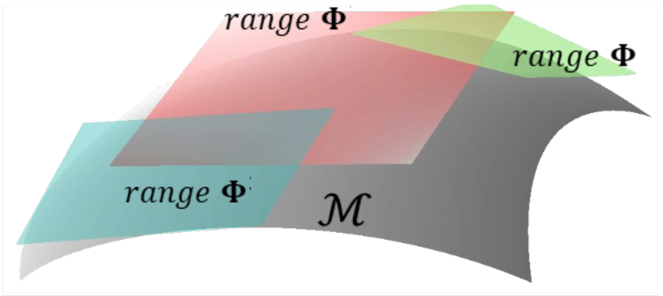


Let $\boldsymbol{u_{new}} \approx \boldsymbol{u_{old}} + \boldsymbol{\Phi}^{\mathbf{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi^2}^{T} \, A \, \boldsymbol{\Phi^2} \, q = \boldsymbol{\Phi^2}^{T} \, b$$

$$A^* \, q = b^*$$



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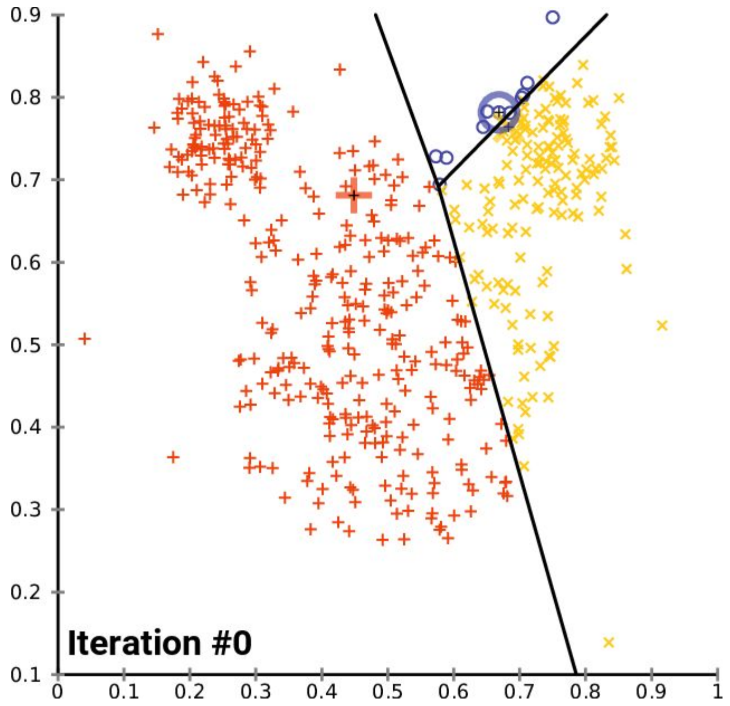
Local POD. K-means

Given: $\{\boldsymbol{x}_j\}_{j=1}^{N}$

Find centroids: $\{\boldsymbol{c}_i\}_{i=1}^{n}$ and assignments: s_{ij}

$$\min \sum_{j=1}^{n} \sum_{i}^{N} s_{ij} \left\| \boldsymbol{x}_j - \boldsymbol{c}_i \right\|_2^2$$

$$s.t. \sum_{i} s_{ij} = 1, \qquad s_{ij} \in \{0,1\}$$



Animation from Wikipedia

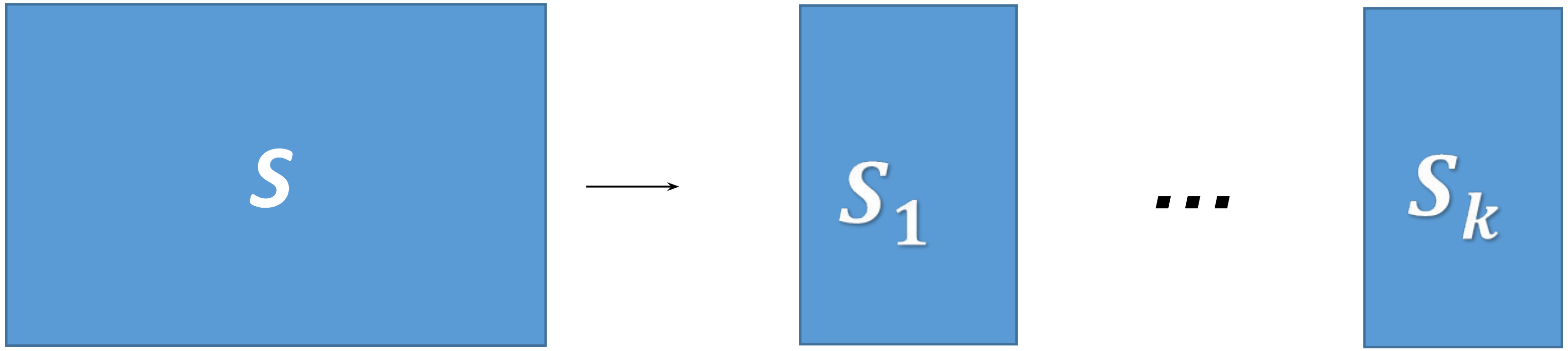
Solve via alternating minimization:

$$s_{ij} = \begin{cases} 1 & nearest\ centroid \\ 0 & otherwise \end{cases} \qquad c_i = \frac{\sum_{j=1}^{N} s_{ij} \boldsymbol{x}_j}{\sum_{j=1}^{N} s_{ij}}$$

Local POD. Building multiple bases

- Use an unsupervised learning method to build clusters

1. Get Non-overlapping clusters $\boldsymbol{S_i = kmeans(S)}$

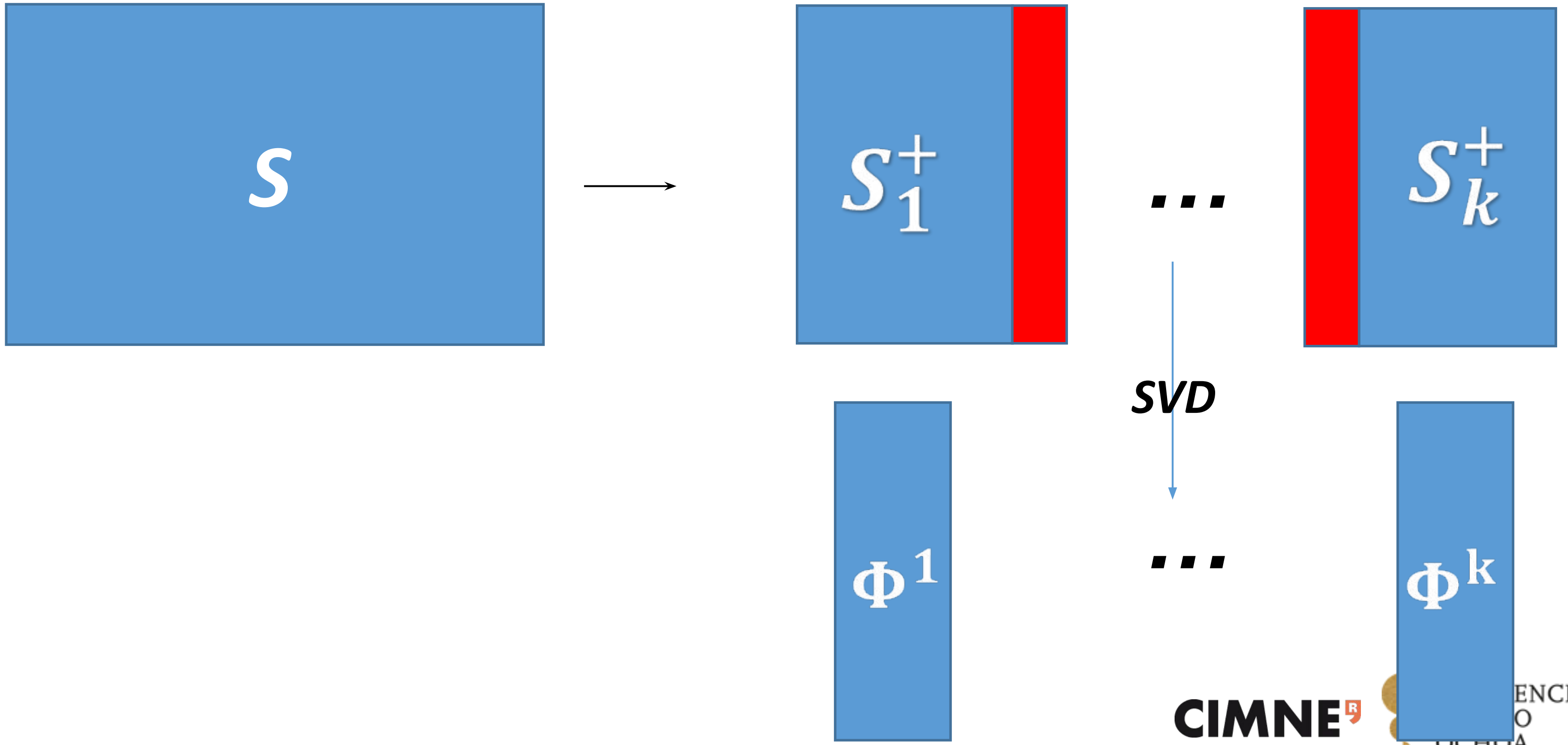


Local POD. Building multiple bases

- Use an unsupervised learning method to build clusters

1. Get Non-overlapping clusters $\boldsymbol{S_i = kmeans(S)}$

2. Add fixed overlapping $\boldsymbol{S_i^{+} = overlap(S_i)}$ (Farhat, 2012): doi.org/10.2514/6.2012-2686



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Local POD. Overlapping proposal

Locally Linear Embedding LLE:

$$\min_{c} \sum_{j=1}^{N} \|\boldsymbol{x}_j - \sum c_{ij} \boldsymbol{x}_i\|_2^2$$

$$s.t. \quad c_{ij} = 0 \quad if\ \boldsymbol{x}_i\ not\ k - NN\ to\ \boldsymbol{x}_j$$

$$\sum_{i=1}^{N} c_{ij} = 1$$

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

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

Each cluster $\boldsymbol{S_i^+}$ should consist on its snapshots, and the neighbours of its snapshots

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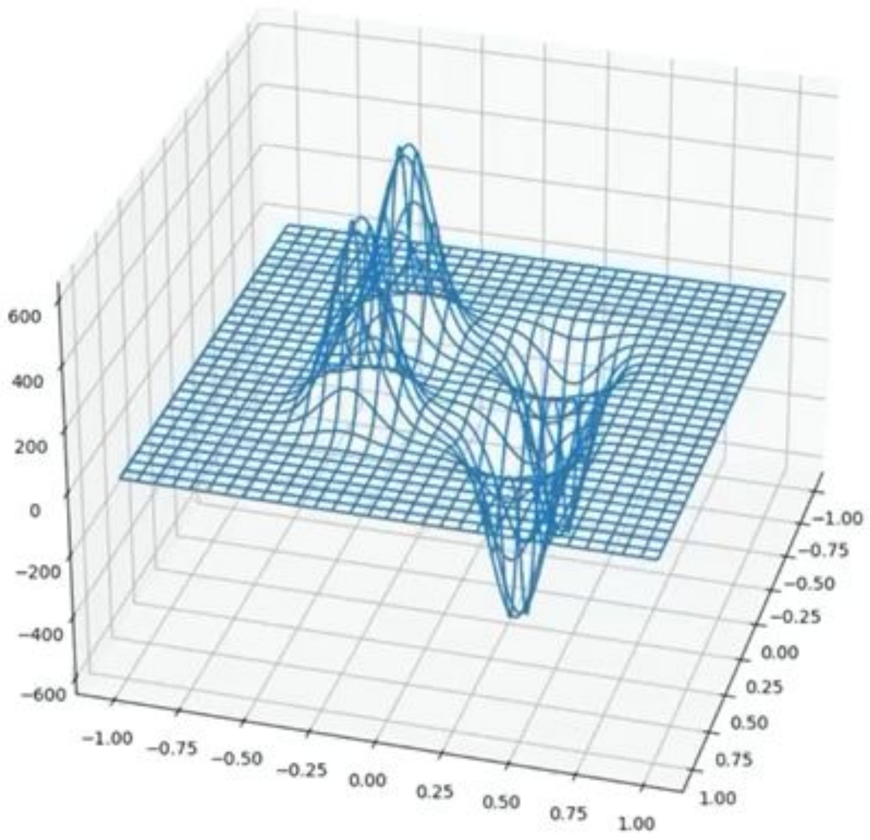
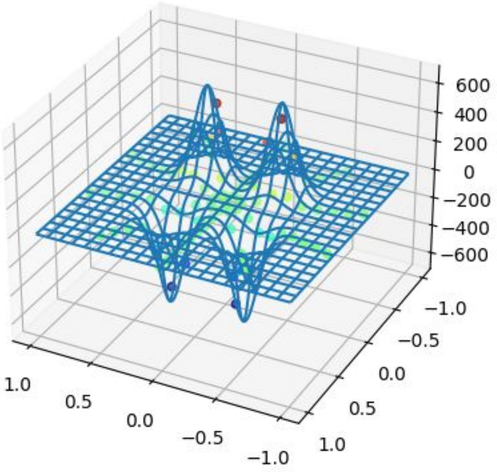
Local POD. Overlapping comparison

$$\mathcal{M} \subset \mathbb{R}^3, \qquad \dim(\mathcal{M}) = 2$$

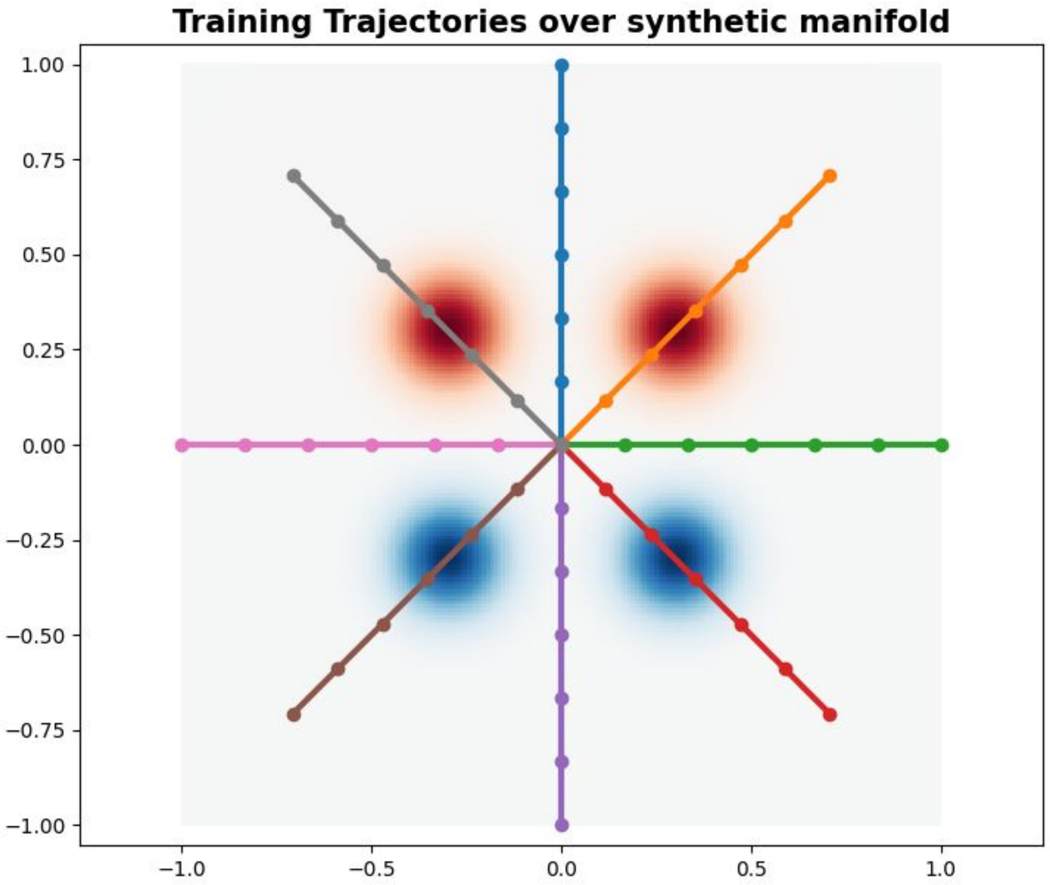


Synthetic 2-Manifold

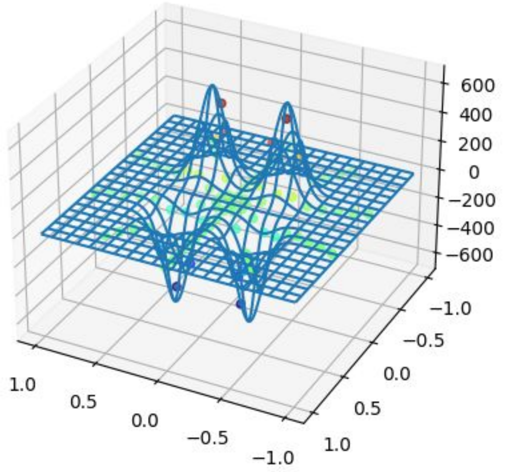
Local POD. Overlapping comparison



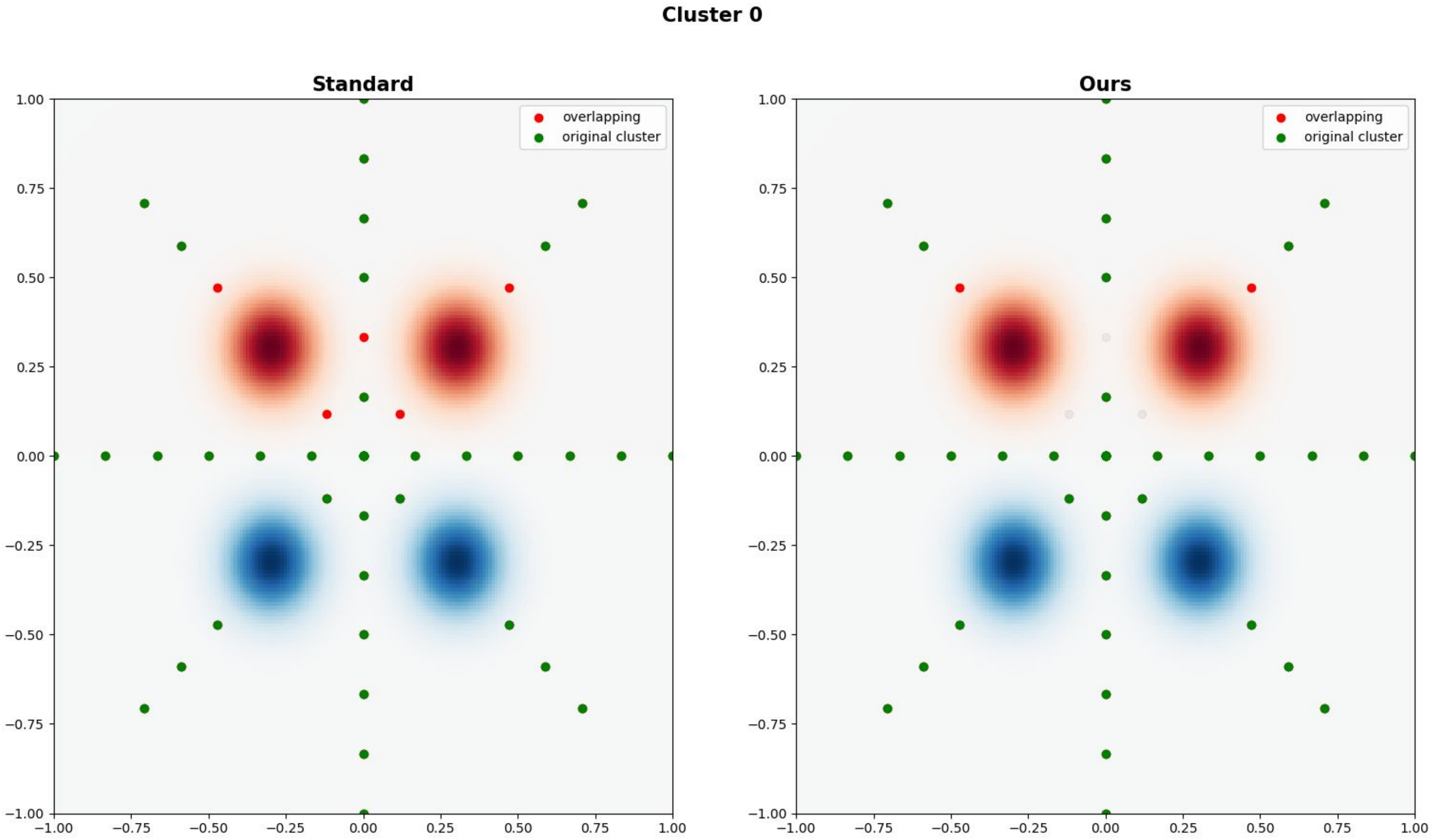
Synthetic 2-Manifold



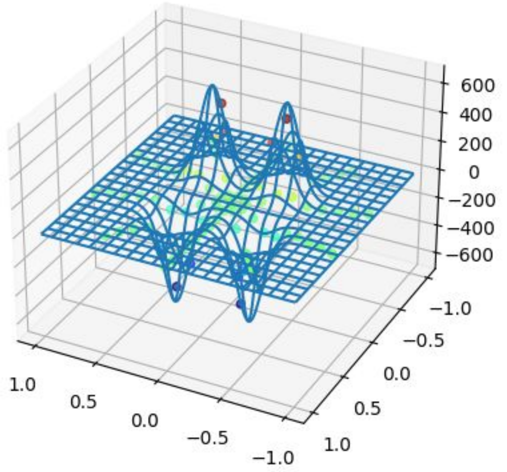
Local POD. Overlapping comparison



Synthetic 2-Manifold



Local POD. Overlapping comparison



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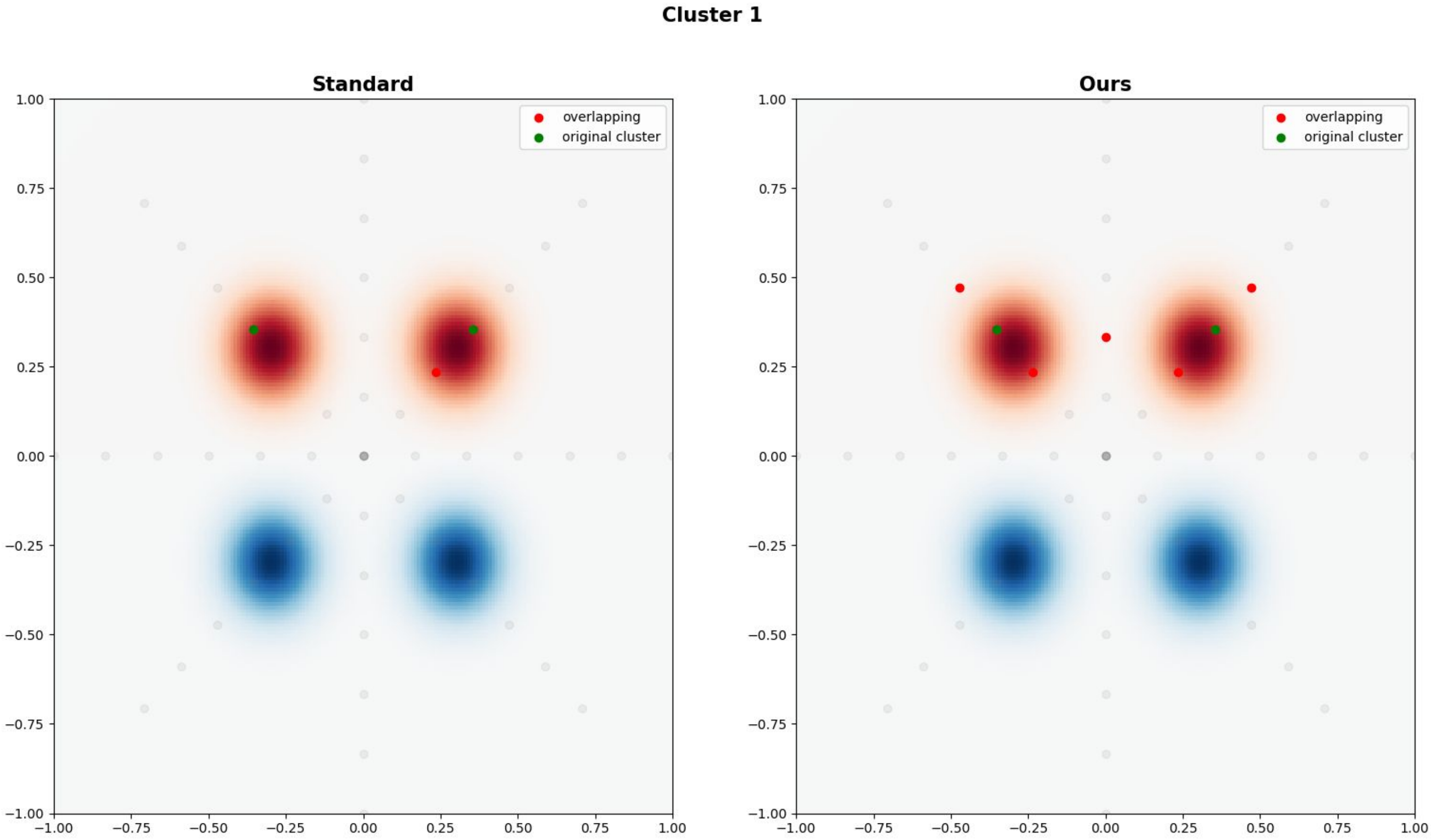
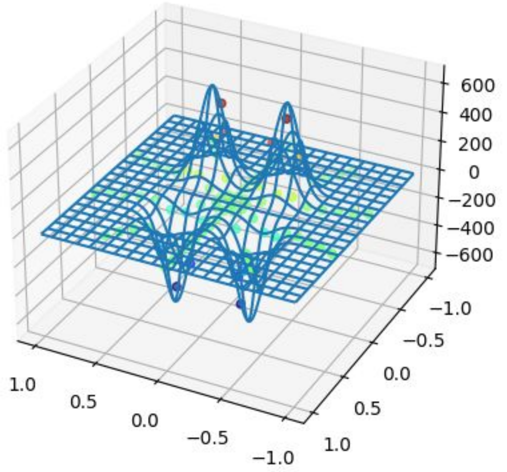


Local POD. Overlapping comparison



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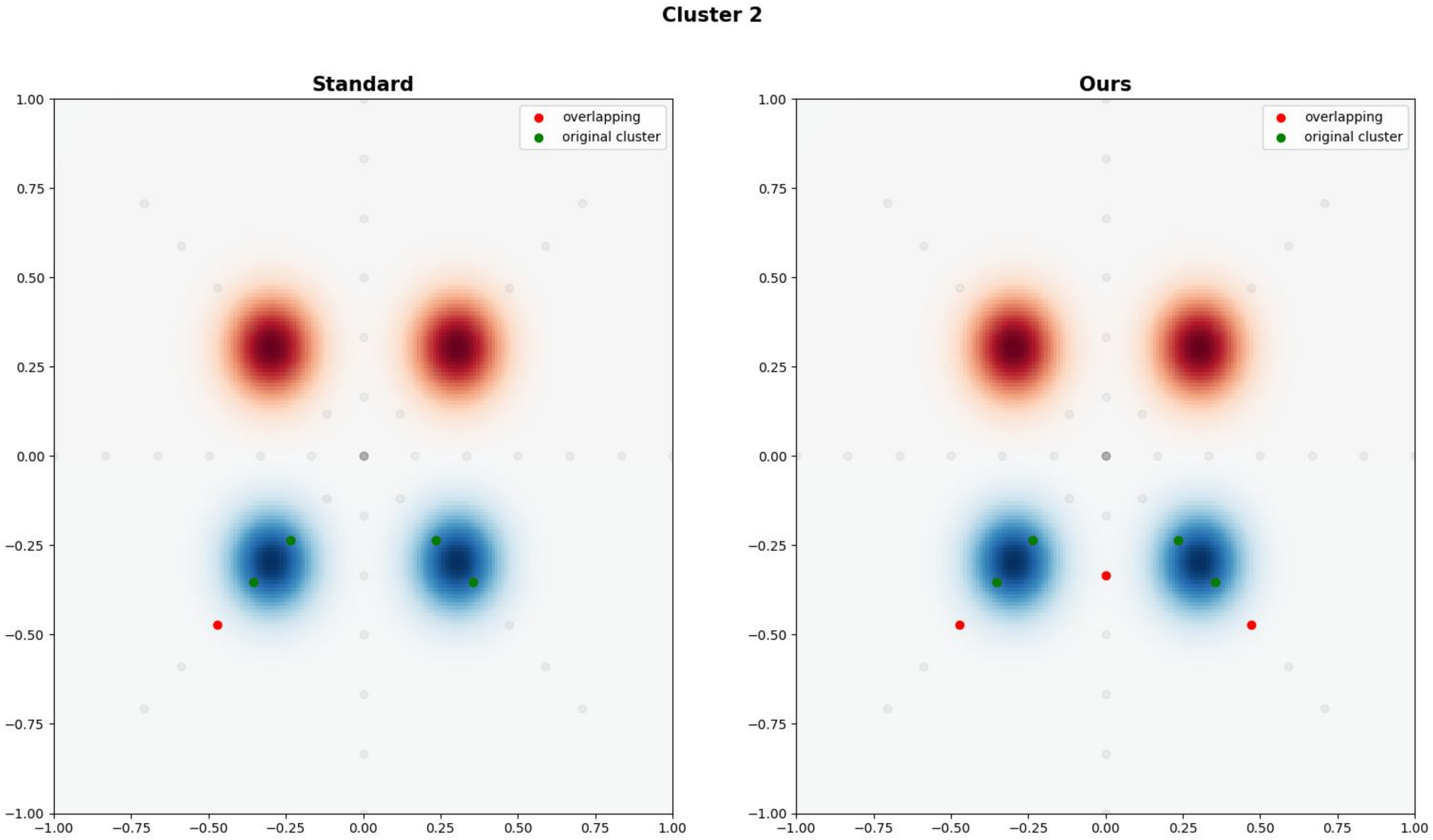
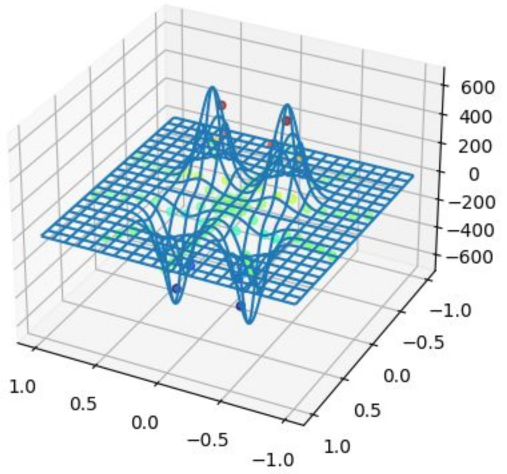
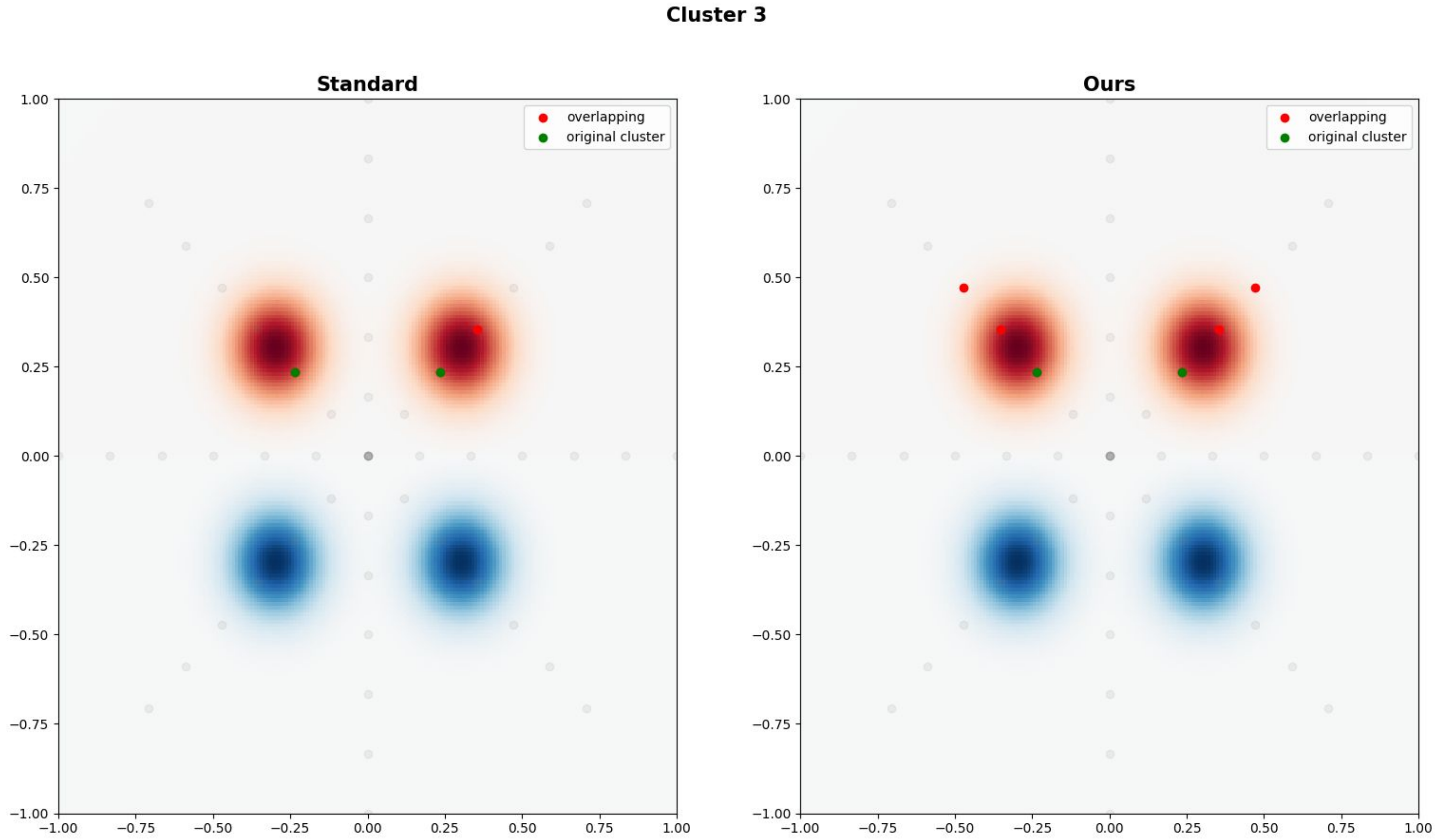


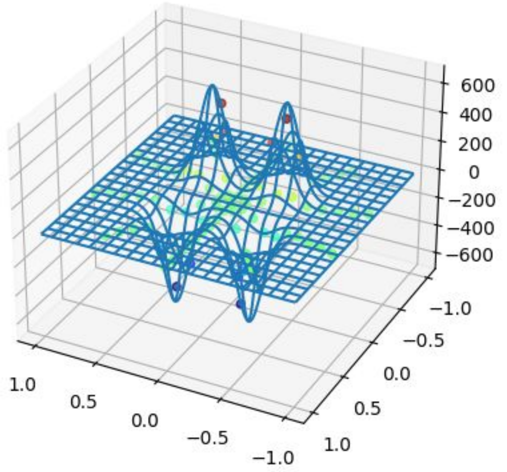
Local POD. Overlapping comparison



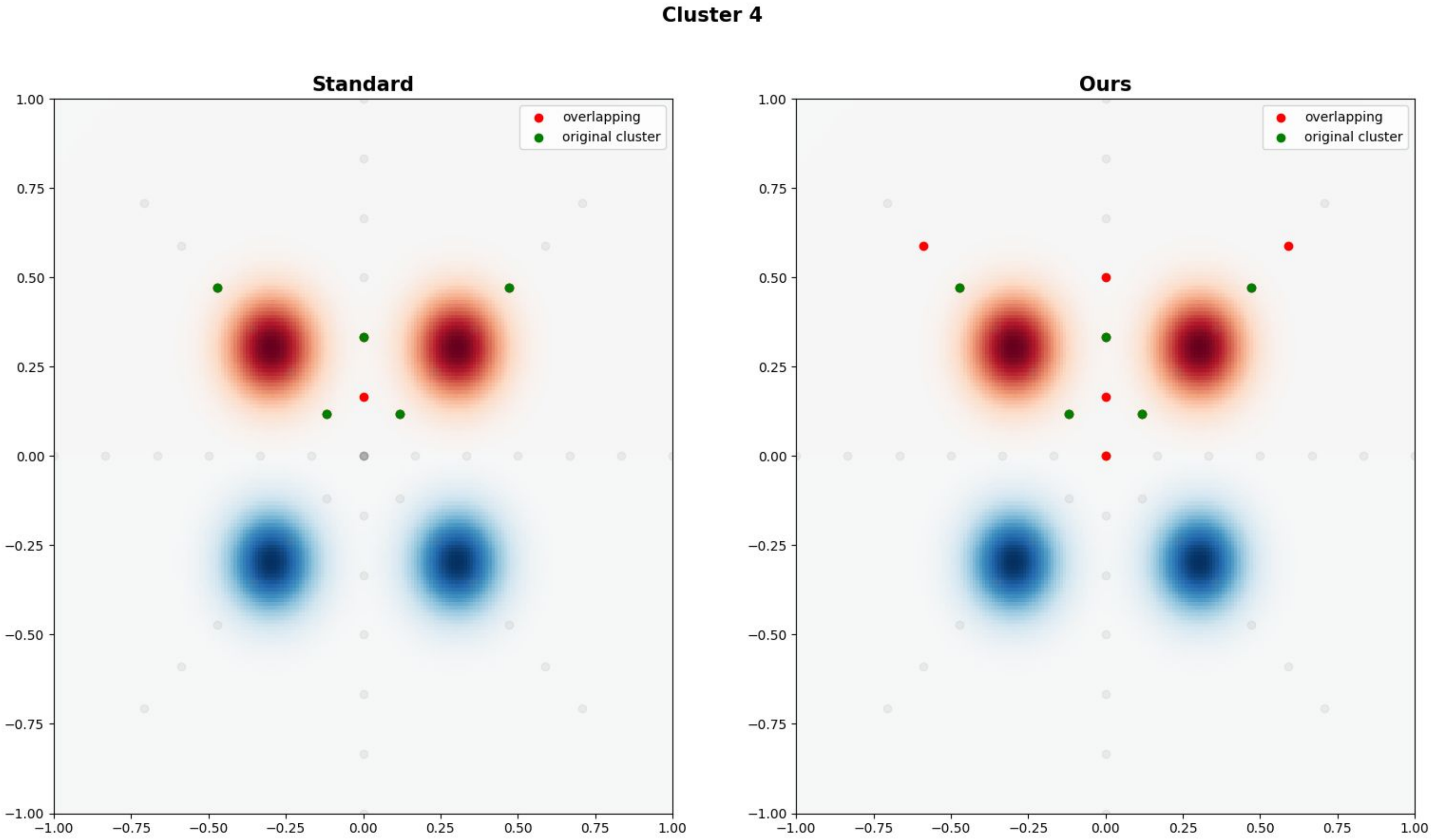
Synthetic 2-Manifold



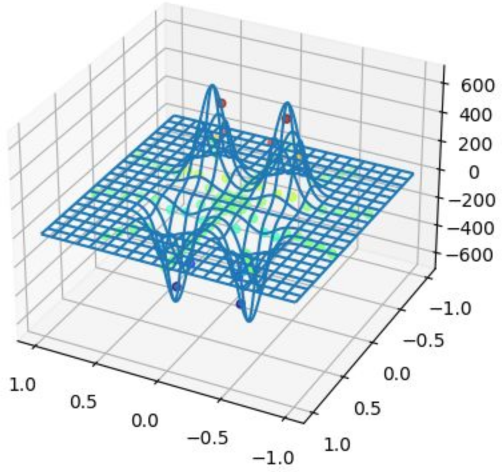
Local POD. Overlapping comparison



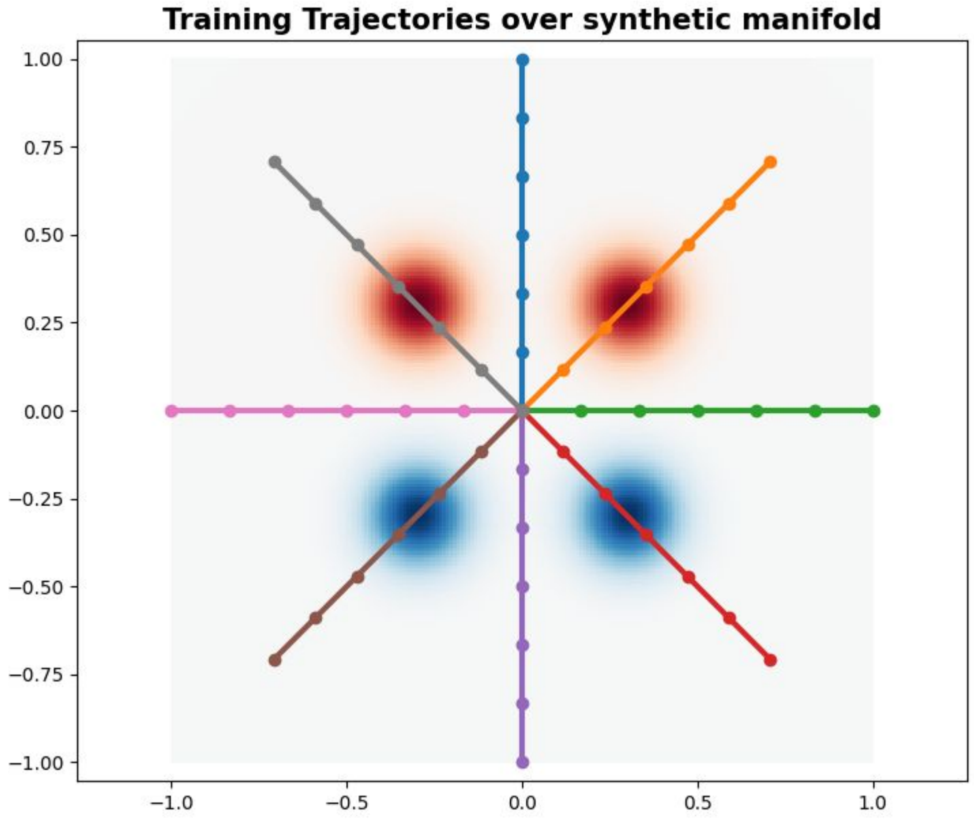
Synthetic 2-Manifold

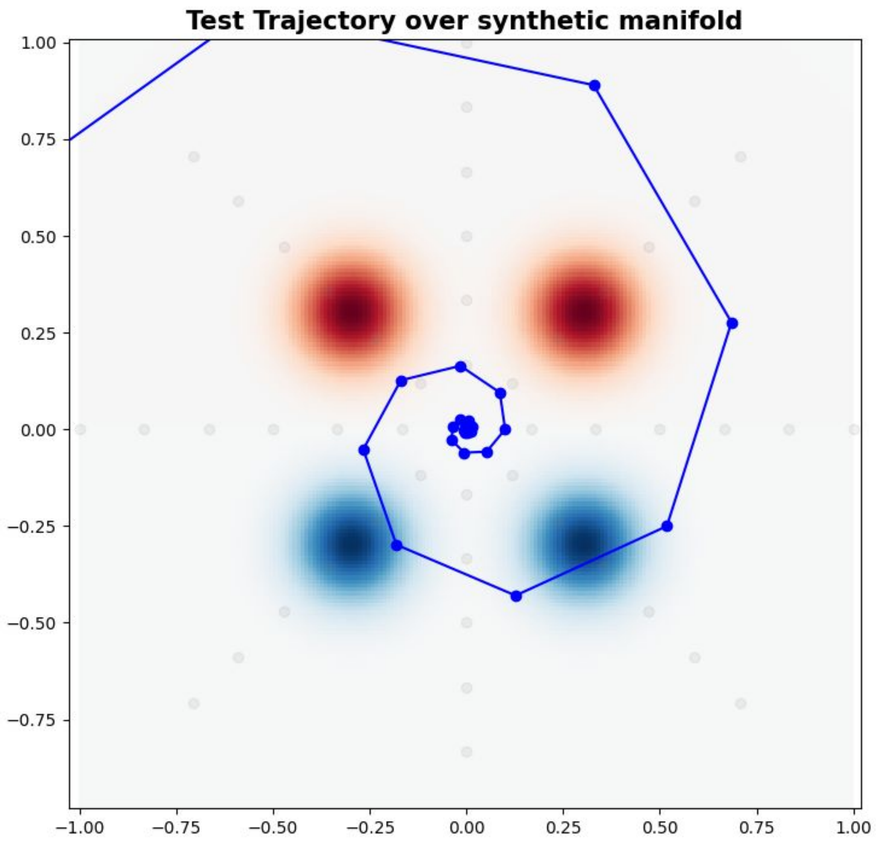


Local POD. Overlapping comparison



Synthetic 2-Manifold





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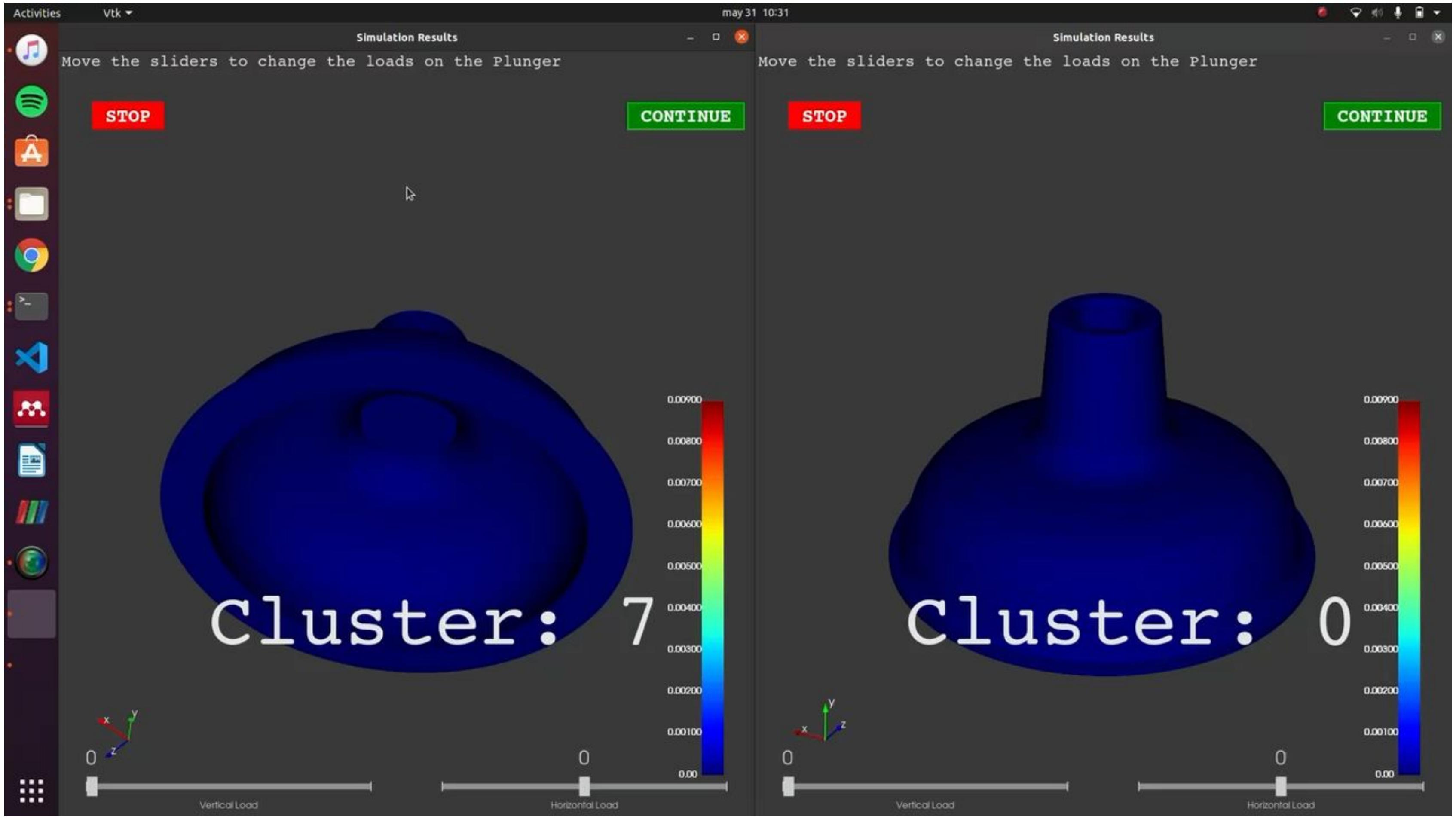
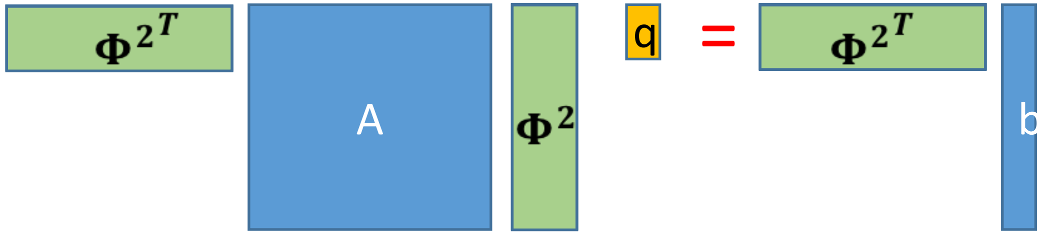
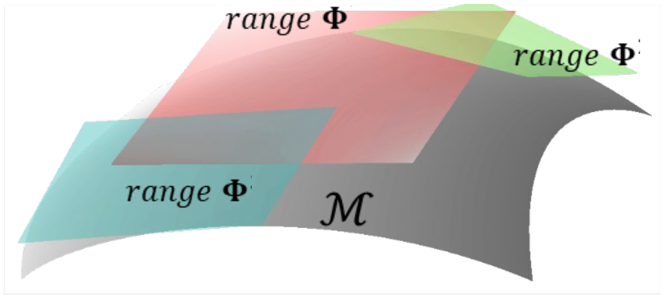
Local POD. Example 1



Local POD. Hyper-reduction

Reduced Order Model (ROM)





$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi}, \boldsymbol{R})$$

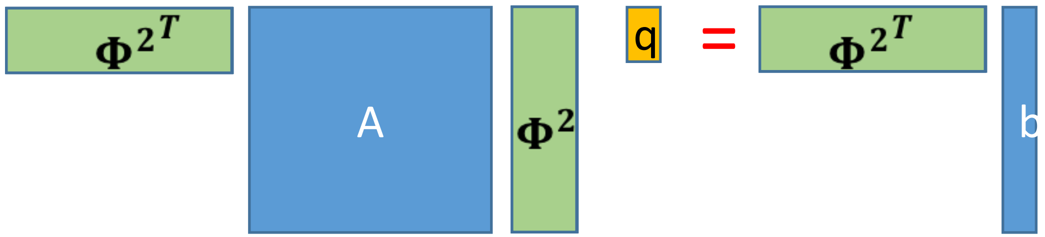
$$(\boldsymbol{E}, \boldsymbol{W}) = \arg min \left\| \sum_{i=1}^{n} \boldsymbol{g}_i - \sum_{i \in E}^{n} \boldsymbol{g}_i \boldsymbol{\omega}_i \right\|_2^2$$

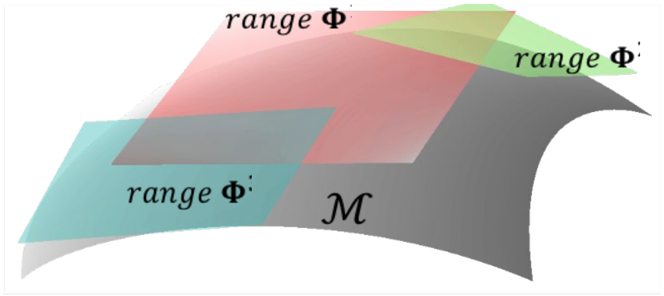
$$s.t. \quad \omega_i > 0$$

(Grimberg, 2020): doi.org/10.1002/nme.6603

Local POD. Improved hyper-reduction

Reduced Order Model (ROM)

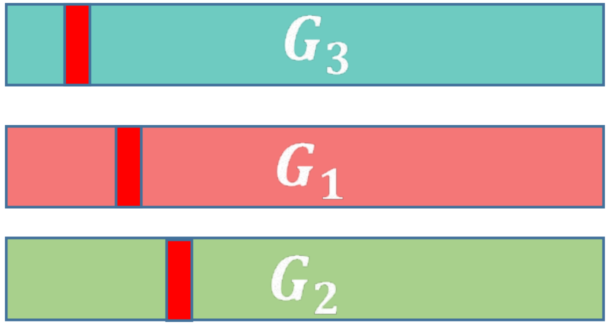




$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi}, \boldsymbol{R})$$

$$(\boldsymbol{E}, \widehat{\boldsymbol{W}}) = \arg min \left\| \sum_{i=1}^{n} \boldsymbol{g}_i^k - \sum_{i \in E}^{n} \boldsymbol{g}_i^k \widehat{\boldsymbol{\omega}}_i \right\|_2^2$$

$$s.t. \quad \widehat{\omega}_i \geq 0$$



Find a single set of elements and as many sets of weights as bases

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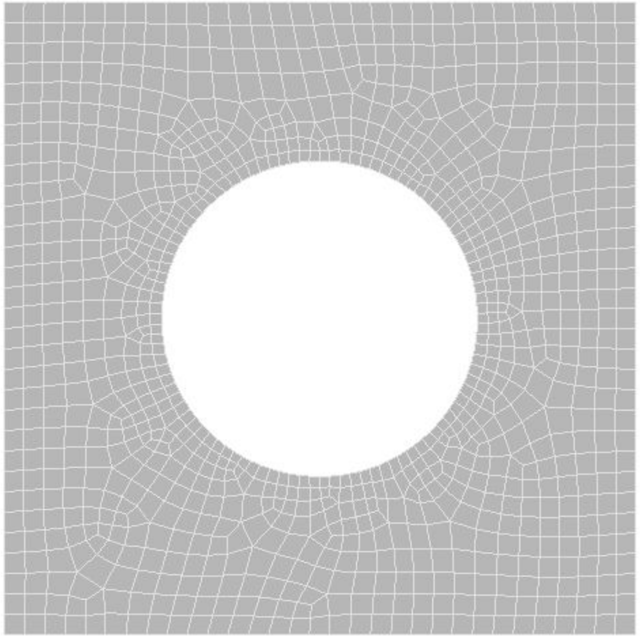
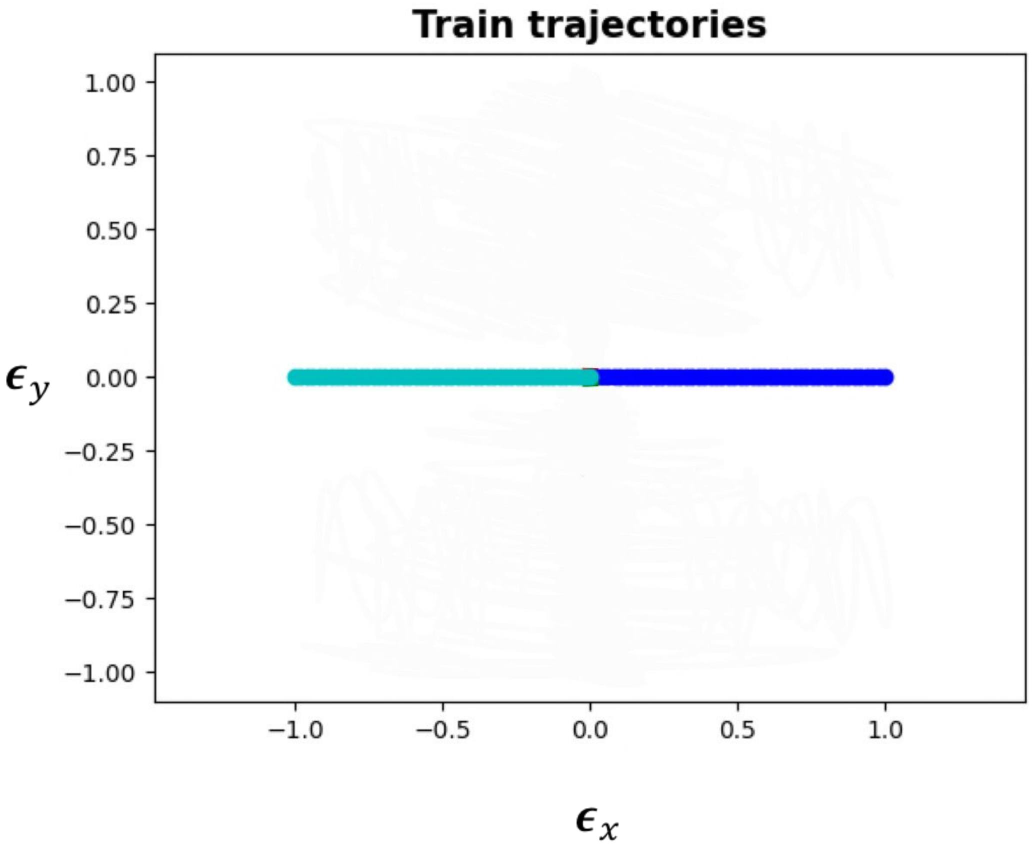
Local POD. Example 2

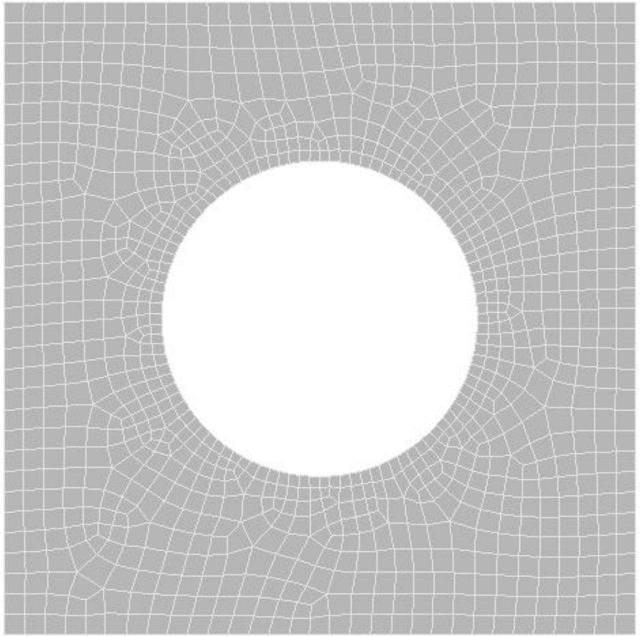


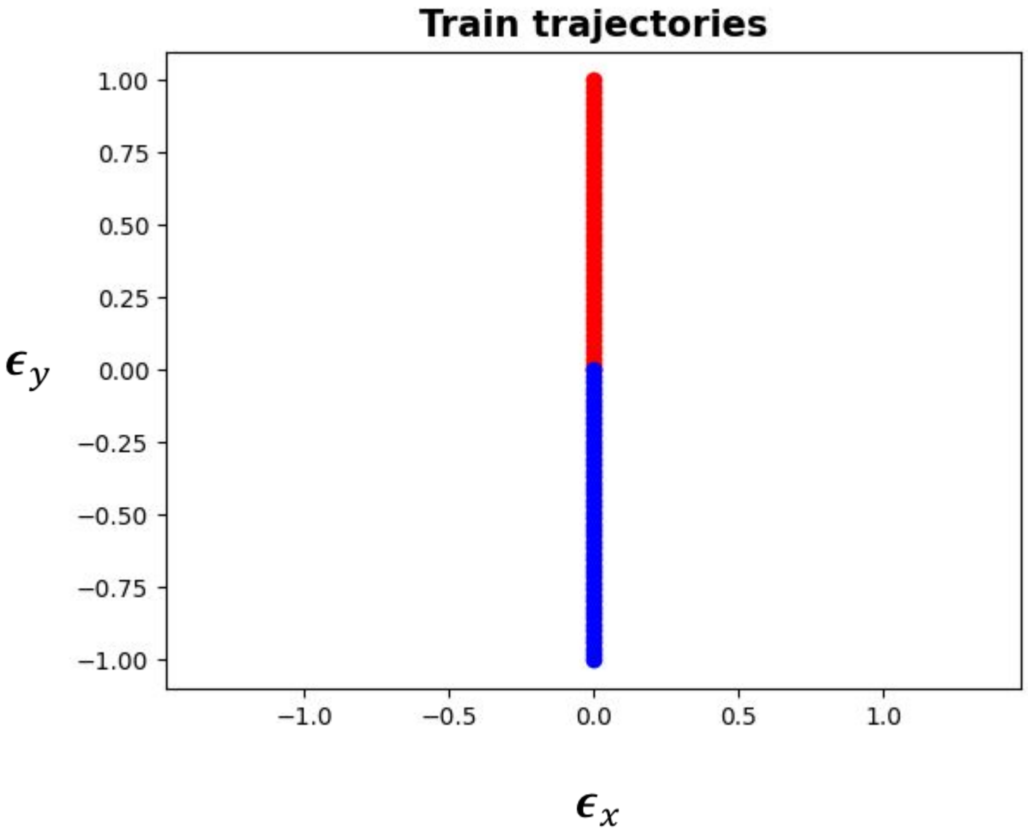
ϵ_x



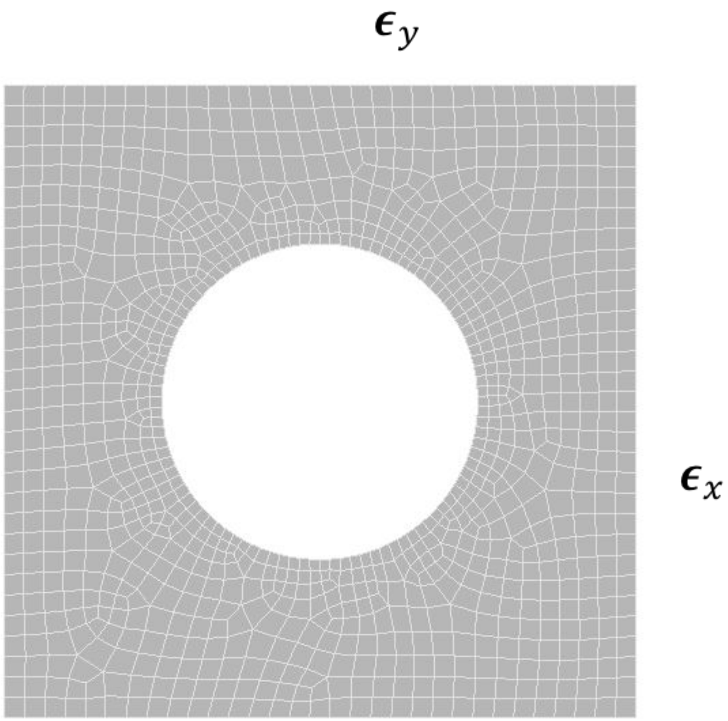
Local POD. Example 2

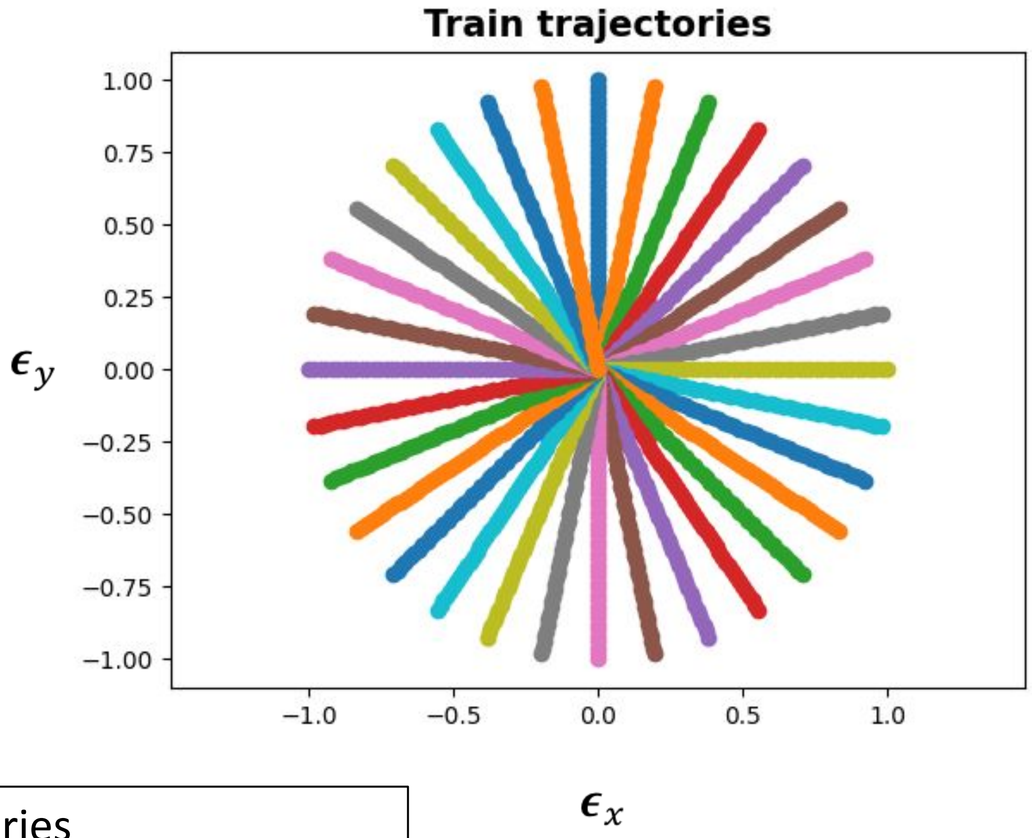
ϵ_y





Local POD. Example 2

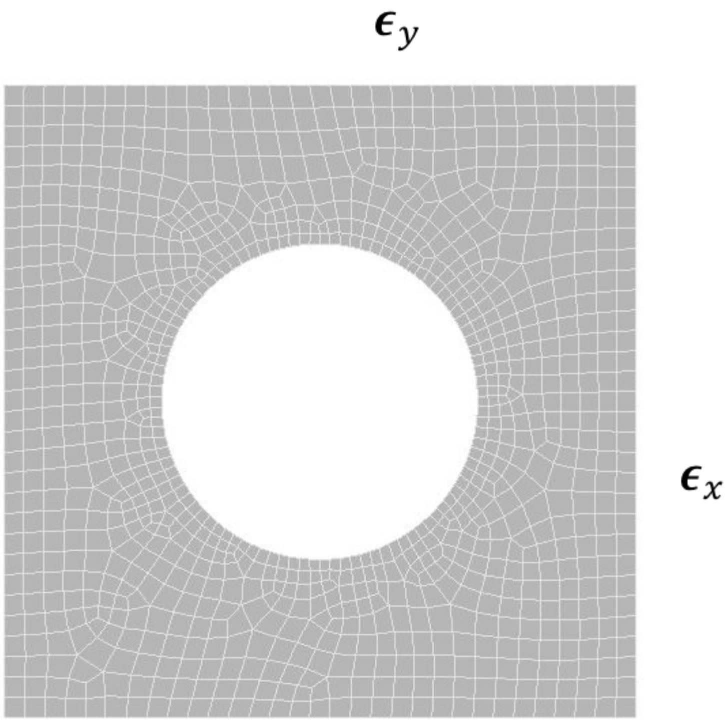


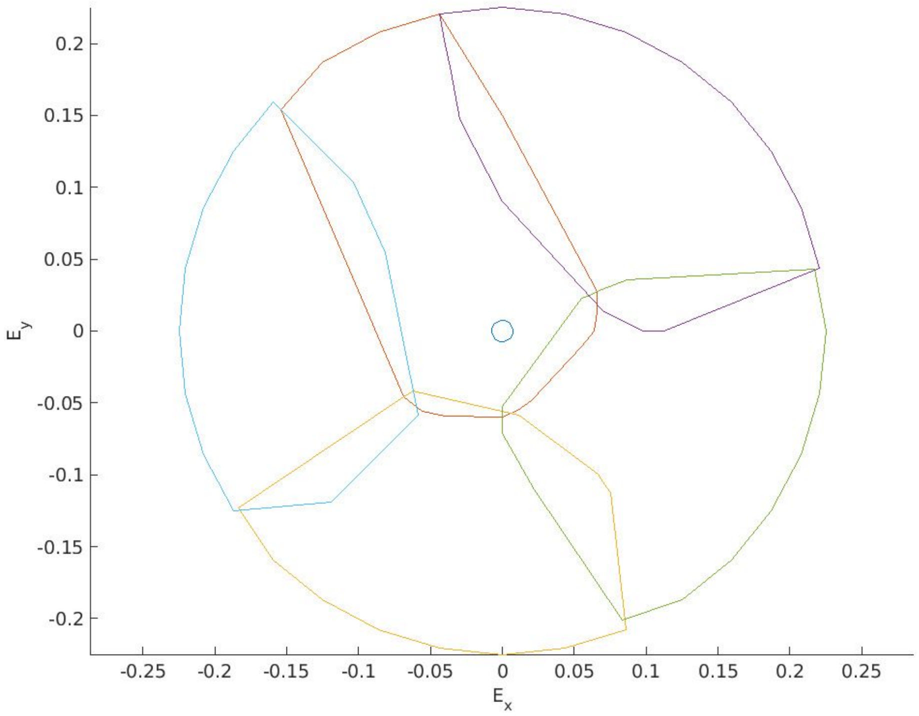


32 trajectories
50 snapshots per trajectory
1600 snapshots

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Example 2

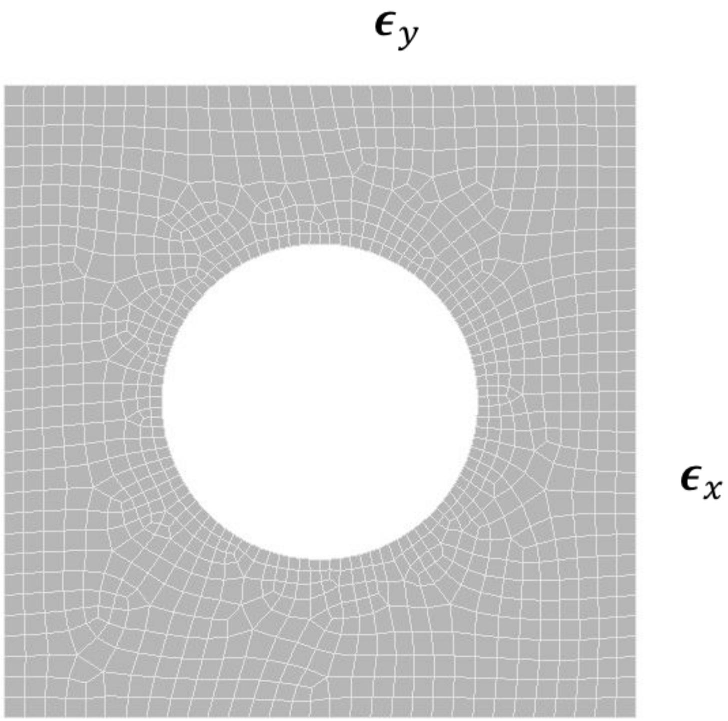


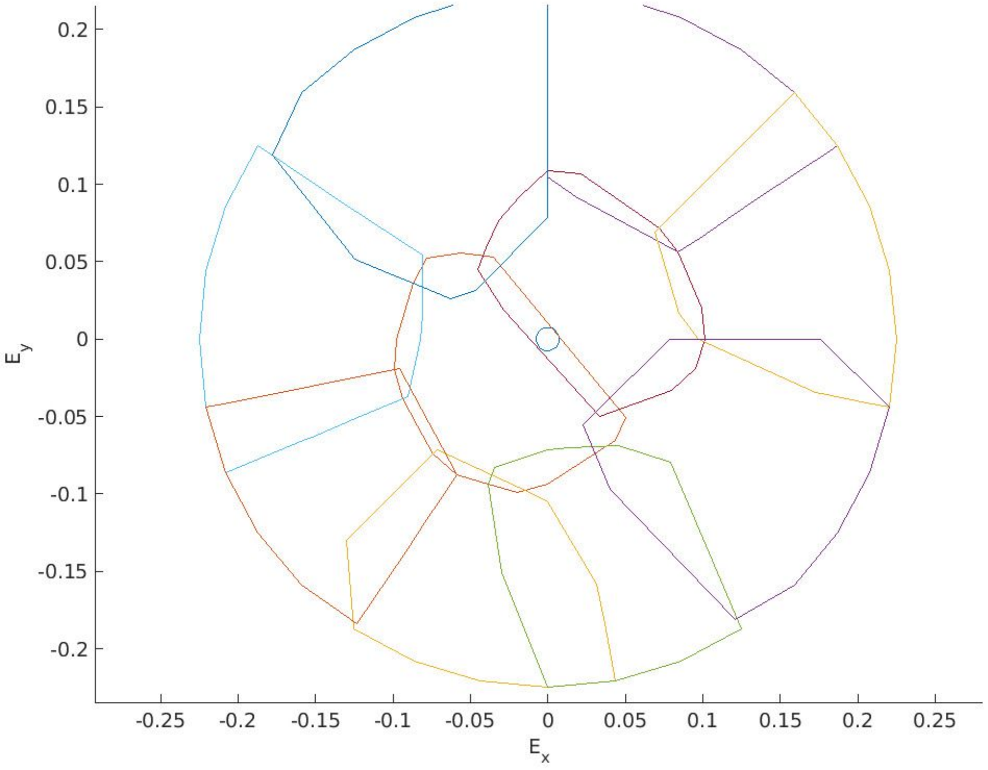


32 trajectories
50 snapshots per cluster
1600 snapshots

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

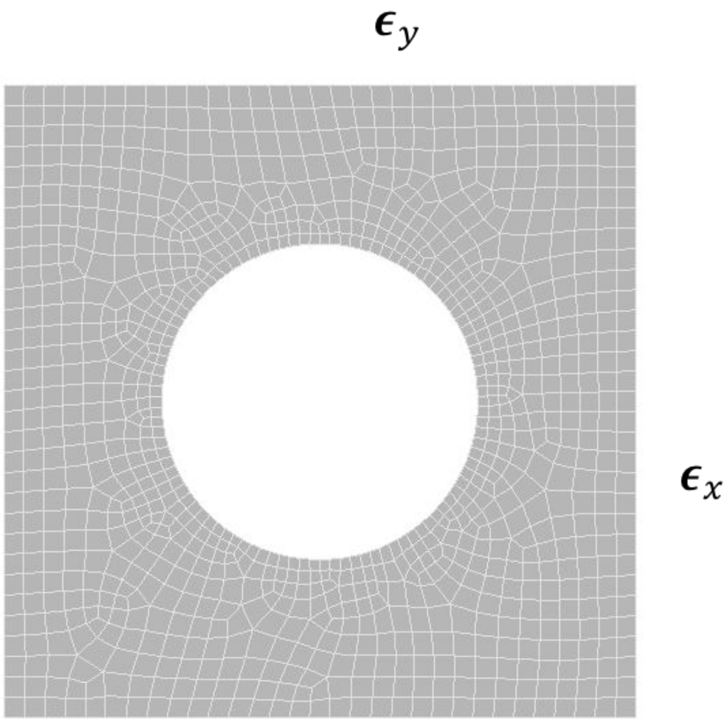
Local POD. Example 2

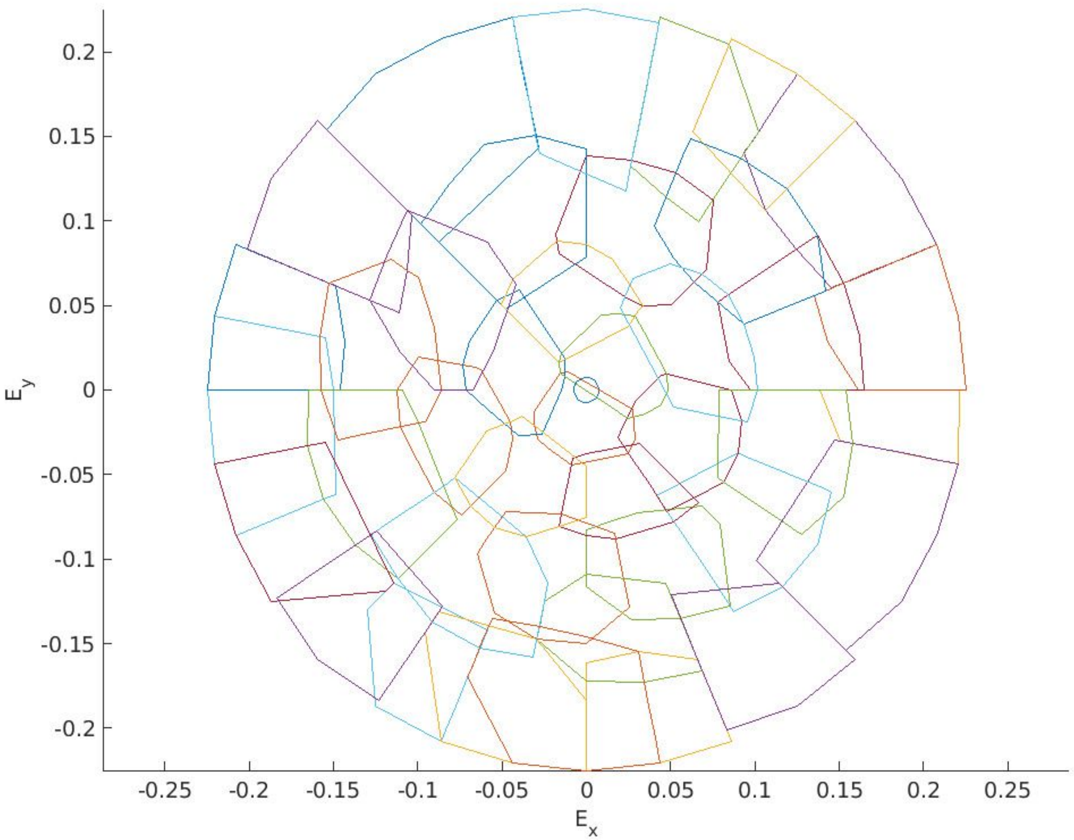




32 trajectories
50 snapshots per cluster
1600 snapshots

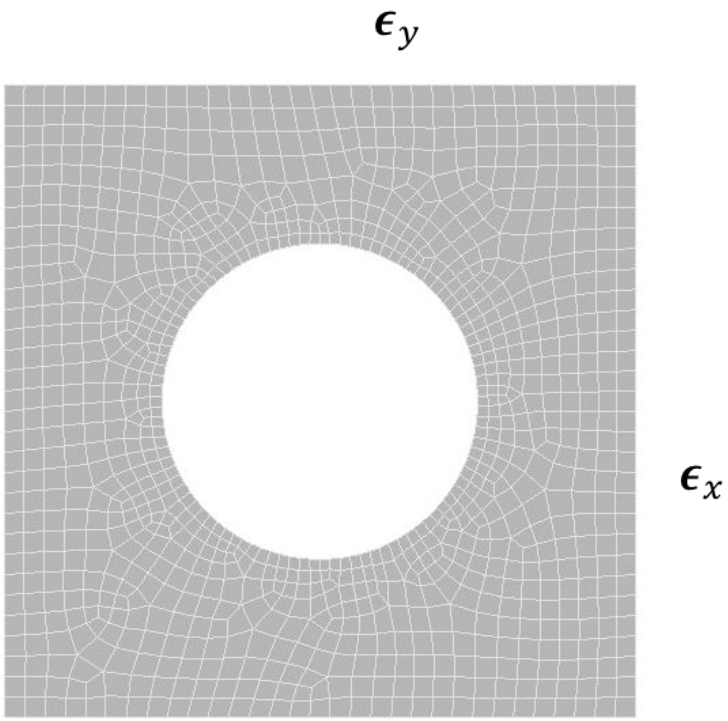
Local POD. Example 2

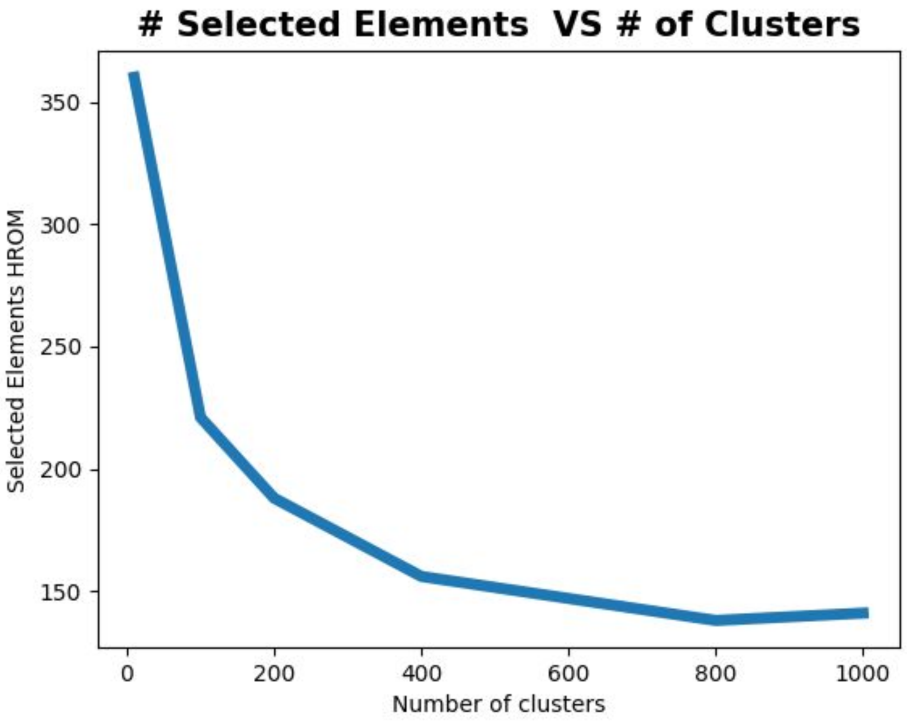




32 trajectories
50 snapshots per cluster
1600 snapshots

Local POD. Example 2

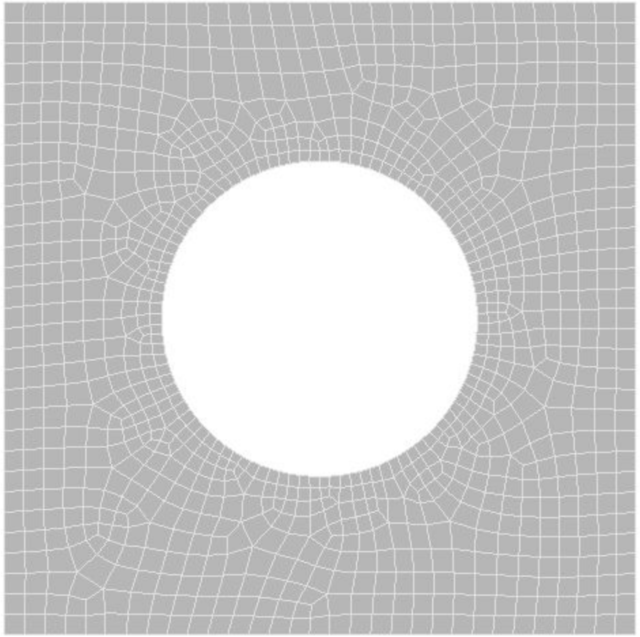




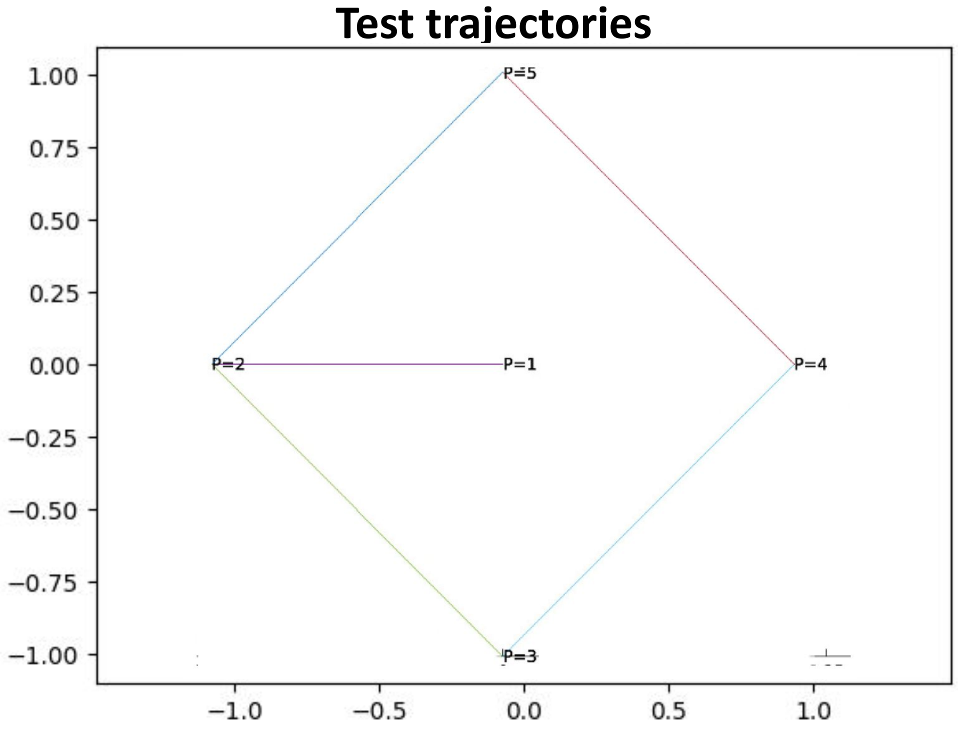
32 trajectories
50 snapshots per cluster
1600 snapshots

Local POD. Example 2

ϵ_y



ϵ_x

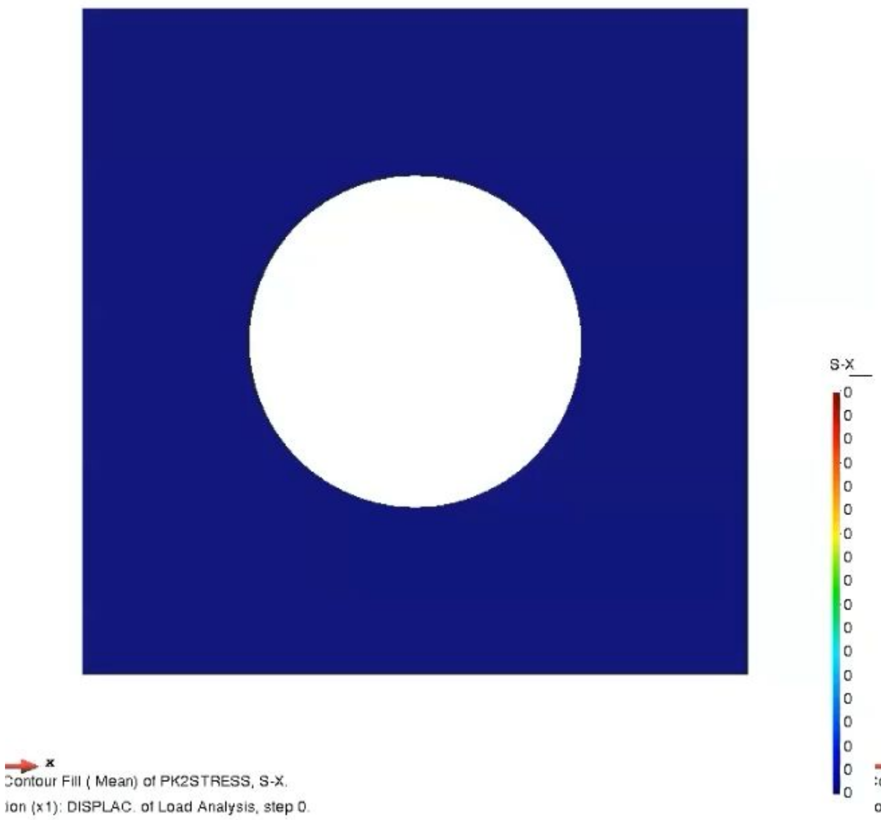


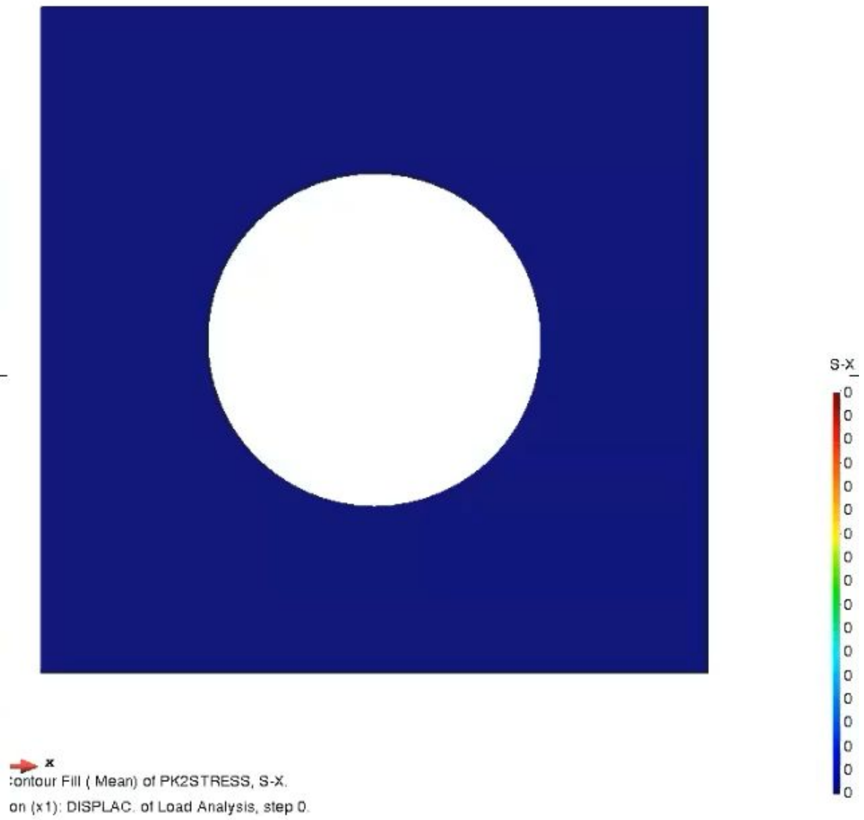
32 trajectories
50 snapshots per cluster
1600 snapshots

Local POD. Example 2

FOM

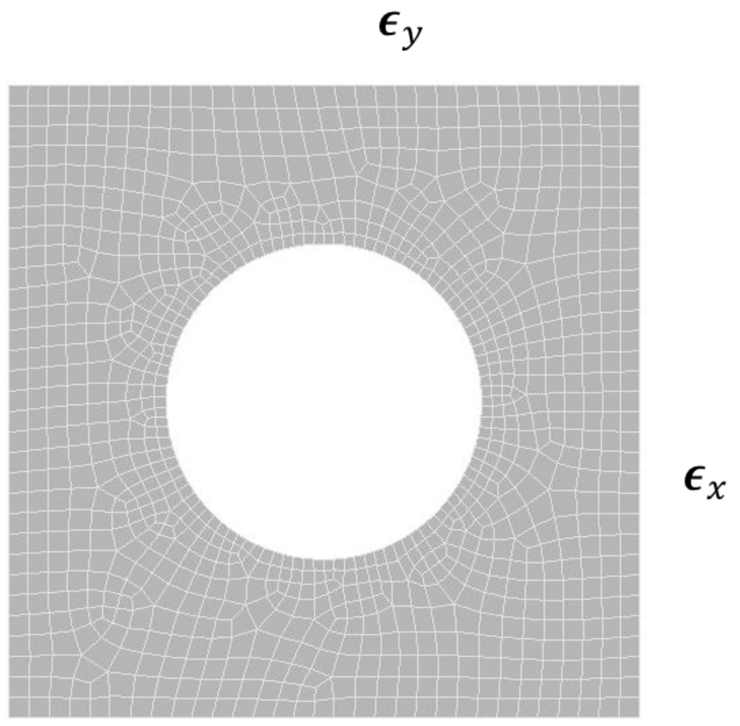
HROM





CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Example 2



10X less elements required compared with a single basis

5X less modes required compared with a single basis

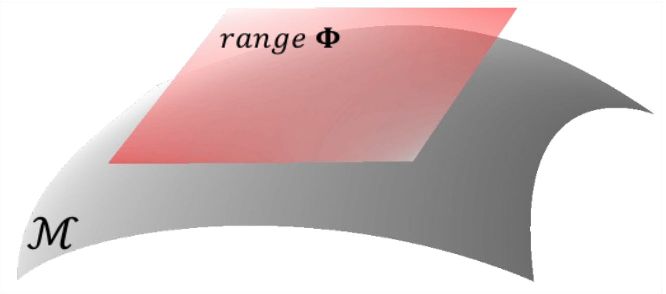
Local POD. Strengths and weaknesses

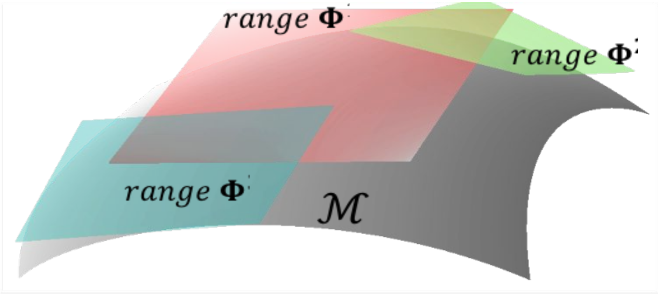
- Reasonable overhead in training and negligible in inference
- Smaller bases and elements sets, therefore faster ROMs

- Easy to overfit to training trajectories

General conclusions

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





THANK YOU

GRATEFUL TO:

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Link to Kratos github site

References:

[1] Hernández, J. A. (2020). A multiscale method for periodic structures using domain decomposition and ECM-hyperreduction. *Computer Methods in Applied Mechanics and Engineering*, *368*, 113192.

[2] Washabaugh, K., Amsallem, D., Zahr, M., & Farhat, C. (2012, June). Nonlinear model reduction for CFD problems using local reduced-order bases. In *42nd AIAA Fluid Dynamics Conference and Exhibit* (p. 2686).

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[4] Grimberg, S., Farhat, C., Tezaur, R., & Bou-Mosleh, C. (2021). Mesh sampling and weighting for the hyperreduction of nonlinear Petrov–Galerkin reduced-order models with local reduced-order bases. *International Journal for Numerical Methods in Engineering*, *122*(7), 1846-1874.