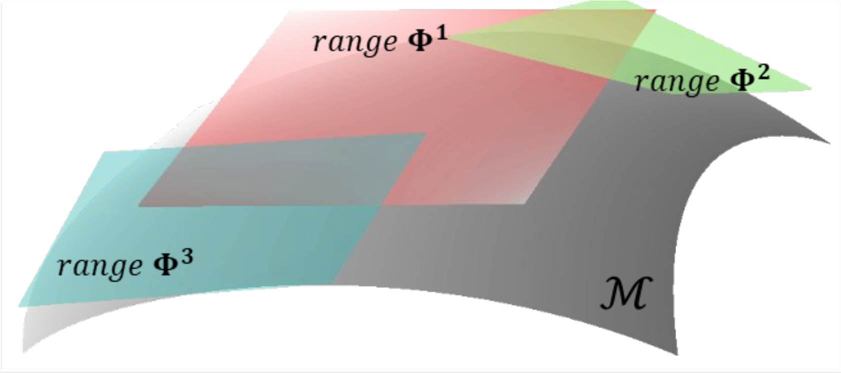
Minimally intrusive nonlinear Model Order Reduction



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Prof. Joaquin Hernandez

Mr. J Raul Bravo M

Mr. Carlos Roig

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Presenting ourselves

Kratos github site

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CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Outline of the talk

- Proper Orthogonal Decomposition POD
- Local POD
- Our proposals:
    - Clustering + “custom” Overlapping
        - Takeaway: take into account training history in the selection of overlap
    - HROM with multiple bases (keep the elements sets – change the weights)
        - Takeaway: “adaptive” basis + cheaper hyperredution
- Examples run in Kratos Multiphysics
- Conclusions

Proper Orthogonal Decomposition

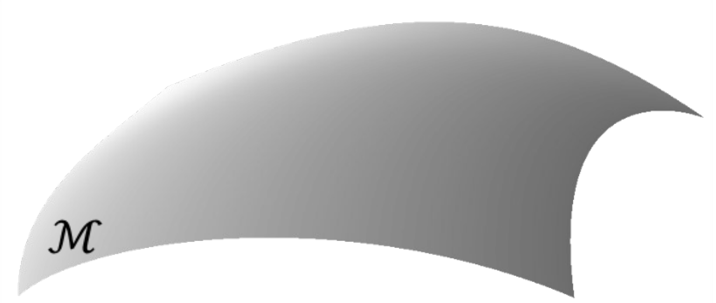
Full Order Model (FOM)

$\boldsymbol{r}(\boldsymbol{u};\boldsymbol{\mu}) = \mathbf{0}$

$\boldsymbol{u} \in \mathbb{R}^n$: state vector

$\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$: parameters vector

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

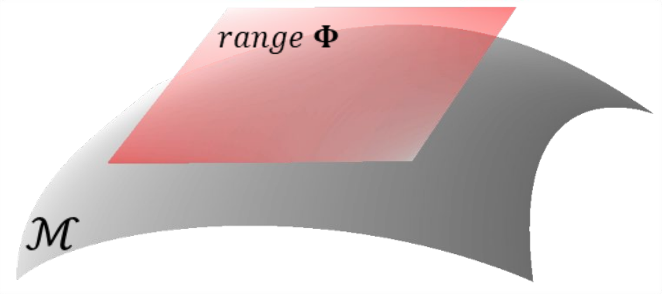


Let $\boldsymbol{u} \approx \mathbf{u}_{\text{old}} + \boldsymbol{\Phi}\,\mathbf{q}$

Reduced Order Model (ROM)

$\boldsymbol{\Phi}^T \boldsymbol{r}(\mathbf{u}_{\text{old}} + \boldsymbol{\Phi}\,\mathbf{q};\boldsymbol{\mu}) = \mathbf{0}$

$\boldsymbol{q} \in \mathbb{R}^k$: reduced state vector



A MUCH SMALLER SYSTEM!

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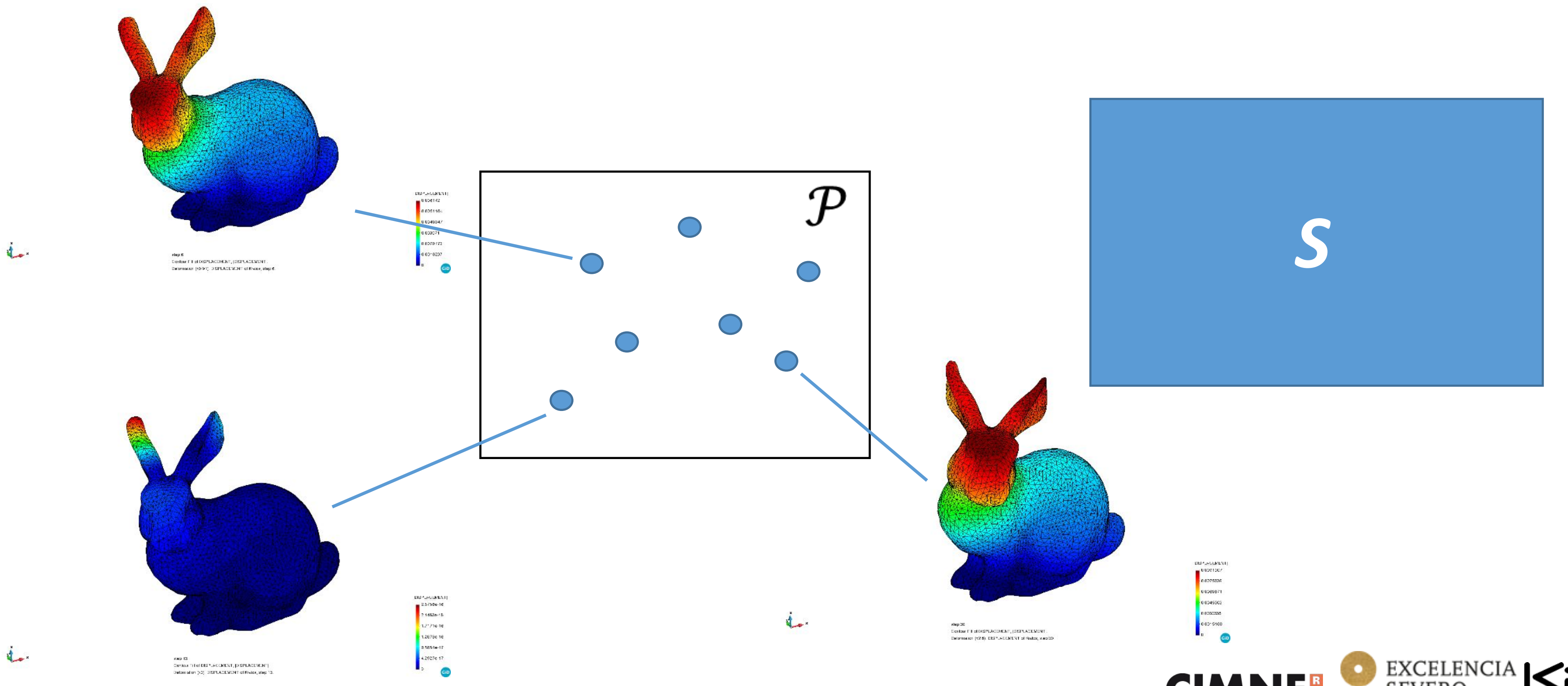
Proper Orthogonal Decomposition

- Solve the FOM using Finite Elements to find $\boldsymbol{u}(\boldsymbol{\mu})$



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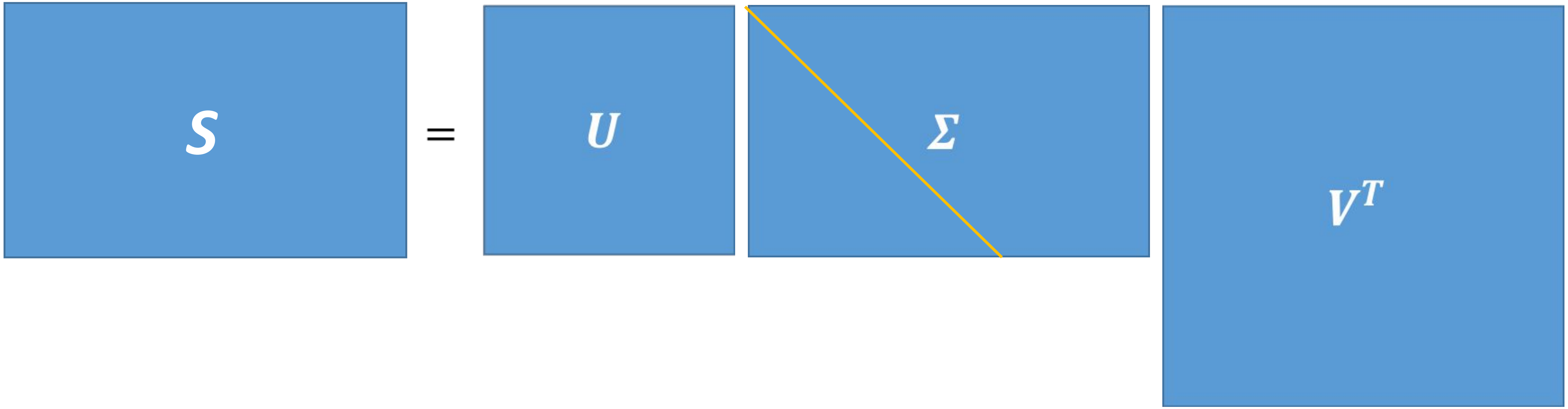
Proper Orthogonal Decomposition

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



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

Proper Orthogonal Decomposition

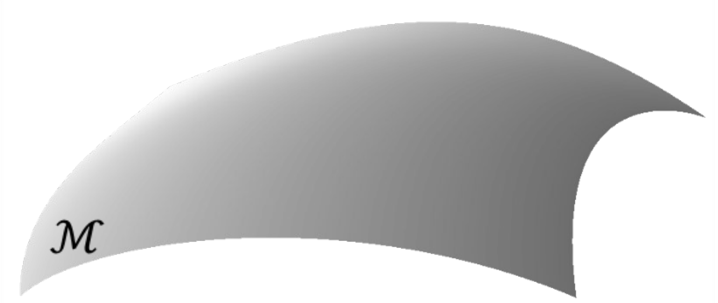
- Take the SVD of $\boldsymbol{S} = \boldsymbol{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathrm{T}} \approx \boldsymbol{U}_k\boldsymbol{\Sigma}_{\mathbf{k}}\mathbf{V}_{\mathbf{k}}^{\mathrm{T}}$

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

Proper Orthogonal Decomposition

Full Order Model (FOM)

Solution manifold: $\mathcal{M} = \{ \boldsymbol{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P} \} \subset \mathbb{R}^n$



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Reduced Order Model (ROM)

$\boldsymbol{\Phi}^T \boldsymbol{r}(\mathbf{u}_{\text{old}} + \boldsymbol{\Phi}\,\mathbf{q}; \boldsymbol{\mu}) = \boldsymbol{0}$

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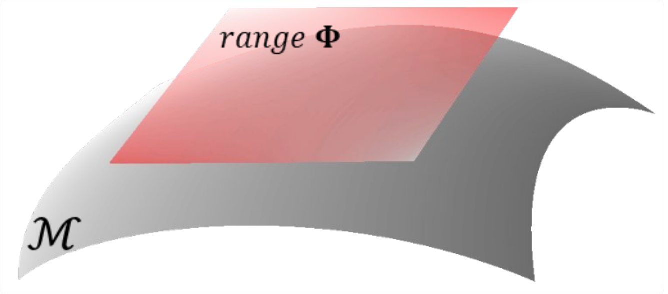

A MUCH SMALLER SYSTEM!

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

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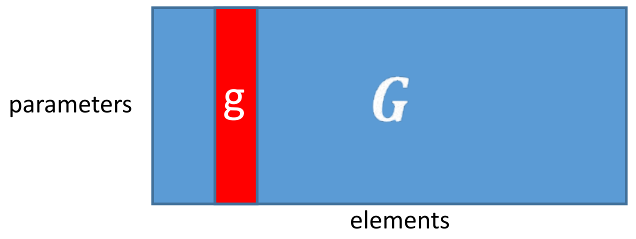
Hyper-reduction

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

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

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

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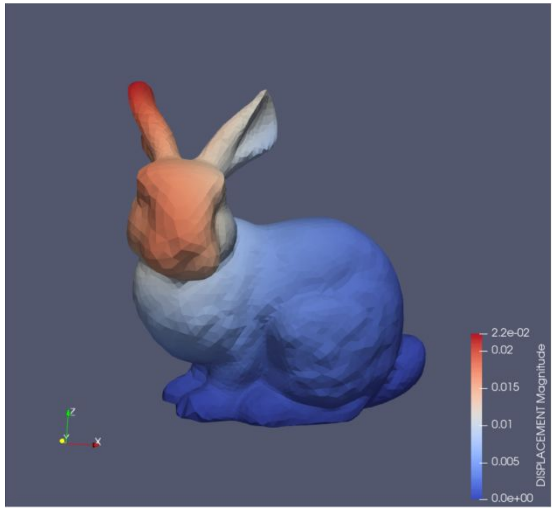
Hyper-reduction

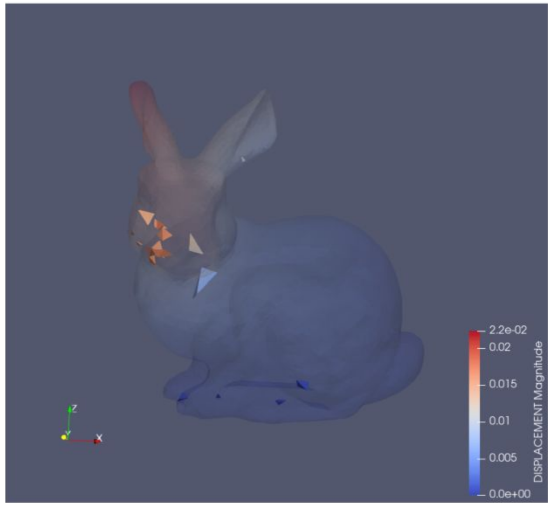
Assembly comparison FOM vs HROM:

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

FOM Simulation



HROM Simulation



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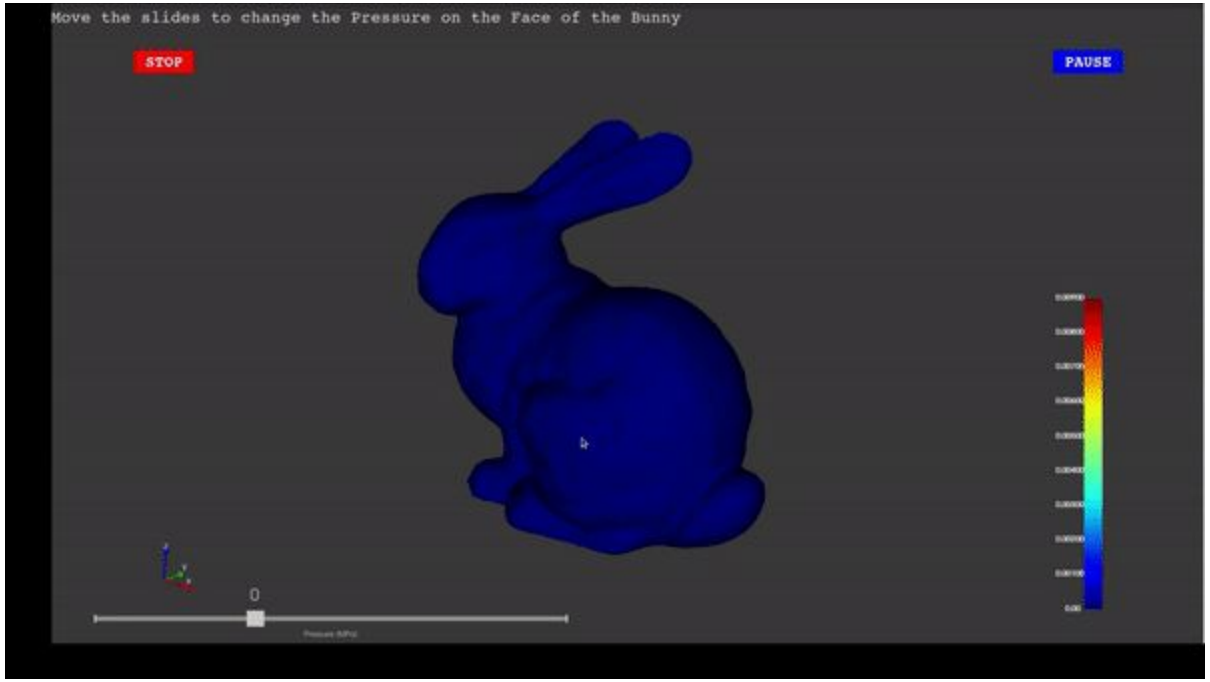
Hyper-reduction

$$\left(\sum_{e \in E} \Phi_e^T A_e \Phi_e \omega_e\right) q = \sum_{e \in E} \Phi_e^T b_e \omega_e$$

HROM Simulation



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)

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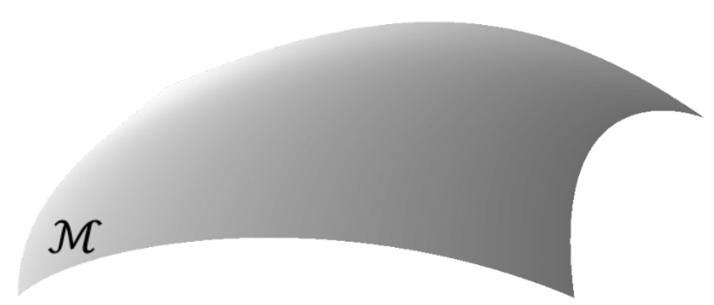
Solution manifold: $\mathcal{M} = \{\, \boldsymbol{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P} \,\} \subset \mathbb{R}^n$

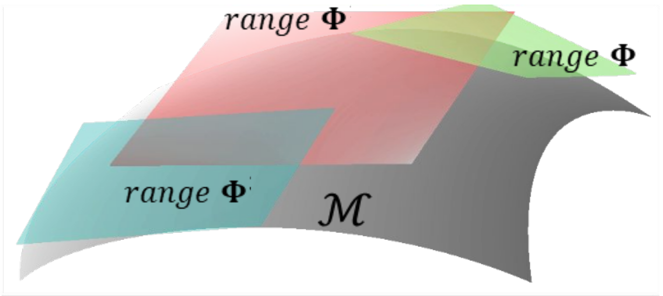


Let $\boldsymbol{u} \approx \boldsymbol{u}_{old} + \boldsymbol{\Phi}^{\mathbf{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^{1^T} \boldsymbol{r}\left(\mathbf{u}_{\mathbf{old}} + \boldsymbol{\Phi}^{1}\boldsymbol{q};\boldsymbol{\mu}\right) = \mathbf{0}$$

$\boldsymbol{q} \in \mathbb{R}^{k^1}$: reduced state vector



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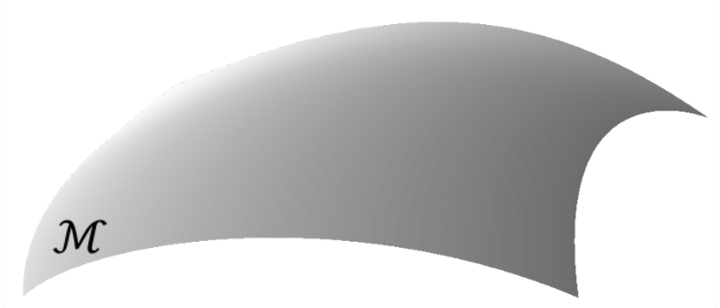
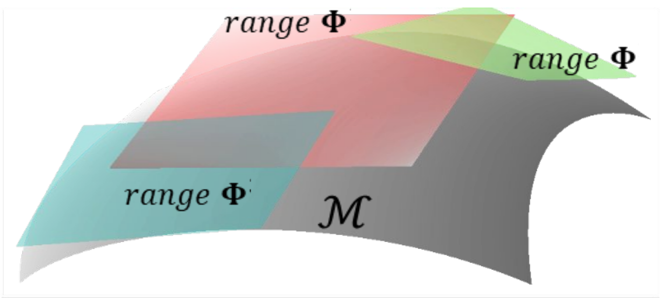


Let $\boldsymbol{u} \approx \boldsymbol{u}_{old} + \boldsymbol{\Phi}^{\mathbf{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

$\boldsymbol{\Phi}^{2^T} \boldsymbol{r}\left(\mathbf{u}_{\text{old}} + \boldsymbol{\Phi}^{2} q; \boldsymbol{\mu}\right) = \mathbf{0}$

$\boldsymbol{q} \in \mathbb{R}^{k^2}$: reduced state vector



Local POD

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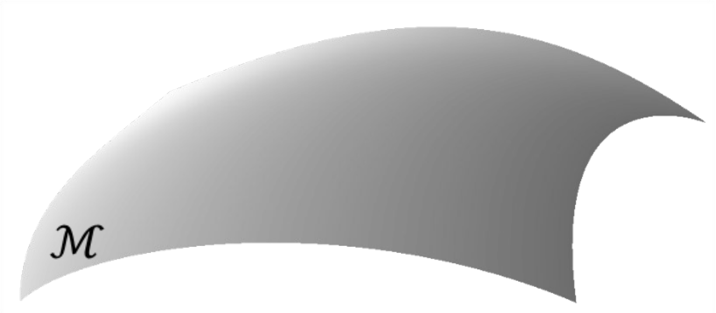
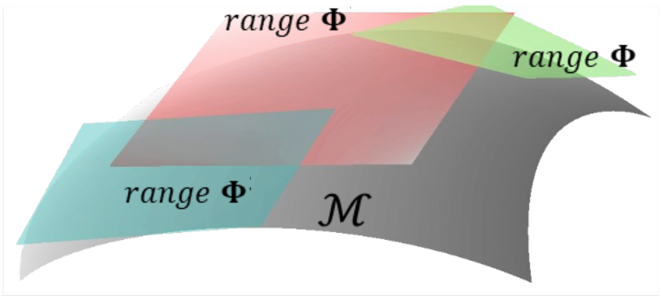


Let $\boldsymbol{u} \approx \boldsymbol{u}_{old} + \boldsymbol{\Phi}^{\mathbf{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^{3^T} \boldsymbol{r}\left(\mathbf{u}_{\text{old}} + \boldsymbol{\Phi}^3 q; \boldsymbol{\mu}\right) = \boldsymbol{0}$$

$\boldsymbol{q} \in \mathbb{R}^{k^3}$: reduced state vector



How to choose the local basis?

K-means

Given: $\{\boldsymbol{u}_j\}_{j=1}^{m}$

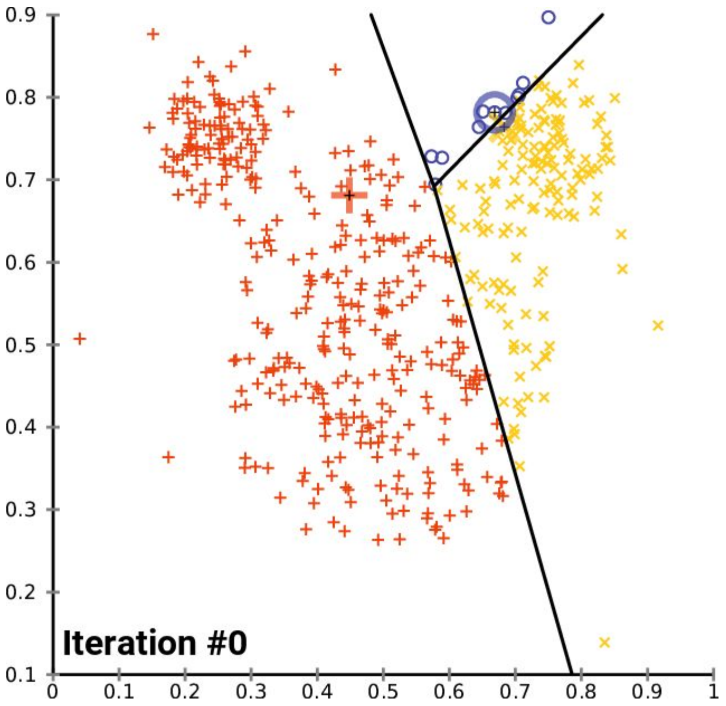
Find centroids: $\{\boldsymbol{c}_i\}_{i=1}^{k}$ and assignments: s_{ij}

$$\min \sum_{j=1}^{k} \sum_{i}^{m} s_{ij} \left\|\boldsymbol{u}_j - \boldsymbol{c}_i\right\|_2^2$$

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

Solve via alternating minimization:

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

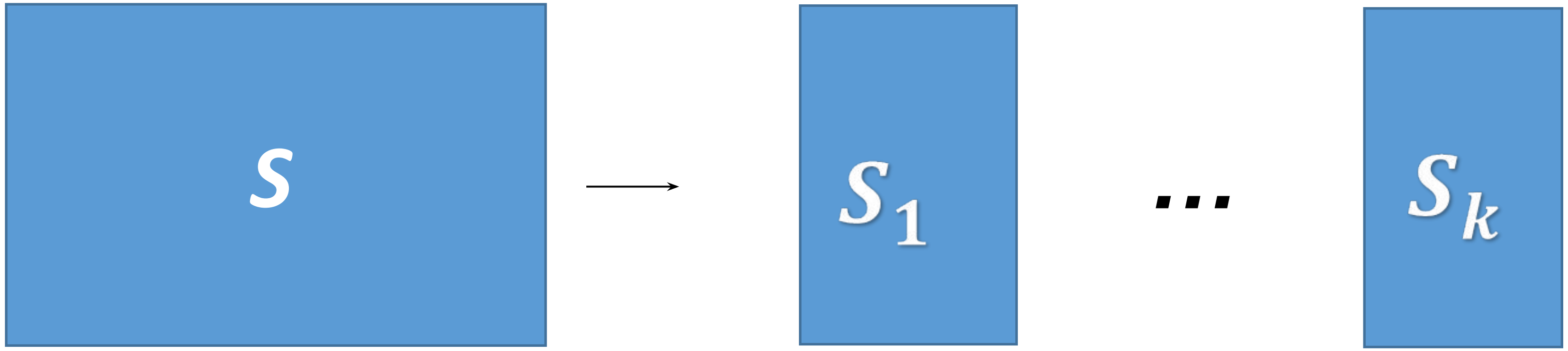


Animation from Wikipedia

Local POD. Building multiple bases

- Use an unsupervised learning method to build clusters

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

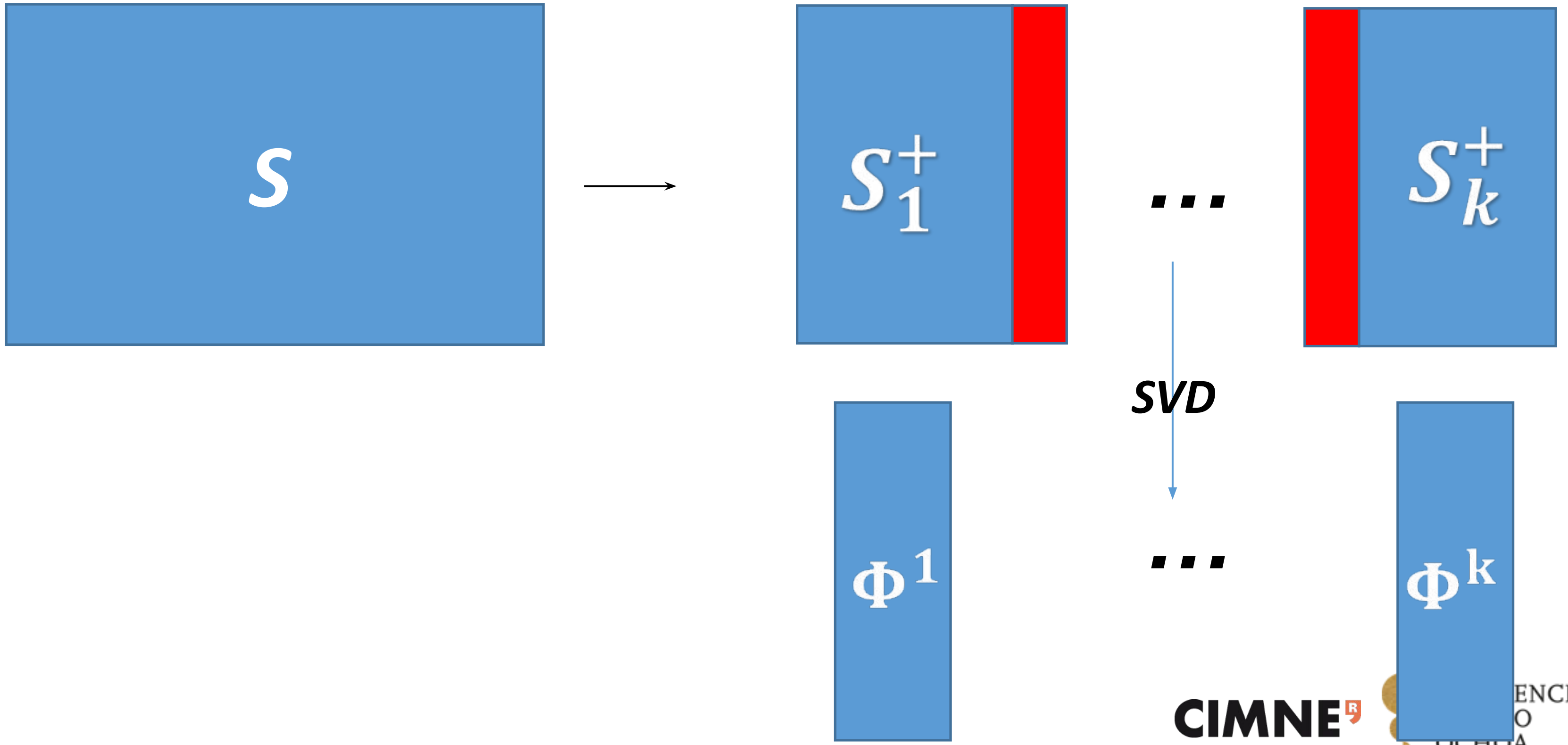


Local POD. Building multiple bases

- Use an unsupervised learning method to build clusters

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

2. Add some (very needed) overlapping $\boldsymbol{S_i^+ = overlap(S_i)}$



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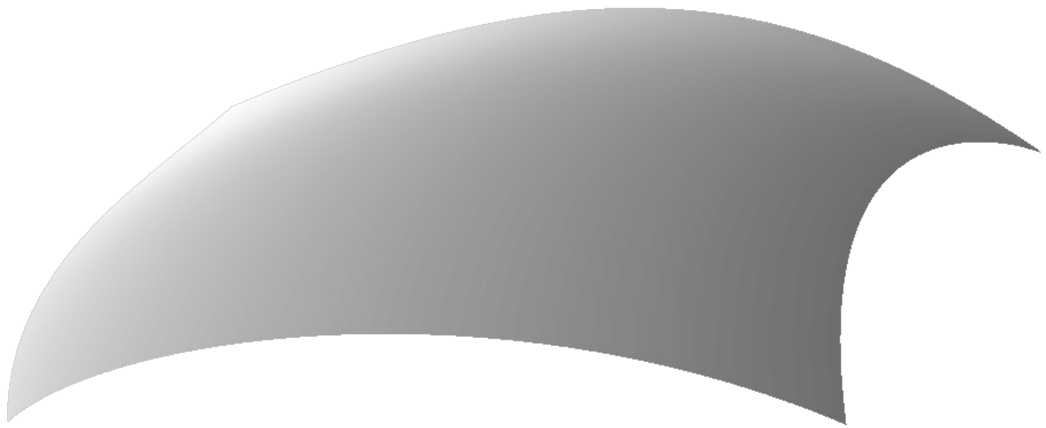
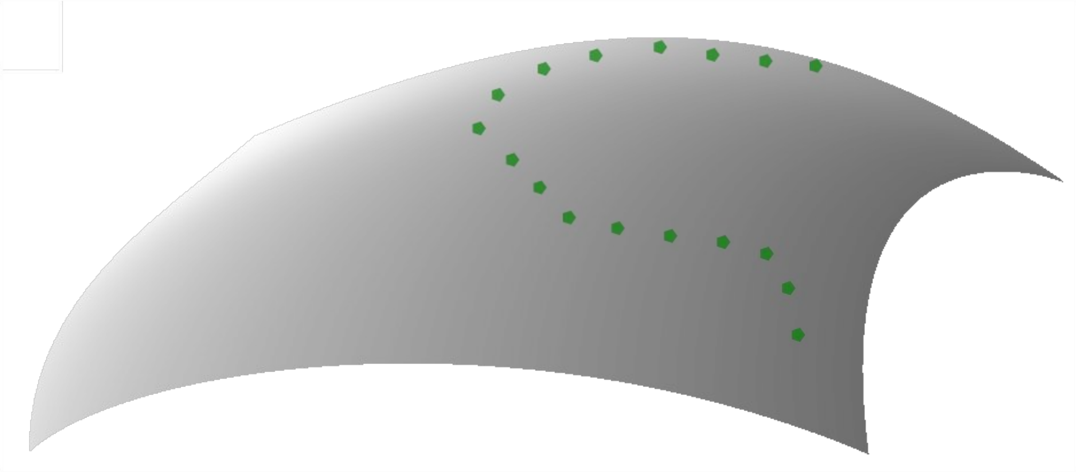
Local POD. Original Idea



(Farhat, 2012): doi.org/10.2514/6.2012-2686

Local POD. Original Idea



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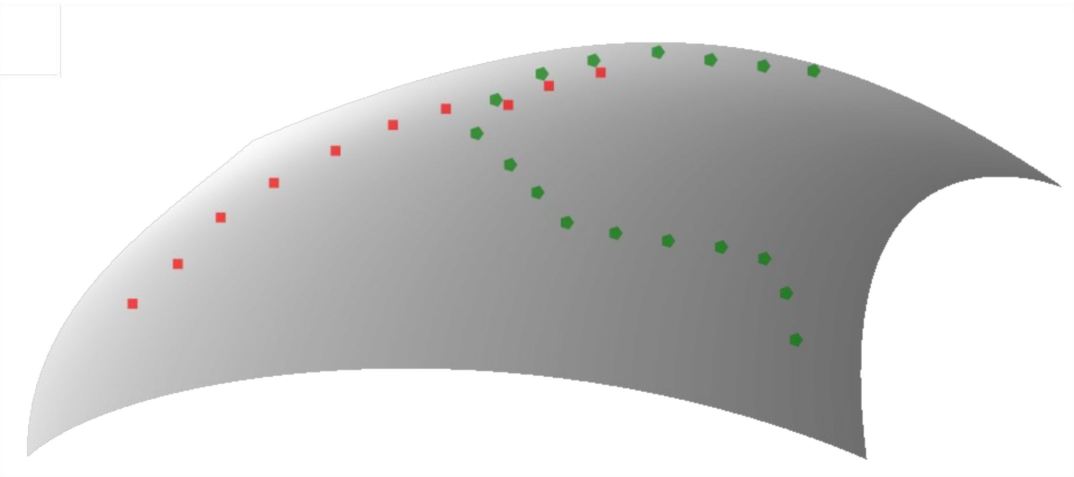
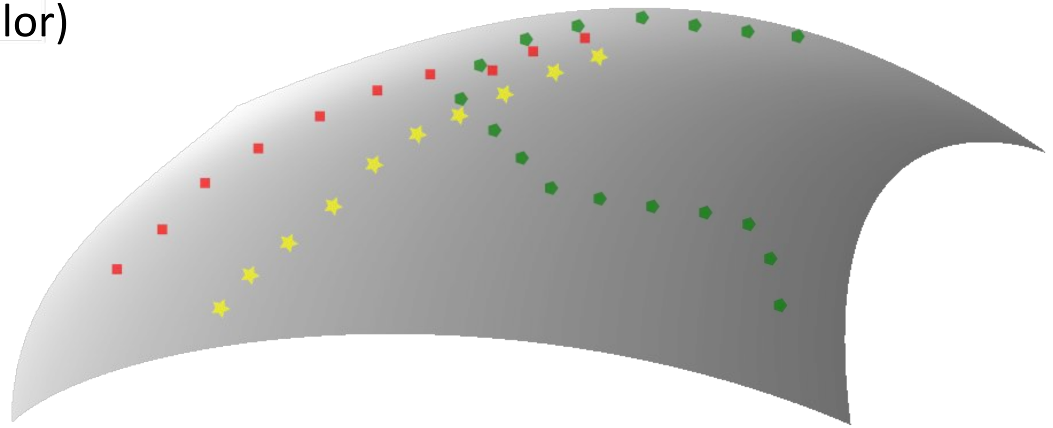
Local POD. Original Idea



(Farhat, 2012): doi.org/10.2514/6.2012-2686

Local POD. Original Idea

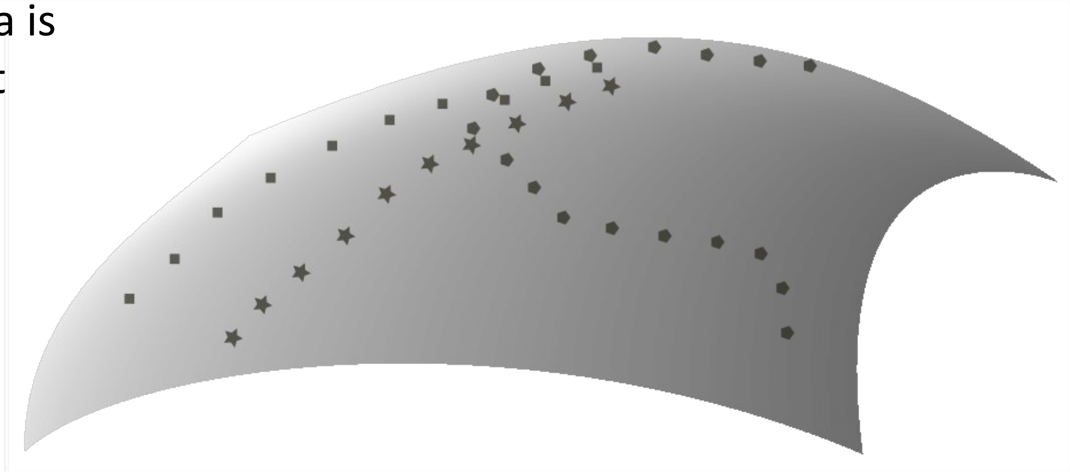
Training data is often collected in “training paths” (each indicated with a different color)



(Farhat, 2012): doi.org/10.2514/6.2012-2686

Local POD. Original Idea

BUT the origin of the data is
Forgotten at the moment
of mounting
The clusters



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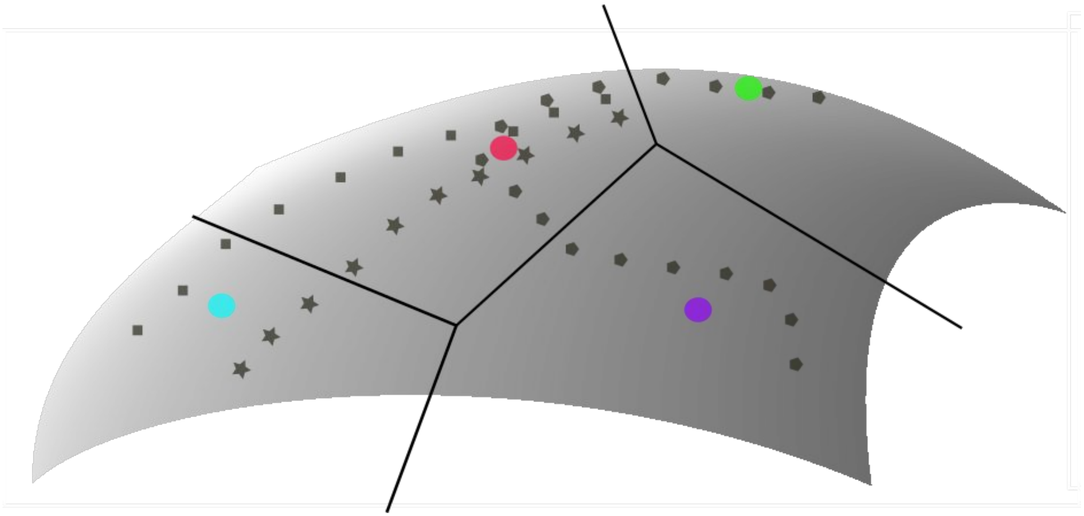
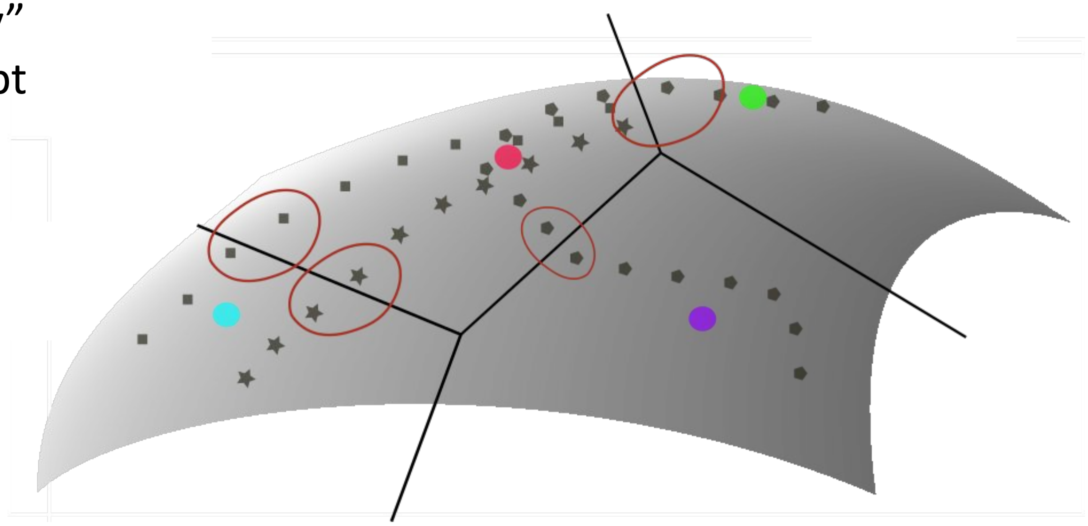
Local POD. Original Idea



(Farhat, 2012): doi.org/10.2514/6.2012-2686

Local POD. Original Idea

In the original idea "vicinity"
Is based only on the concept
Of distance



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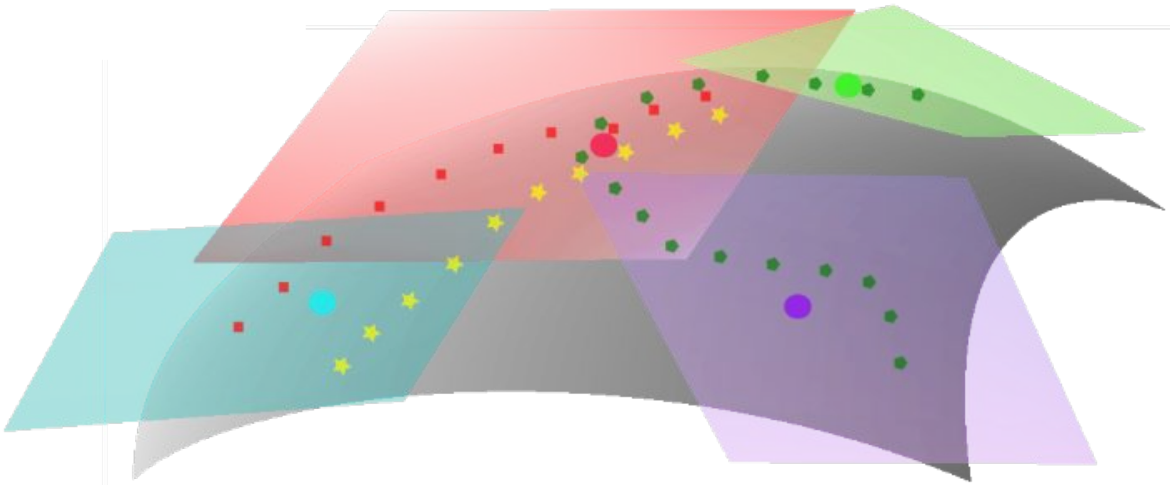
Local POD. Our overlapping proposal



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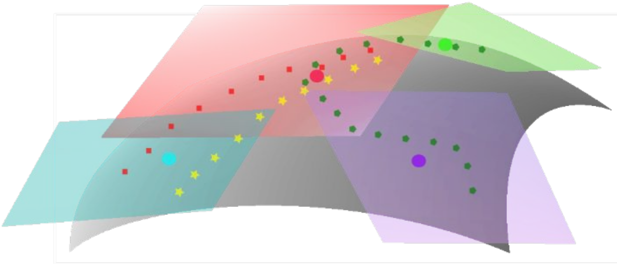

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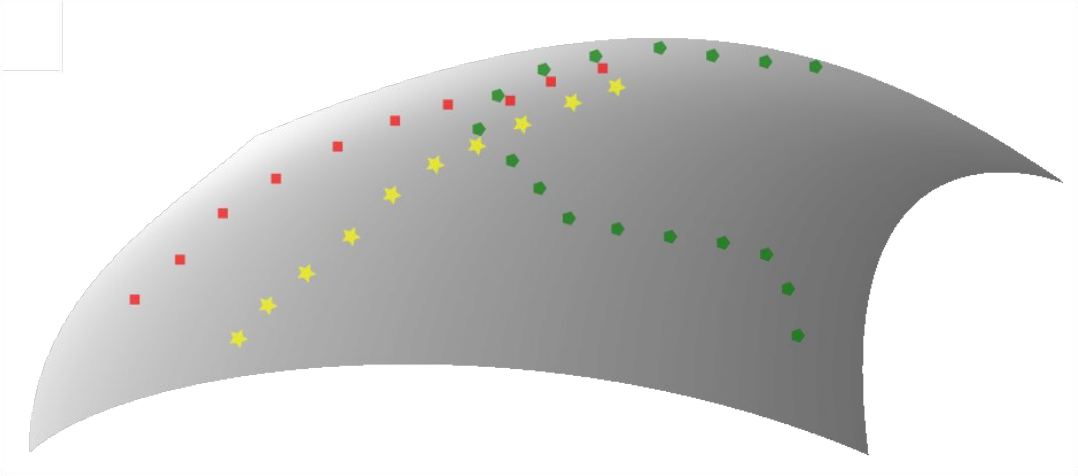
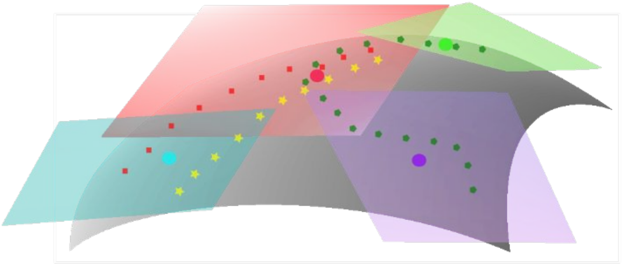


Our overlapping proposal

Local POD. Our overlapping proposal



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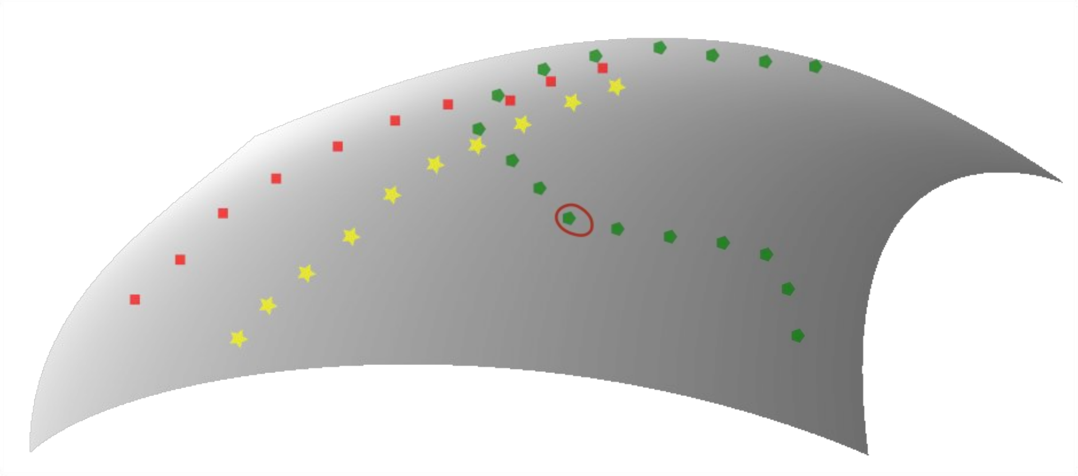
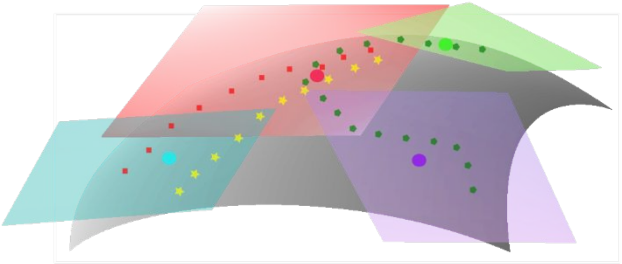


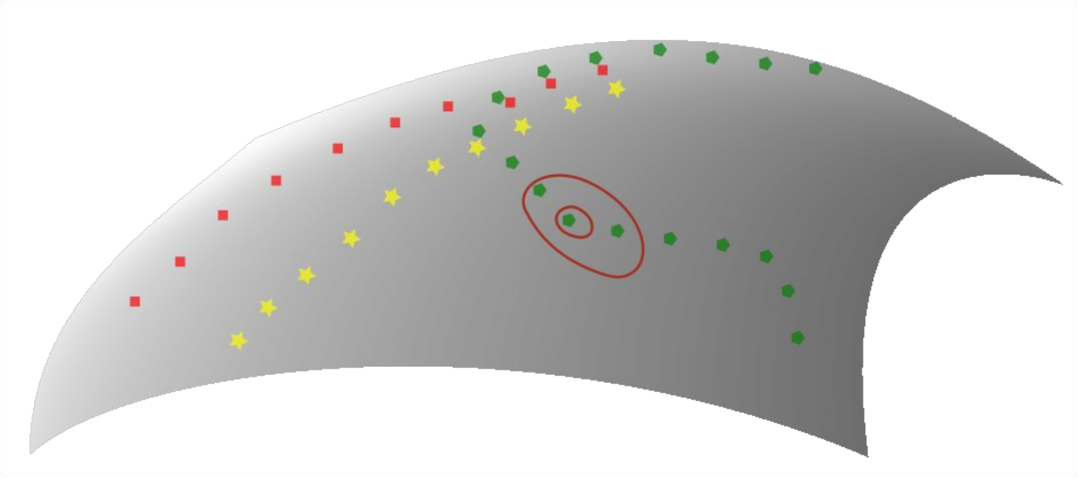
Our overlapping proposal

Local POD. Our overlapping proposal



(Farhat, 2012): doi.org/10.2514/6.2012-2686

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



Our overlapping proposal

Step1: we search for neighbours (In a LLE sense) within the training trajectories

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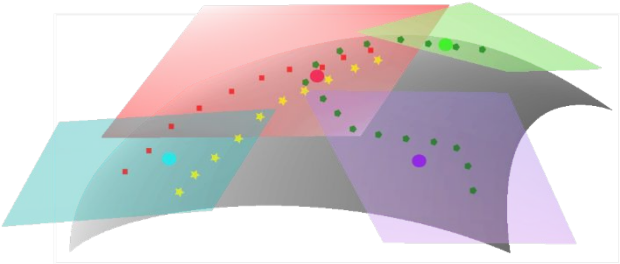
Local POD. Our overlapping proposal



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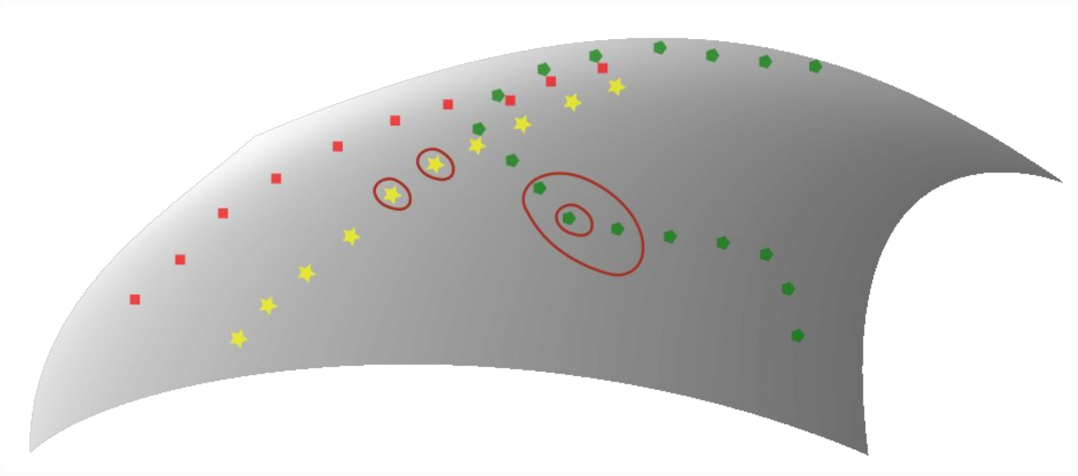

Our overlapping proposal

Step2: we search for neighbours outside of the training trajectories (neighbours in a LLE sense)

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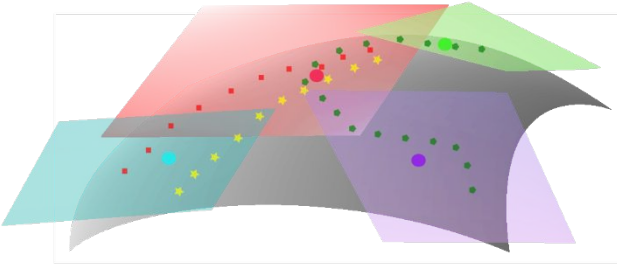
Local POD. Our overlapping proposal



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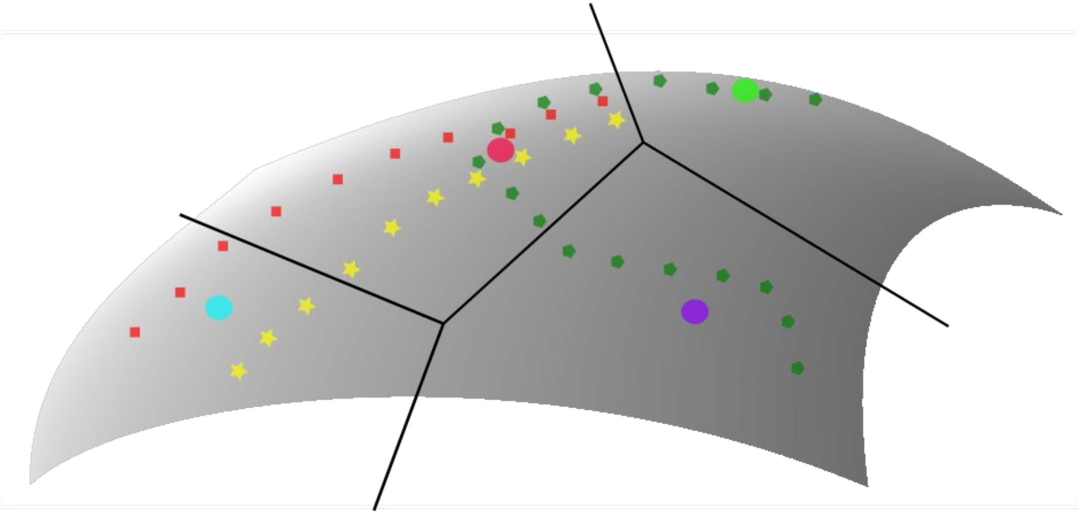
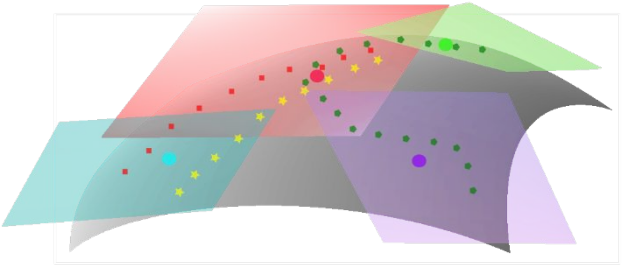


Our overlapping proposal

Local POD. Our overlapping proposal



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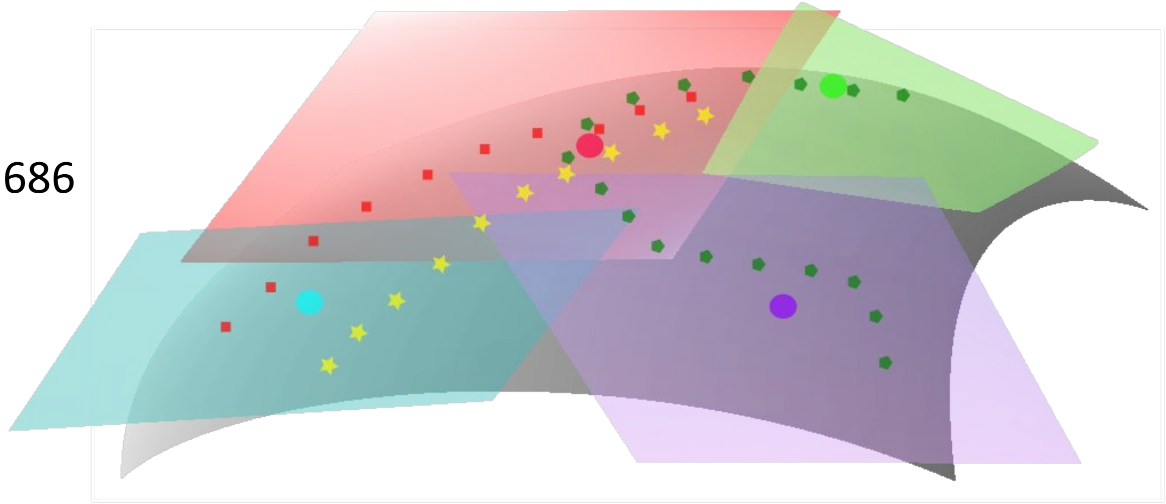
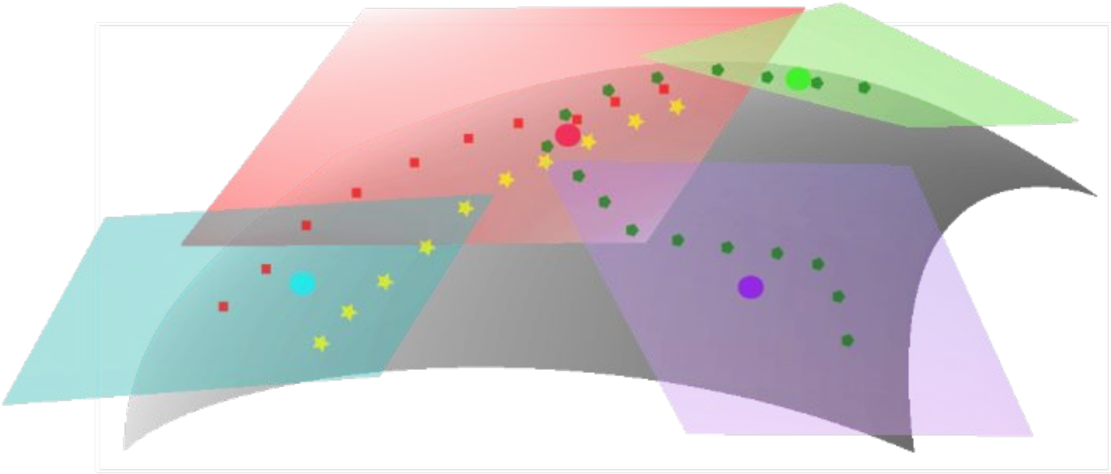


Our overlapping proposal

Local POD. Our overlapping proposal



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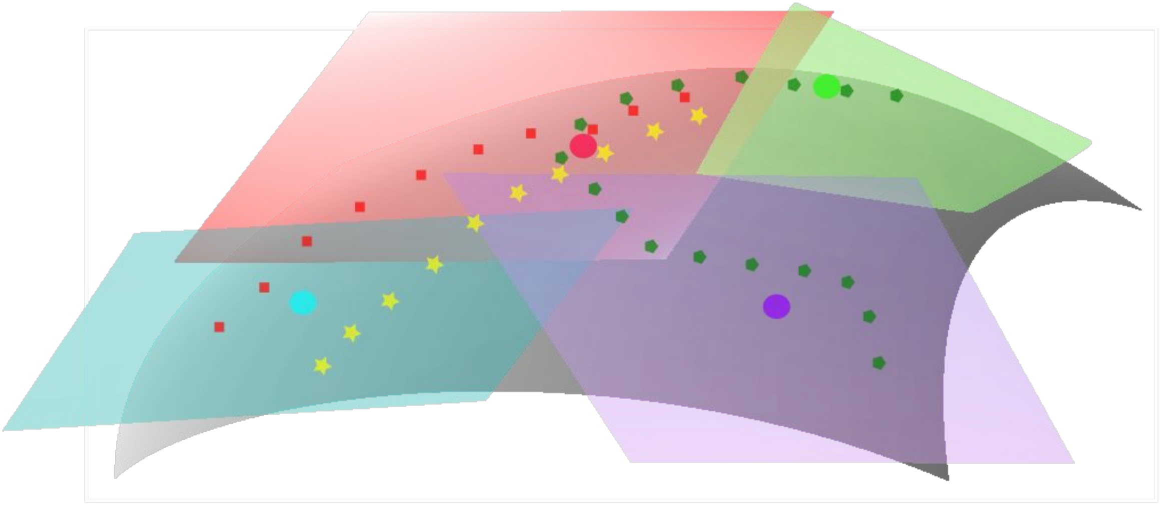
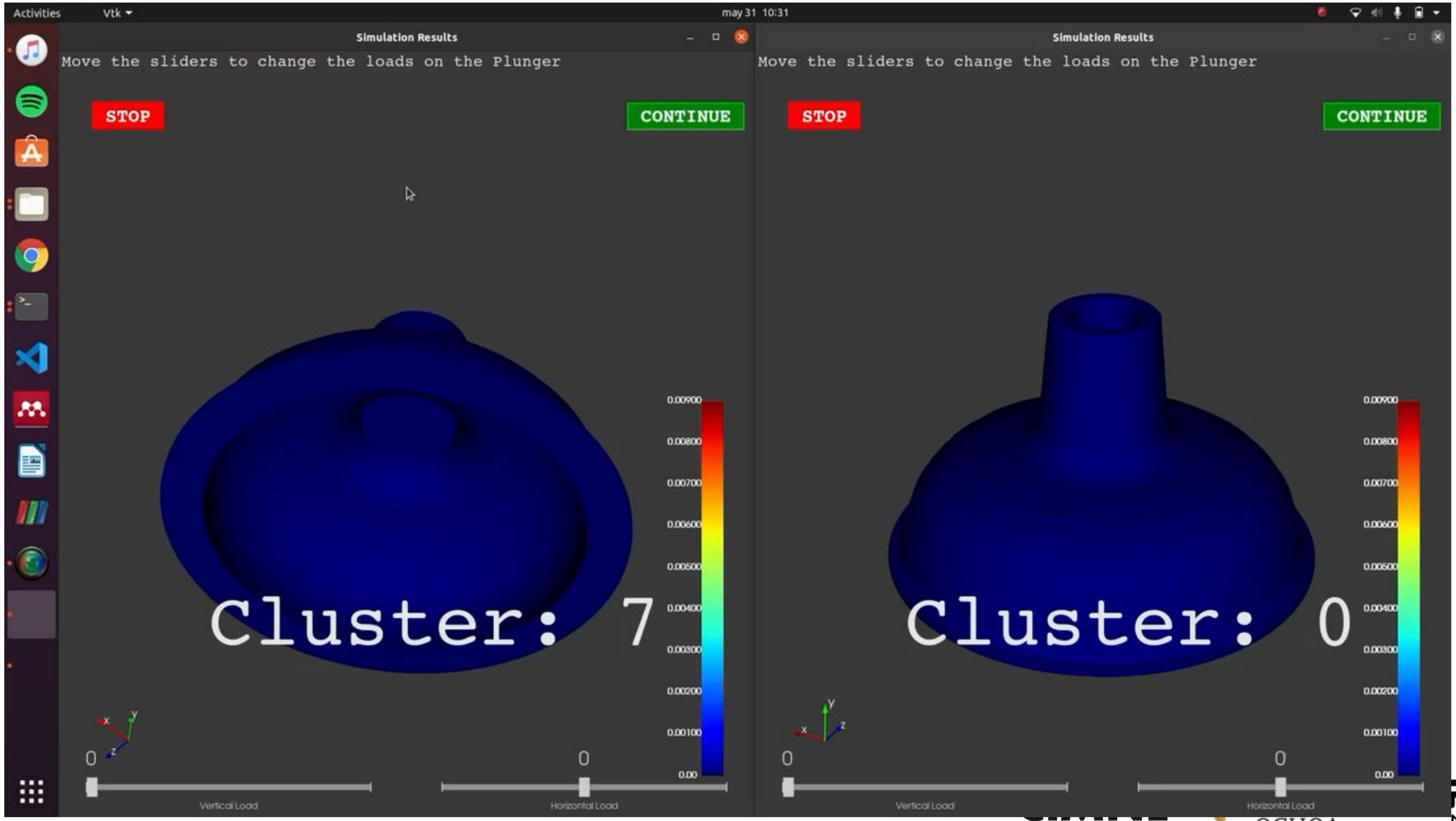


Our overlapping proposal

Local POD. Example 1

(Farhat, 2012): doi.org/10.2514/6.2012-2686

Our overlapping proposal



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 $\boldsymbol{S}_i^+ = \boldsymbol{overlap}(\boldsymbol{S}_i)$

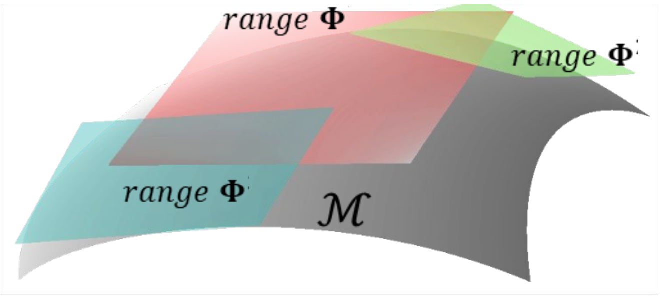
Each cluster $\boldsymbol{S}_i^+$ should consist on its snapshots, and the neighbours of its snapshots

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Classical Hyper-reduction

Reduced Order Model (ROM)

$$\Phi^{3^T} r(u_{old} + \Phi^3 q; \mu) = 0$$



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

G_3

G_1

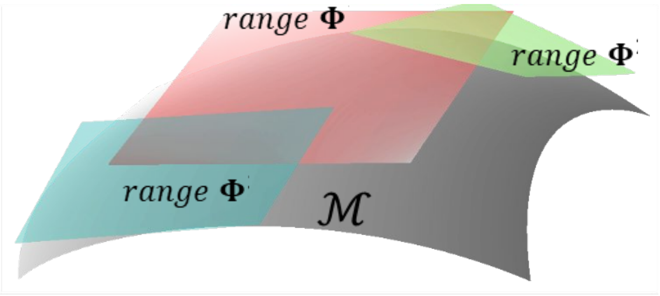
G_2

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Classical Hyper-reduction

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^{1^T} \boldsymbol{r}(\boldsymbol{u}_{old} + \boldsymbol{\Phi}^1 \mathbf{q}; \boldsymbol{\mu}) = \mathbf{0}$$



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

G_3

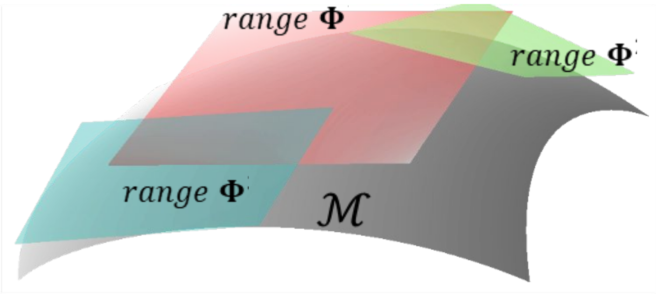
G_1

G_2

Local POD. Classical Hyper-reduction

Reduced Order Model (ROM)

$$\Phi^{2^T} \boldsymbol{r}(u_{old} + \Phi^2 \mathbf{q}; \mu) = \mathbf{0}$$



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

Classical approach: unique set of weights

G_3
G_1
G_2

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Classical Hyper-reduction

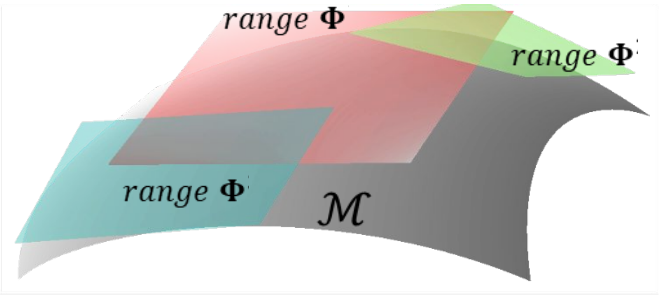
Reduced Order Model (ROM)

$$\Phi^{2^T} \boldsymbol{r}(u_{old} + \Phi^2 \mathbf{q}; \boldsymbol{\mu}) = 0$$

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

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

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



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

Classical approach: unique set of weights

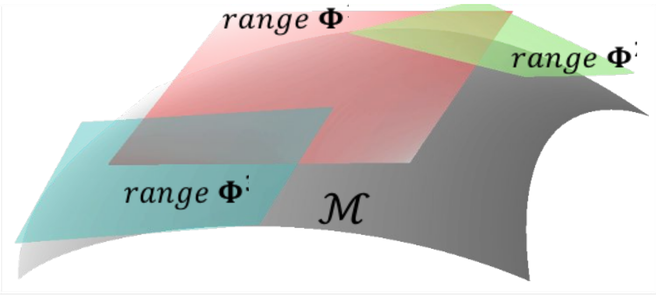
Local POD. Classical Hyper-reduction

Number of clusters **Number of elements**

Local POD. Improved hyper-reduction

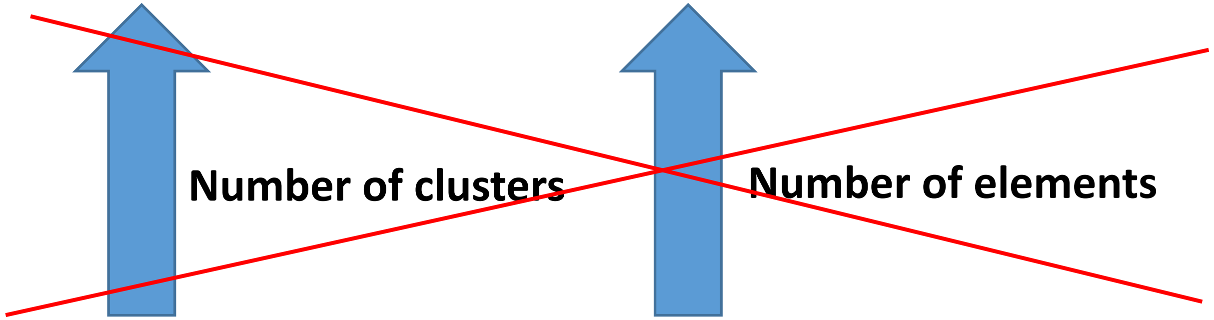
Reduced Order Model (ROM)

$$\Phi^{k^T} r\left(\mathbf{u}_{\text{old}} + \Phi^k q; \mu\right) = 0$$

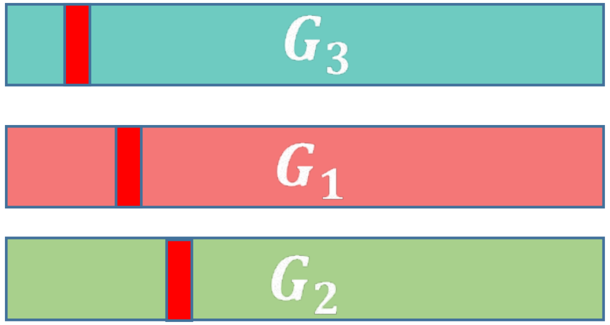


$$G = G(\Phi, R)$$

Expectation:



Our approach: **hyperreduced basis remains the same, but weights change!**



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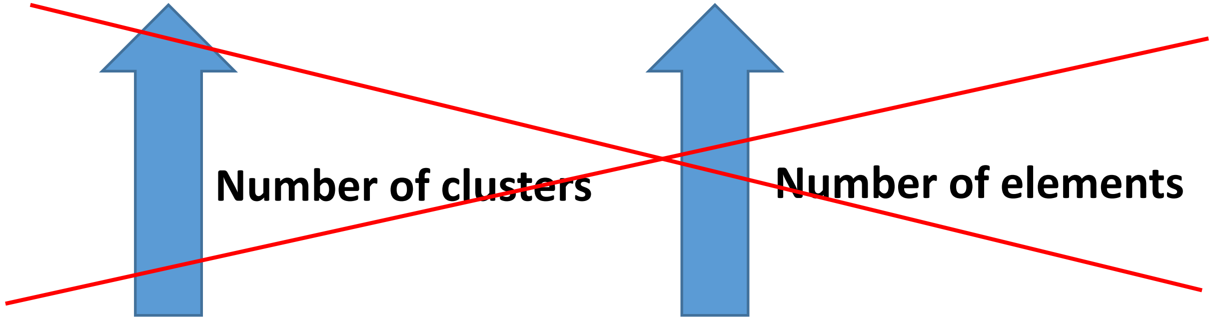
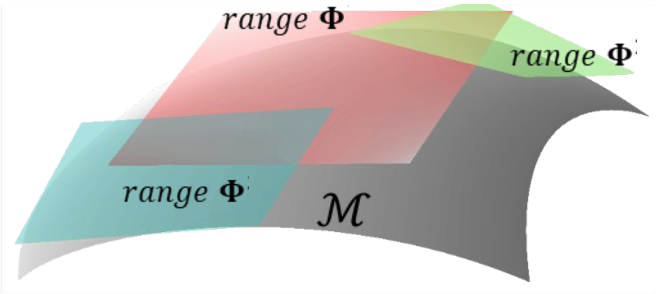
Local POD. Improved hyper-reduction

Reduced Order Model (ROM)

$$\Phi^{k^T} \boldsymbol{r}(\mathbf{u}_{\text{old}} + \Phi^k \boldsymbol{q}; \boldsymbol{\mu}) = \mathbf{0}$$

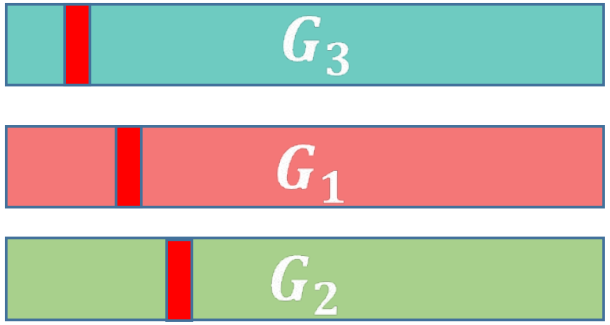
Expectation:





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

Our approach: **hyperreduced basis remains the same, but weights change!**



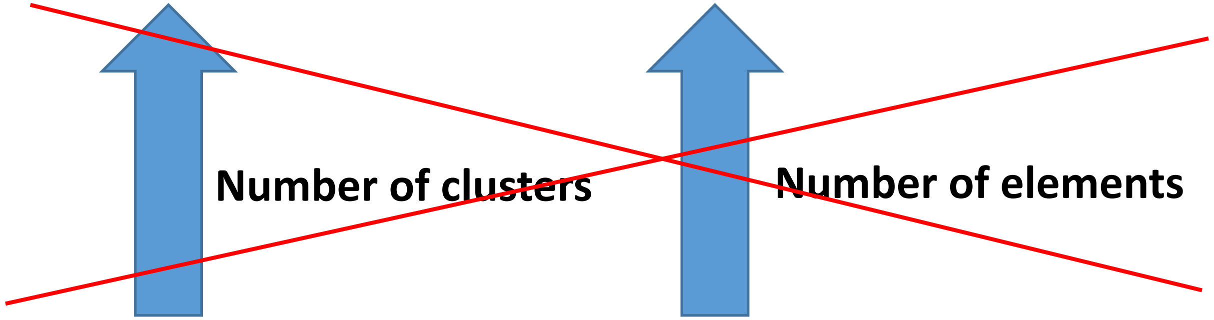
CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Improved hyper-reduction

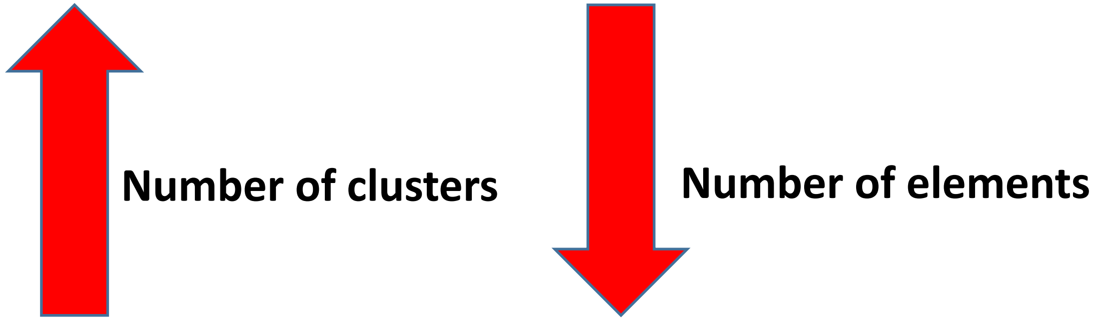
Reduced Order Model (ROM)

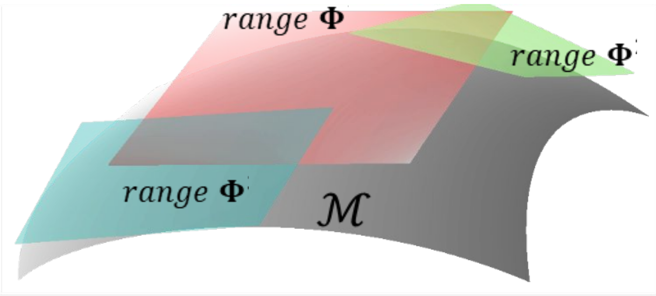
$$\Phi^{k^T} r\left(\mathbf{u}_{\text{old}} + \Phi^k q; \mu\right) = 0$$

Expectation:



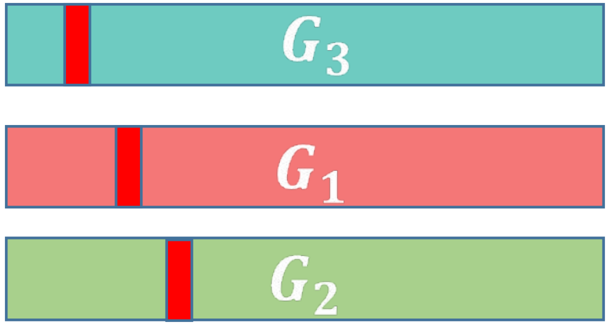
In reality:





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

Our approach: **hyperreduced basis remains the same, but weights change!**

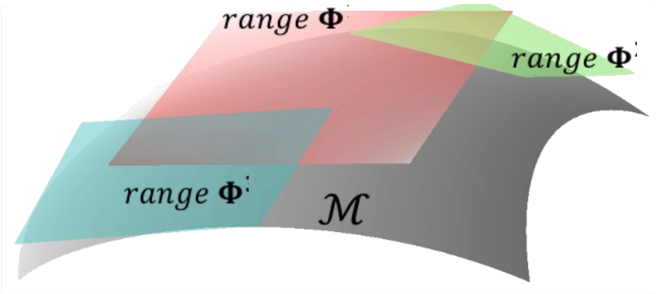


CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Improved hyper-reduction

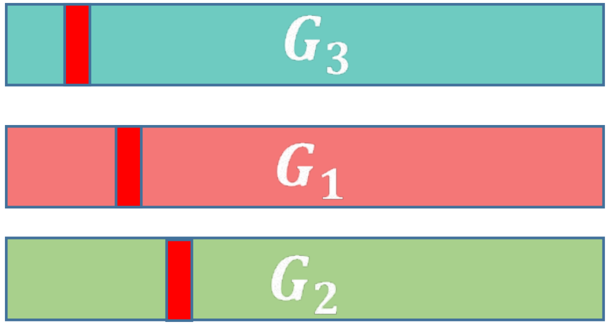
Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^{k^T} \boldsymbol{r}\left(\mathbf{u}_{\text{old}} + \boldsymbol{\Phi}^k \boldsymbol{q}; \boldsymbol{\mu}\right) = \mathbf{0}$$



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

Our approach: **hyperreduced basis remains the same, but weights change!**

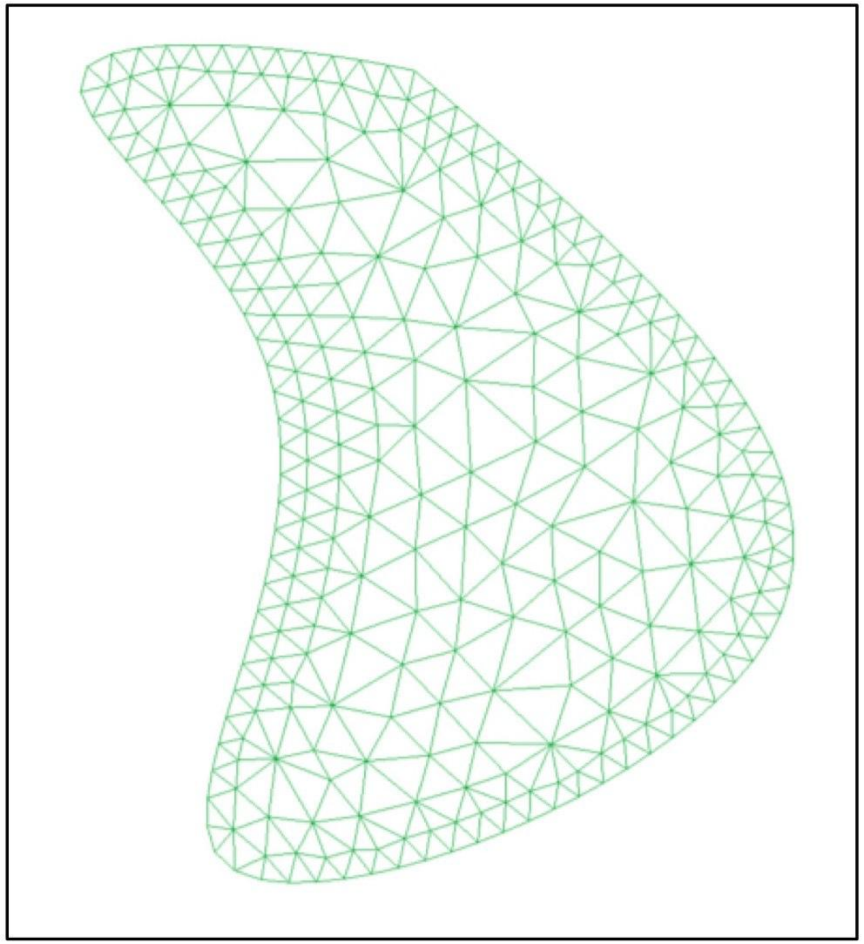


$$(\boldsymbol{E}, \widehat{\boldsymbol{W}}) = \arg min \left\| \sum_{i=1}^{n} \boldsymbol{g}_i^k - \sum_{i \in E} \boldsymbol{g}_i^k \widehat{\boldsymbol{\omega}}_i \right\|_2^2$$

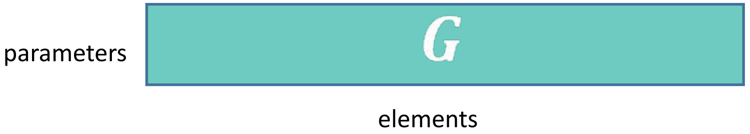
$$s.t. \quad \widehat{\omega}_i \geq 0$$

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

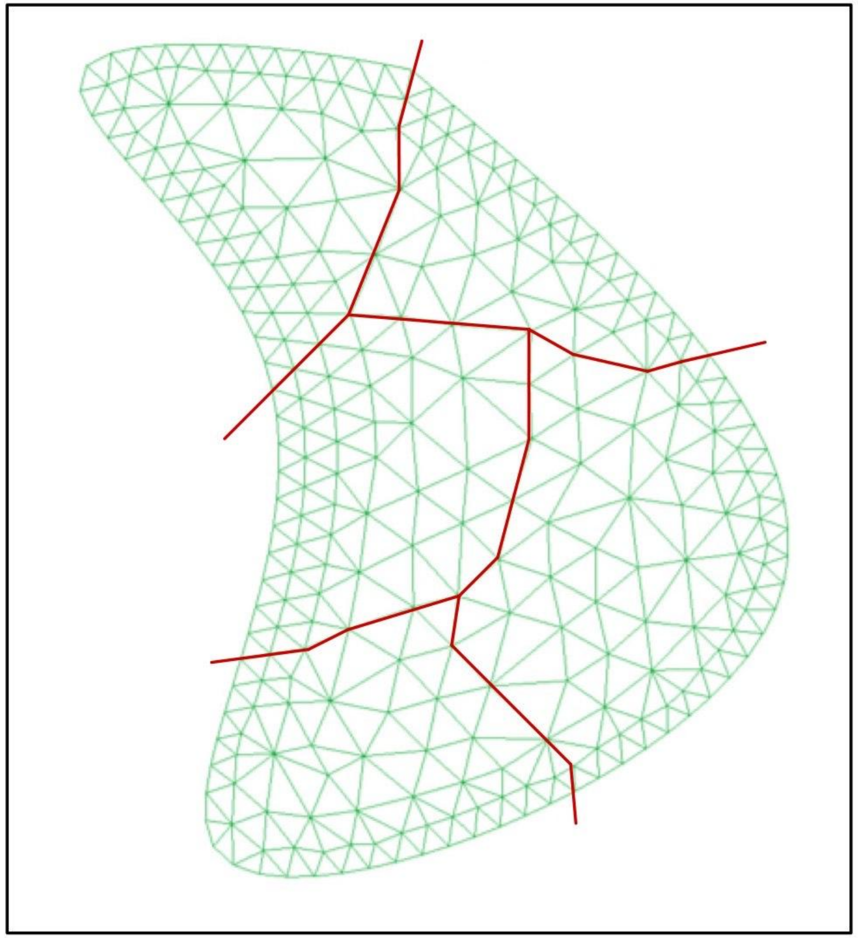
Local POD. Parallelisation of ECM



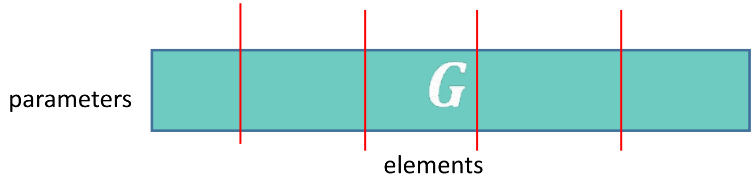
$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi}, \boldsymbol{R})$$



Local POD. Parallelisation of ECM



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



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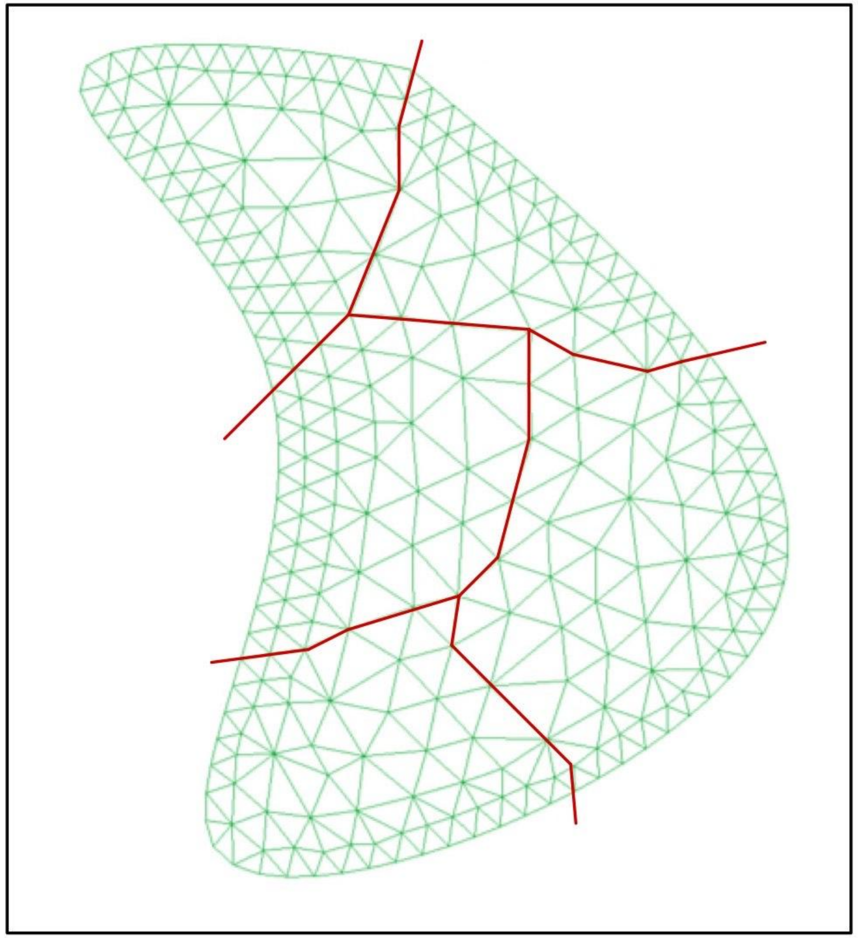
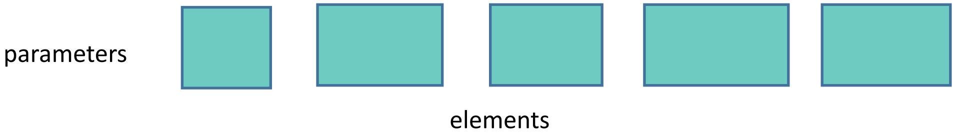
Local POD. Parallelisation of ECM

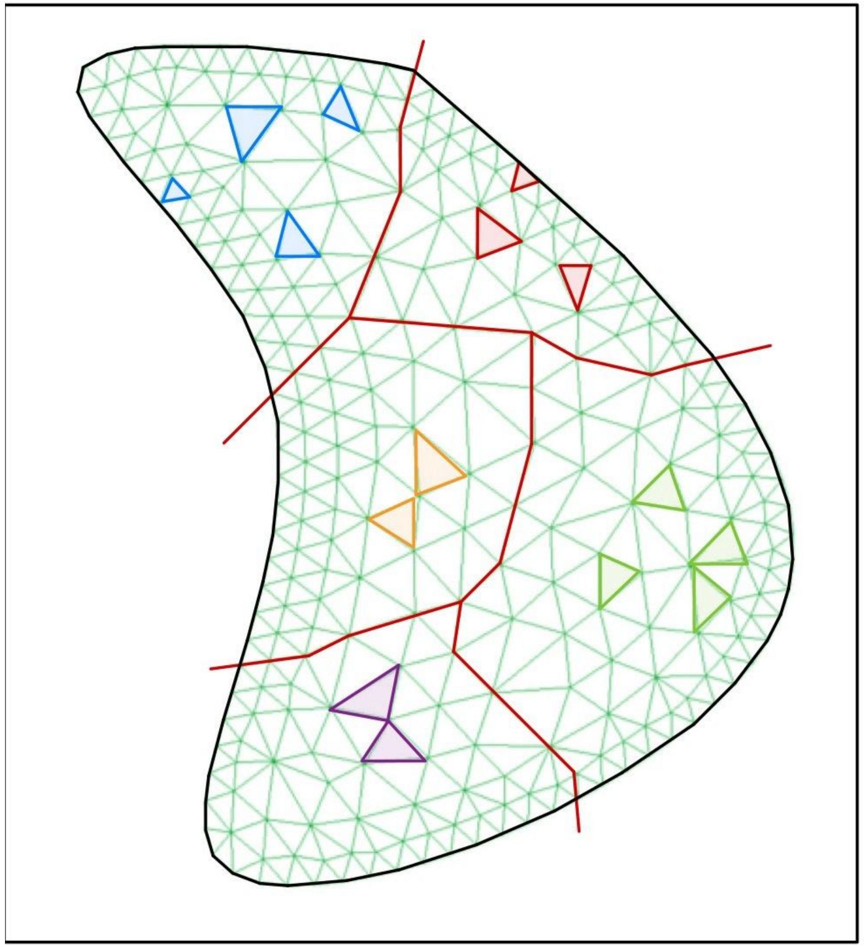


$$(\boldsymbol{E},\boldsymbol{W}) = ECM(\boldsymbol{G})$$

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



Local POD. Parallelisation of ECM



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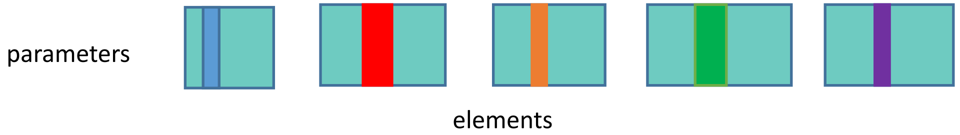
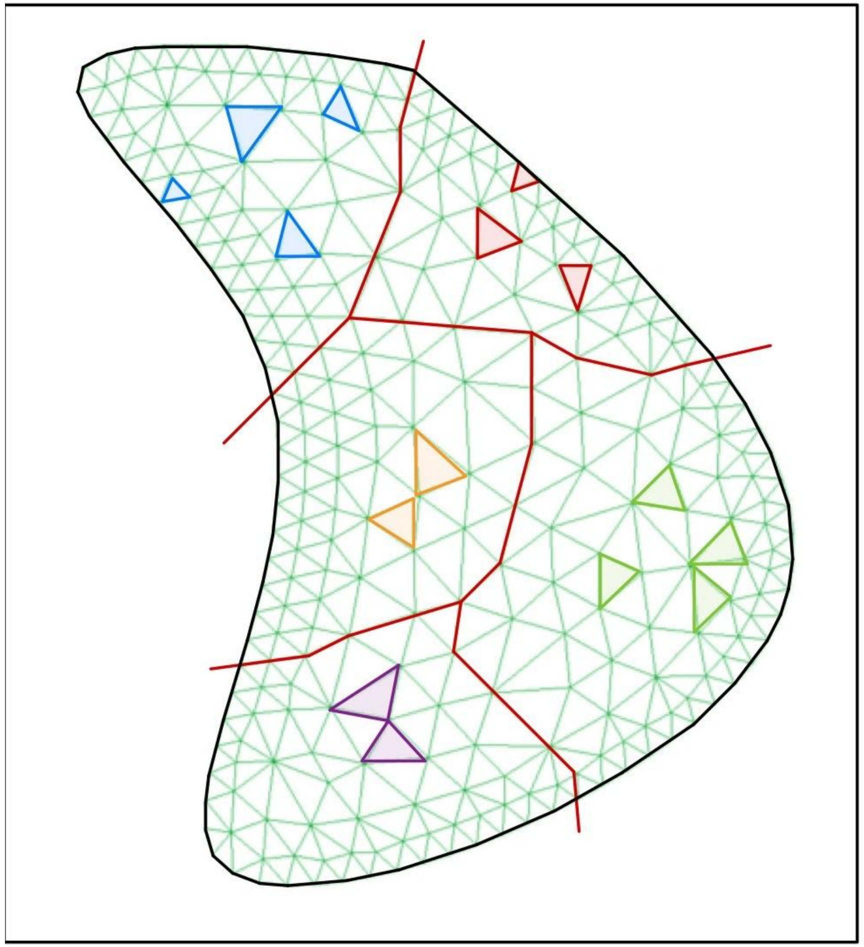


Local POD. Parallelisation of ECM



$$(\boldsymbol{E}, \boldsymbol{W}) = ECM(\boldsymbol{G})$$

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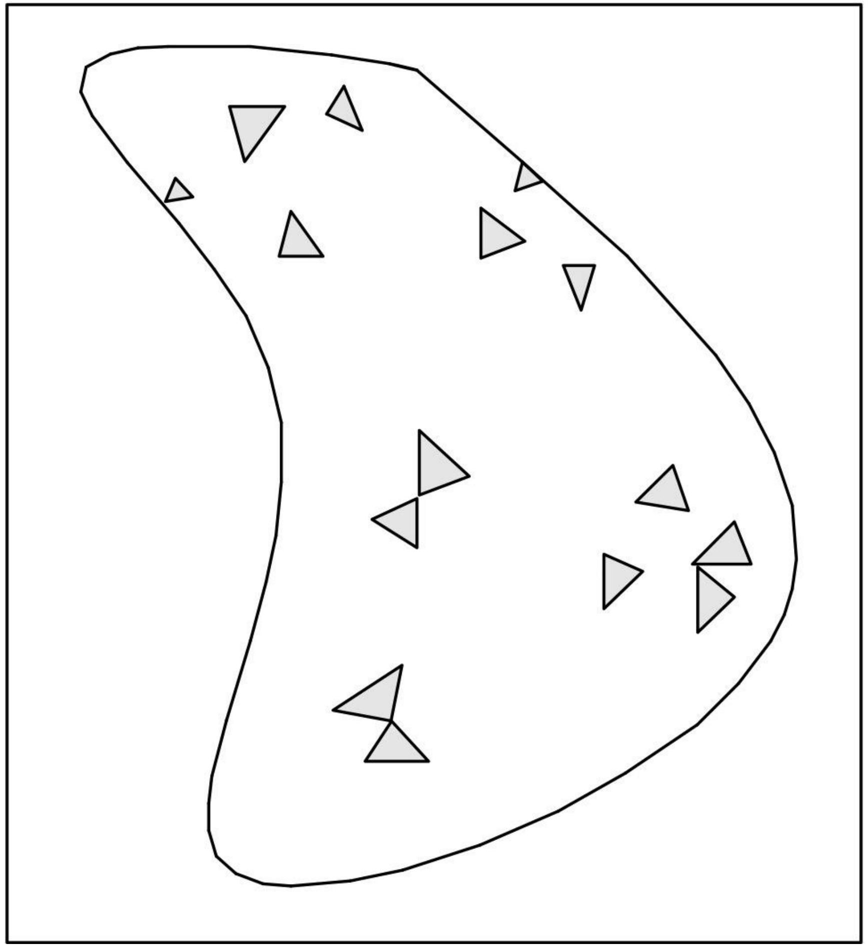
Local POD. Parallelisation of ECM



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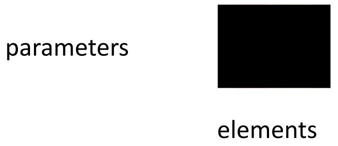
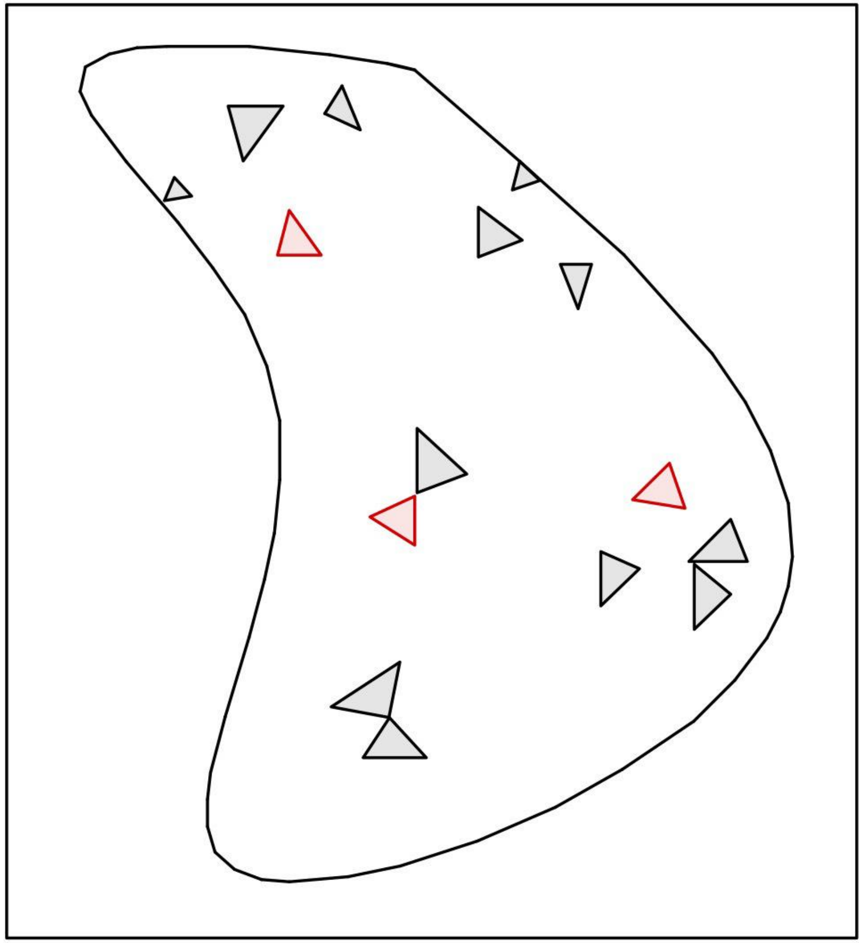
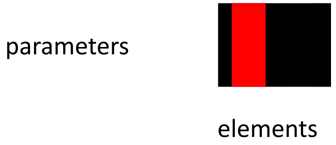


Local POD. Parallelisation of ECM

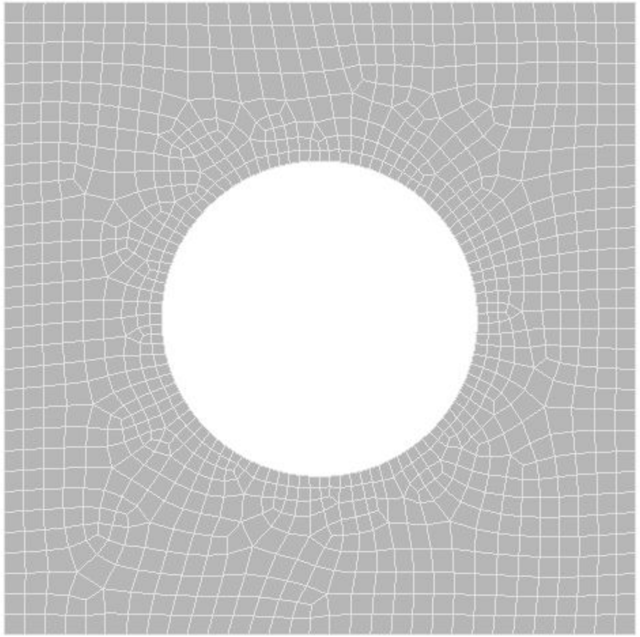


$$(\boldsymbol{E}, \boldsymbol{W}) = ECM(\boldsymbol{G})$$

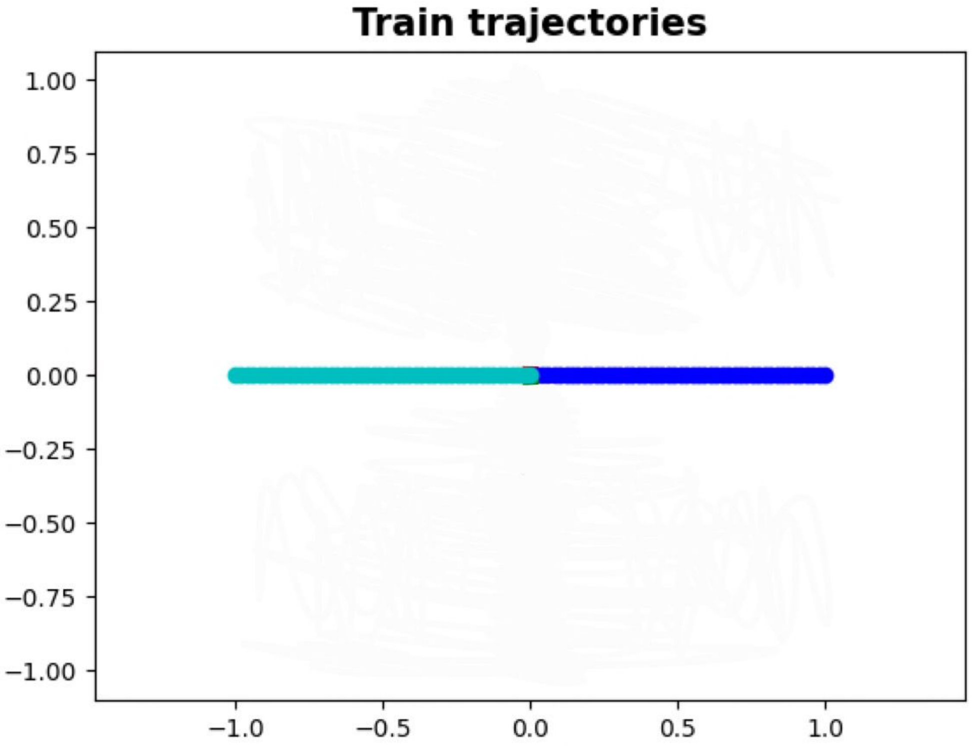
$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi}, \boldsymbol{R})$$



Local POD. Example 2



ϵ_x

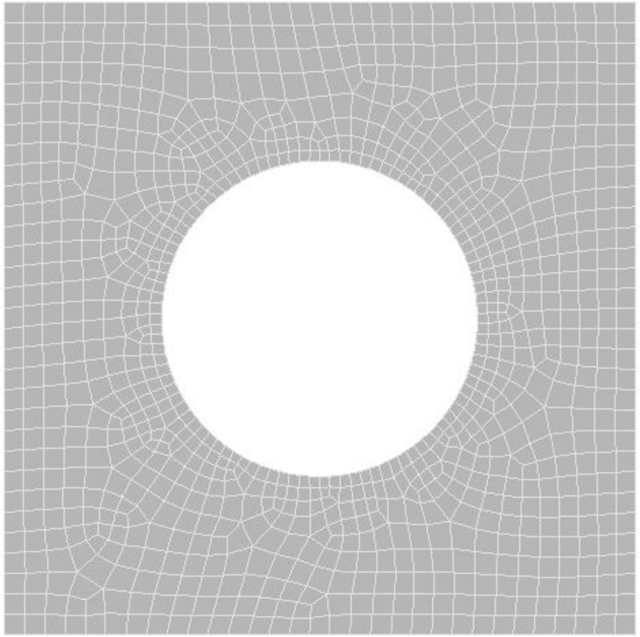


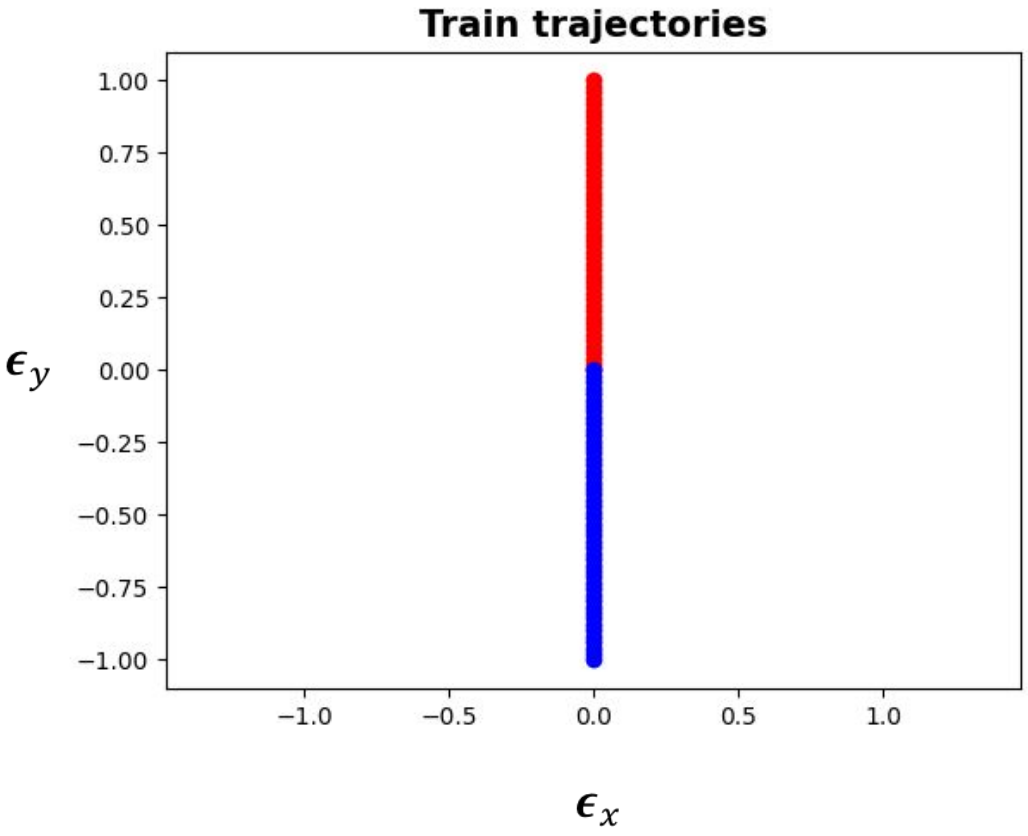
ϵ_y

ϵ_x

Local POD. Example 2

ϵ_y





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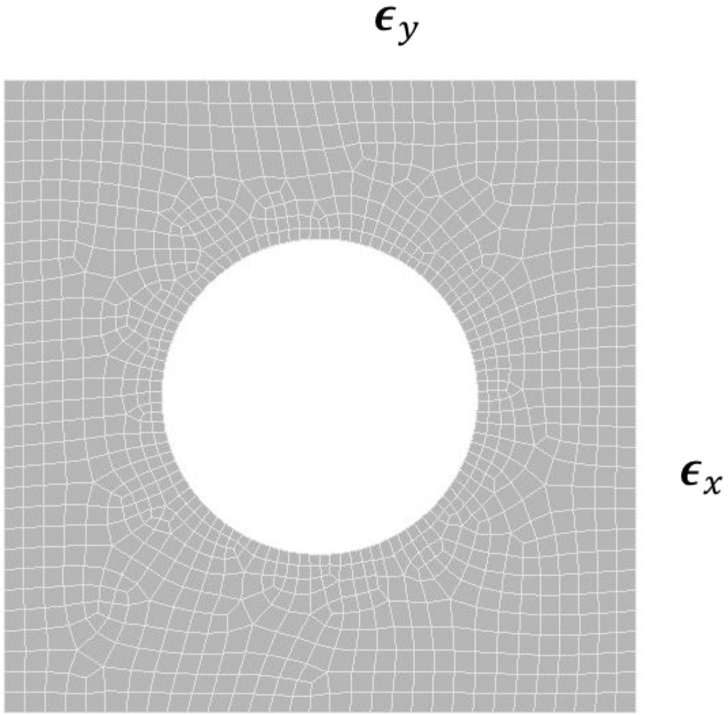
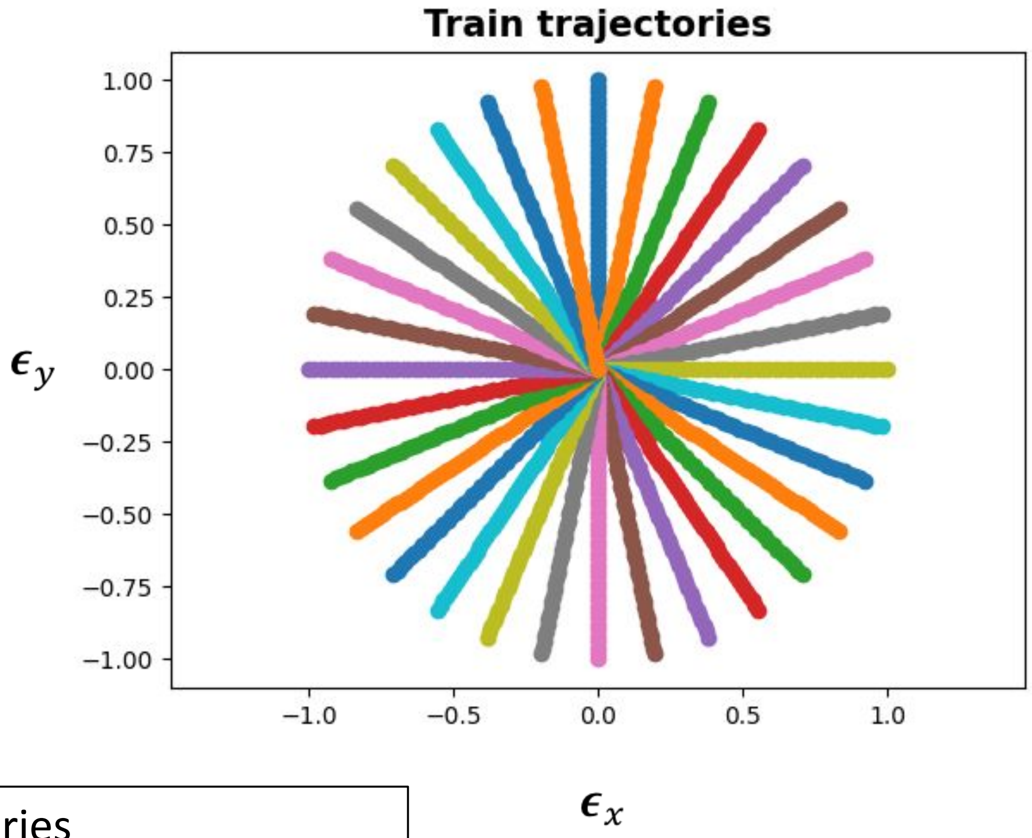
Local POD. Example 2





32 trajectories
50 snapshots per trajectory
1600 snapshots

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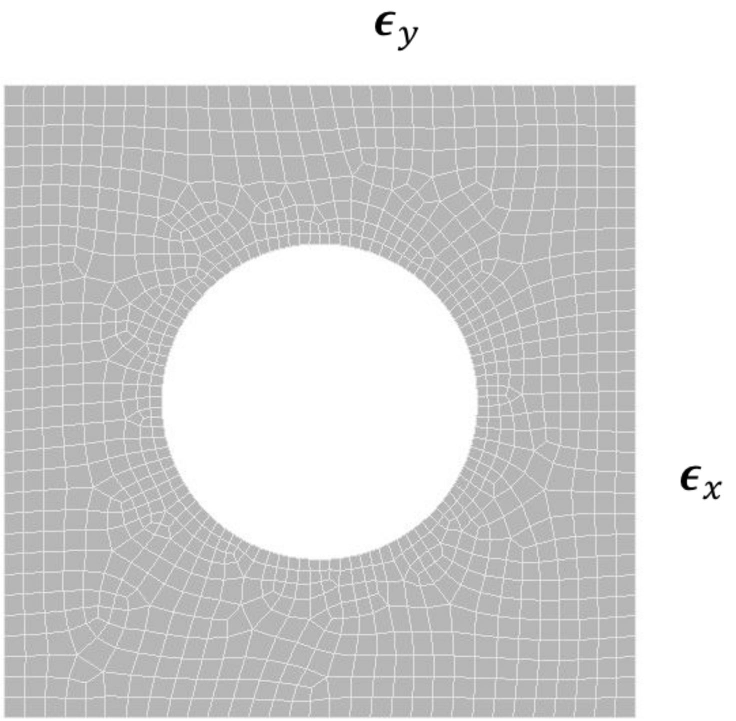
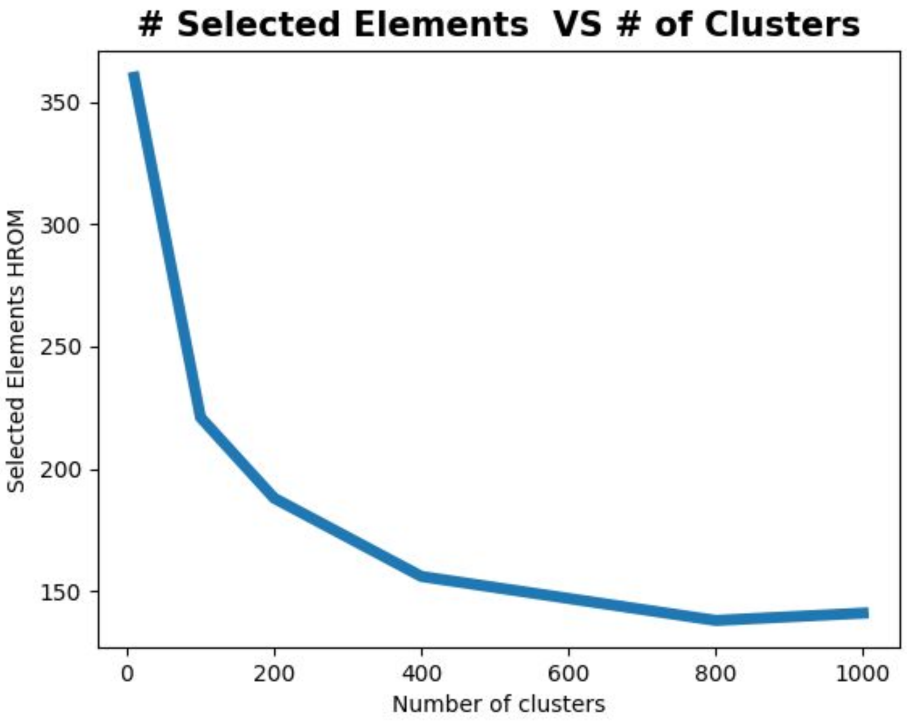
Local POD. Example 2

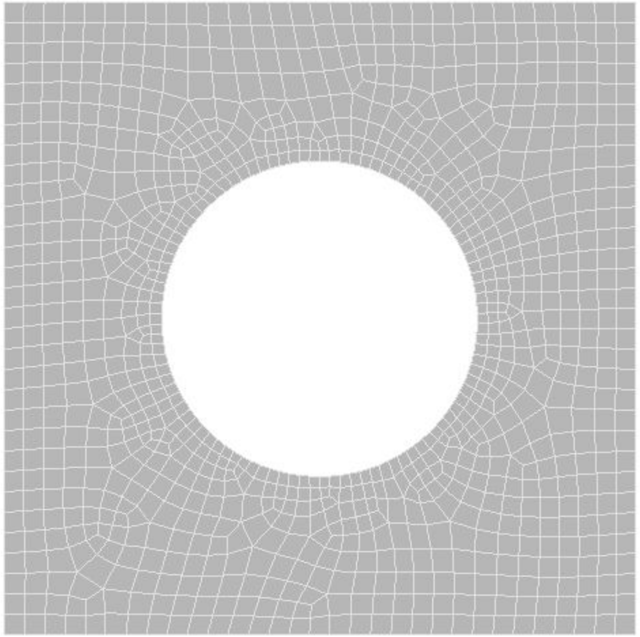




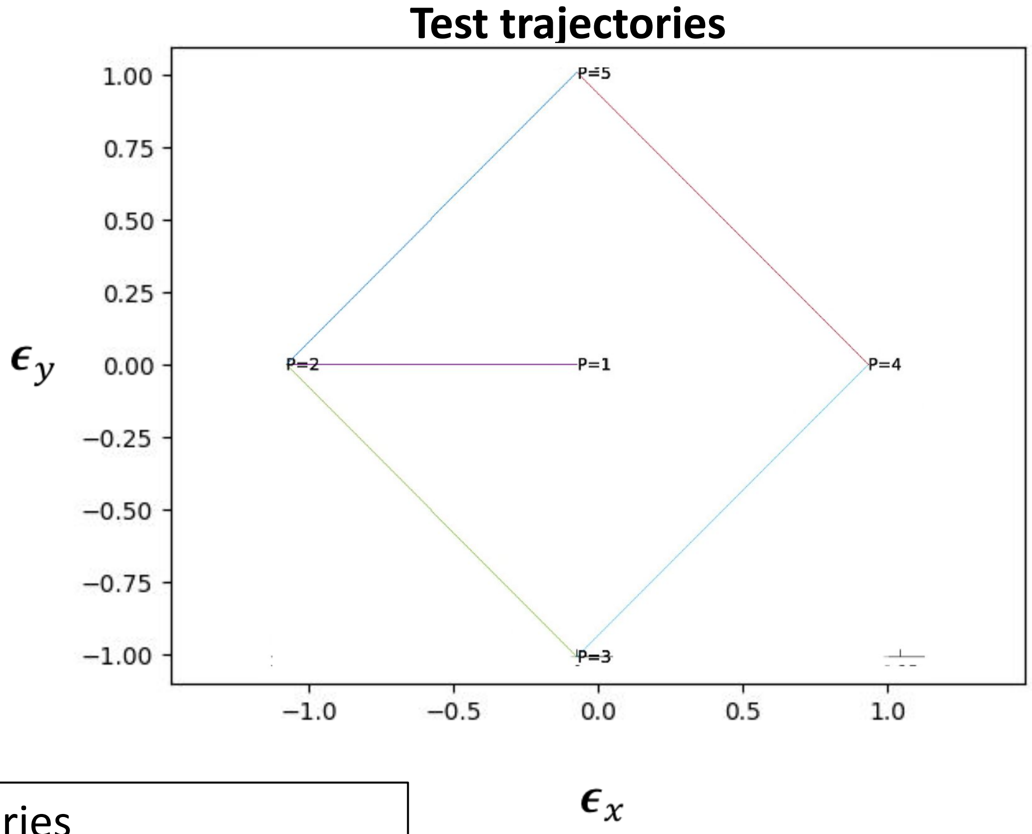
32 trajectories
50 snapshots per trajectory
1600 snapshots

Local POD. Example 2

ϵ_y



ϵ_x



32 trajectories
50 snapshots per trajectory
1600 snapshots

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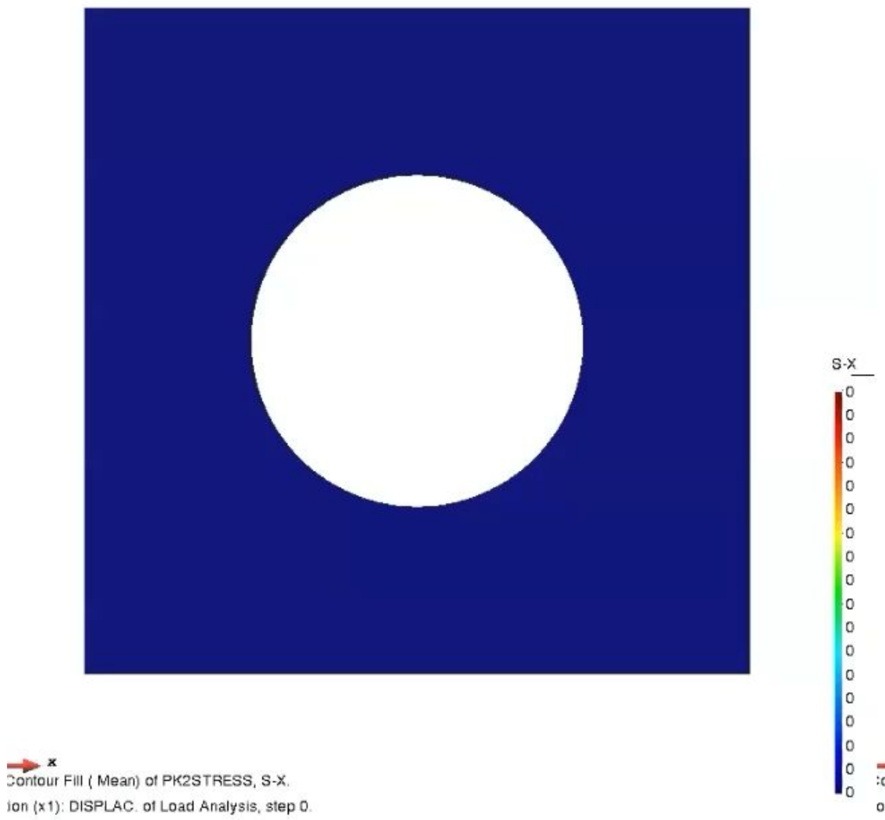
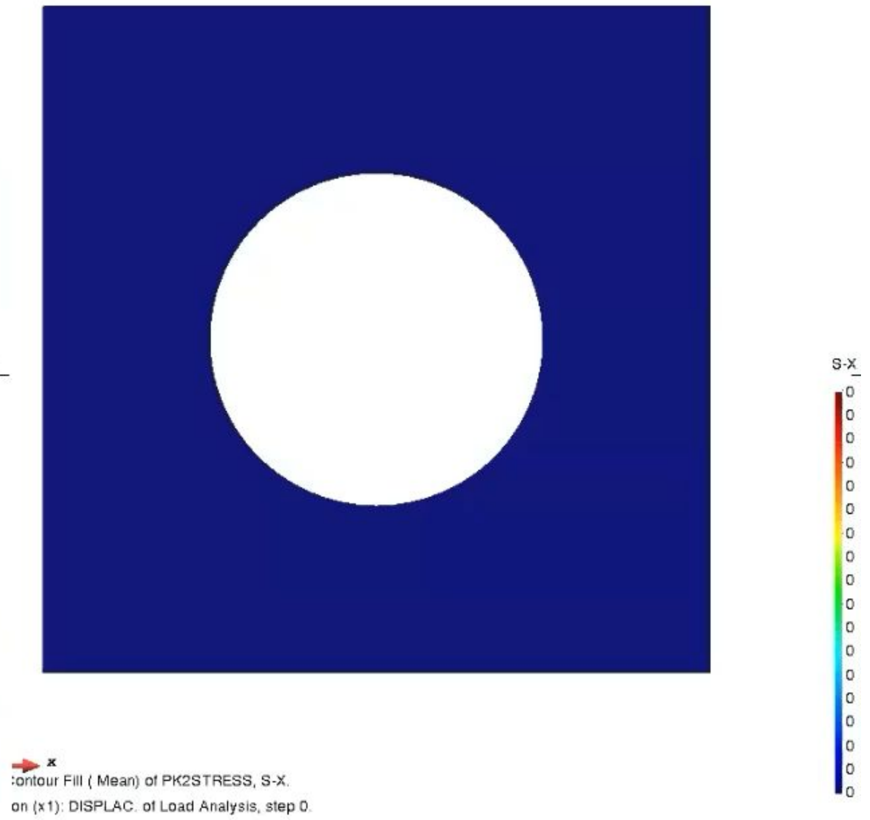
Local POD. Example 2

FOM

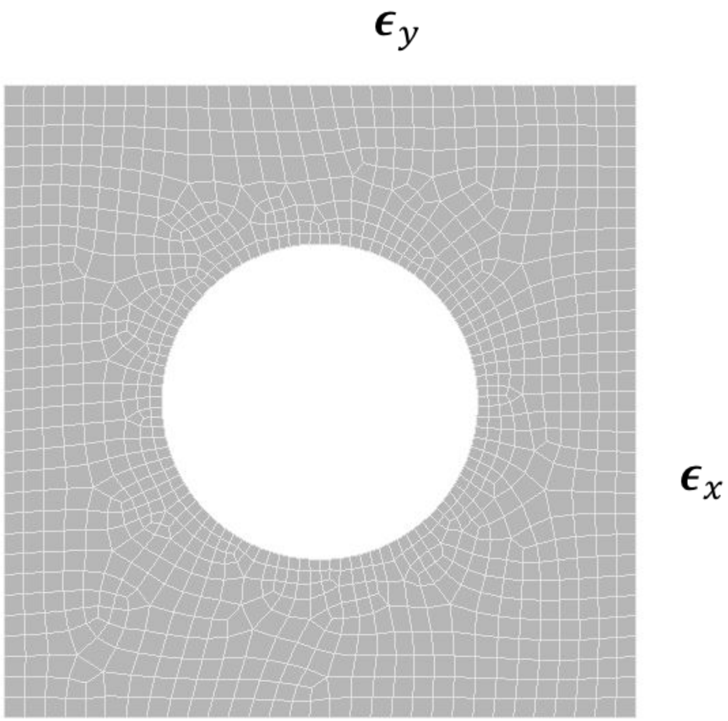


HROM



CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

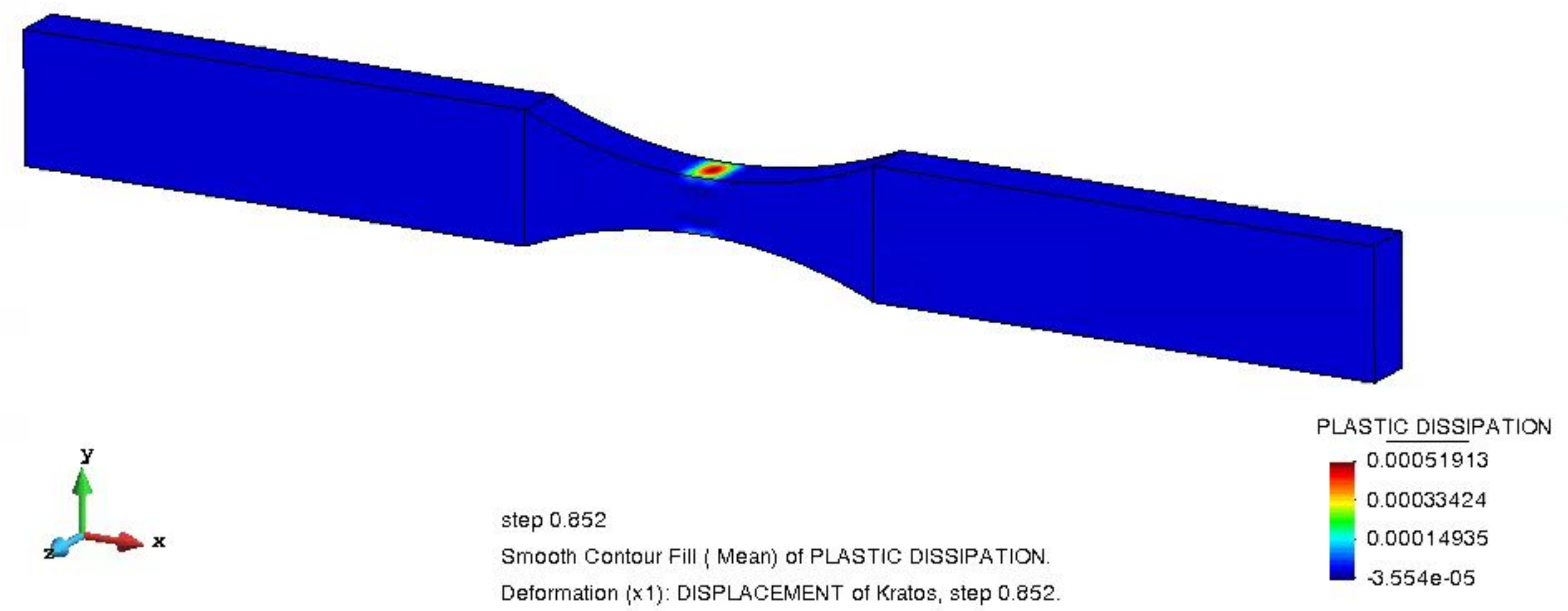
Local POD. Example 2



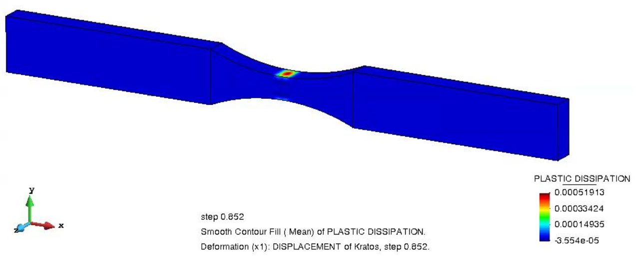
10X less elements required compared with a single basis

5X less modes required compared with a single basis

Local POD. Example 3



Local POD. Example 3



	POD	Local POD
Basis size	260 modes	10 basis ~30 modes
HROM elements	400	240(~150 per basis)
Simulation time	1234 seg	90 seg
L2 error	1e-3%	1e-3%

13X faster than POD

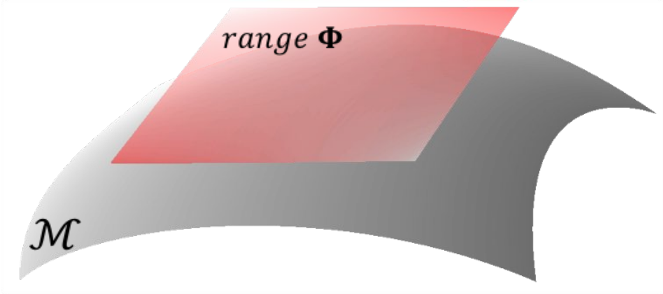
Local POD. Strengths and weaknesses

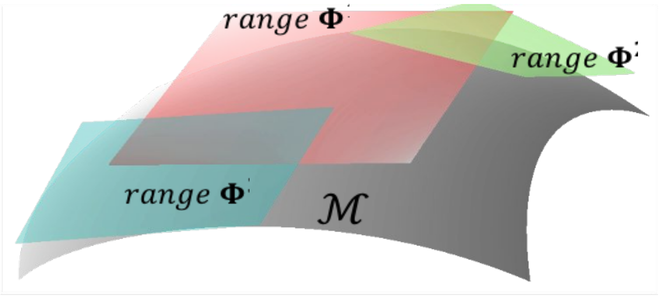
- Reasonable overhead in training and negligible in inference
- Smaller bases and elements sets, therefore faster ROMs

- Still Easy to overfit to training trajectories …but at least a warning can be issued when too many neighbours are found in the clustering algorithm

General conclusions

- The Local POD was presented
  - Taking into account the training paths in the choice of overlapping is important
  - More clusters => smaller basis & smaller integration overhead
- Future work:
  - application of method to multiple escenarios
  - Non-Galerkin hyperreduction





THANK YOU

GRATEFUL TO:

EdgeTwins HPC

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Link to Kratos github site

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

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).

[3] Roweis, S. T., & Saul, L. K. (2000). Nonlinear dimensionality reduction by locally linear embedding. *science*, *290*(5500), 2323-2326.

[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.