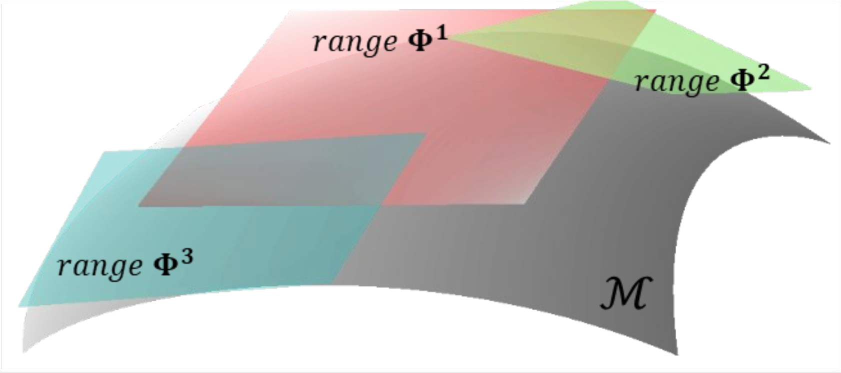
Barcelona

7^{th}–9^{th} September 2021

Clustering Techniques for Enhanced Reduced Order Model Simulations in Structural Mechanics



Mr. J Raul Bravo M

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Prof. Joaquin Hernandez

CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Presenting ourselves

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Kratos github site

Outline of the talk

- Proper Orthogonal Decomposition POD
- Local POD
- Our proposals:
  - Overlapping
  - HROM with multiple bases
- Examples run in Kratos Multiphysics
- Conclusions

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Proper Orthogonal Decomposition

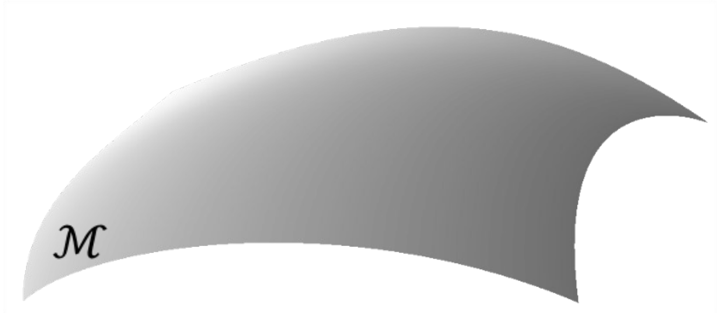
Full Order Model (FOM)

$$r(u;\mu) = 0$$

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

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

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

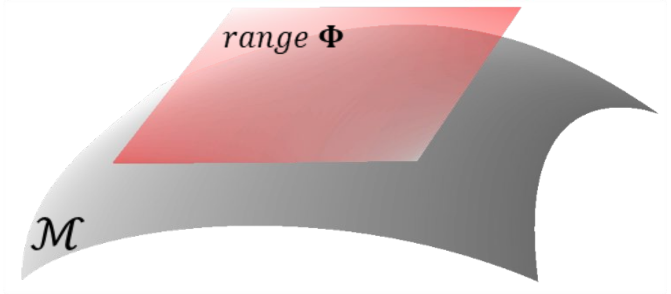


Let $u \approx \Phi\, \mathbf{q}$

Reduced Order Model (ROM)

$$\Phi^T r(\Phi\, \mathbf{q};\mu) = 0$$

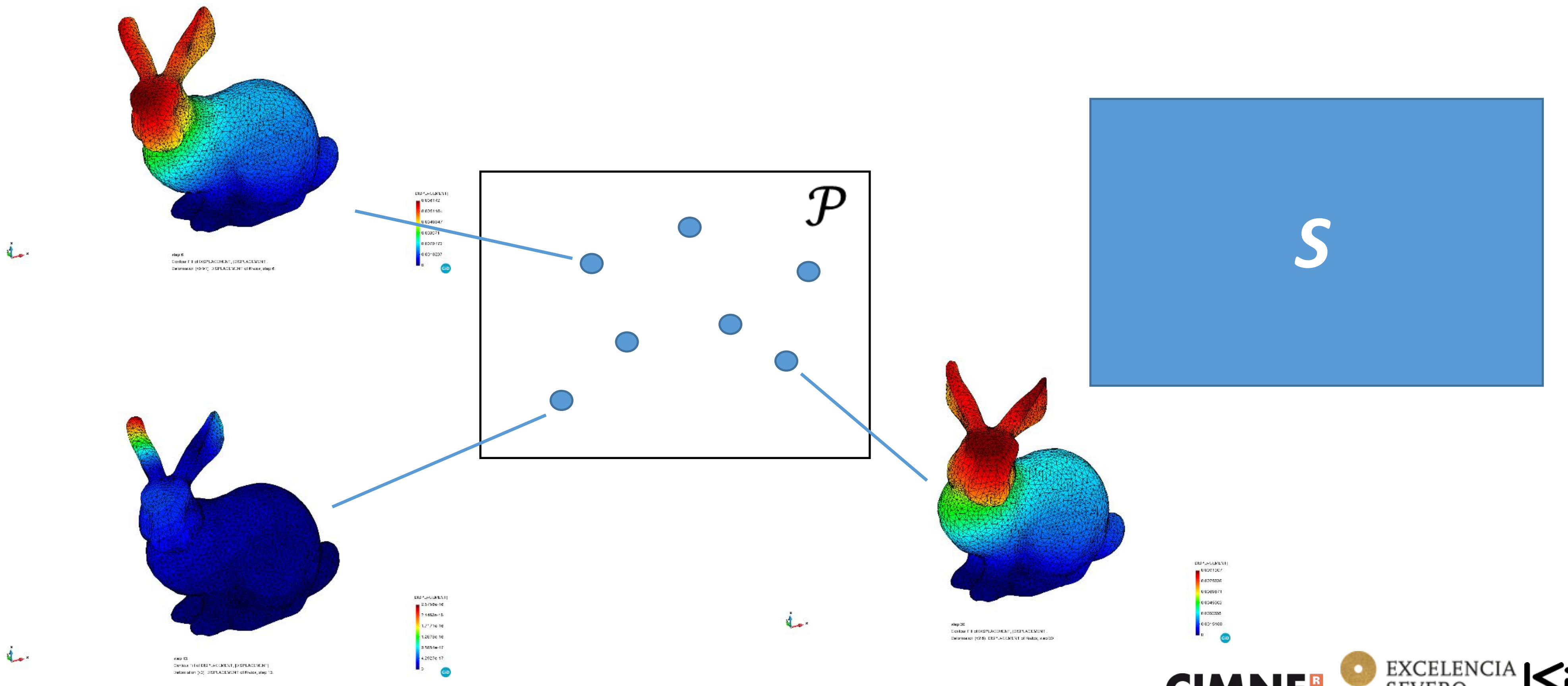
$q \in \mathbb{R}^k$: reduced state vector



A MUCH SMALLER SYSTEM!

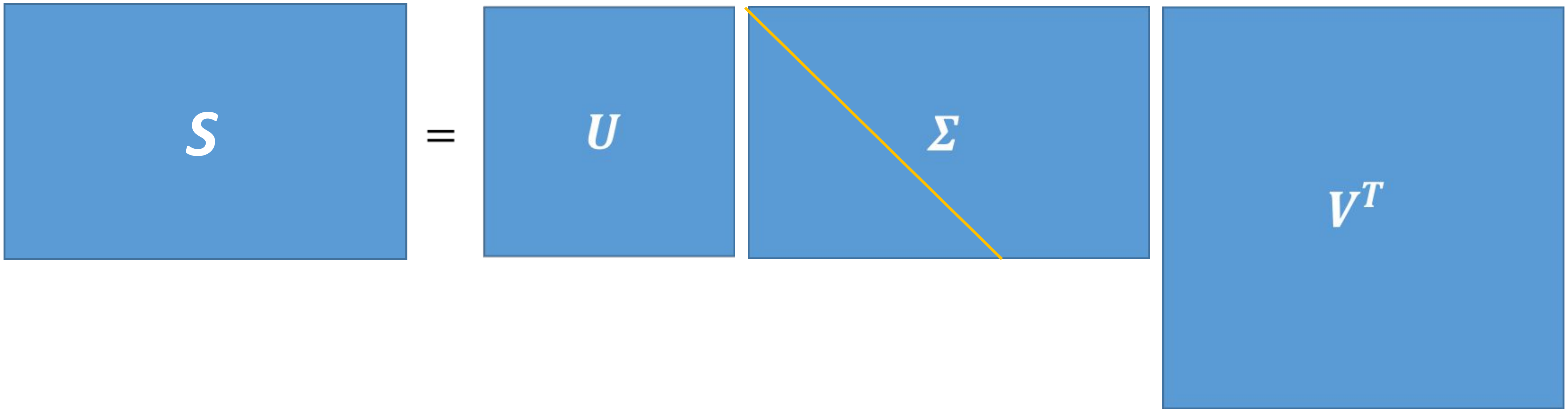
Proper Orthogonal Decomposition

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



Proper Orthogonal Decomposition

- Take the SVD of $\boldsymbol{S} = \boldsymbol{U\Sigma V^{T}} \approx \boldsymbol{U_k \Sigma_k V_k^{T}}$



Proper Orthogonal Decomposition

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Proper Orthogonal Decomposition

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

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

Proper Orthogonal Decomposition

Full Order Model (FOM)

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

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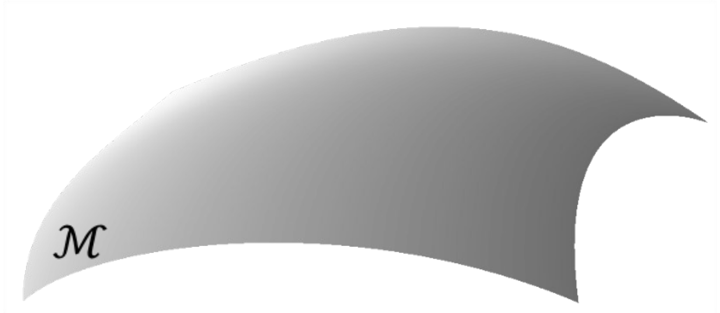
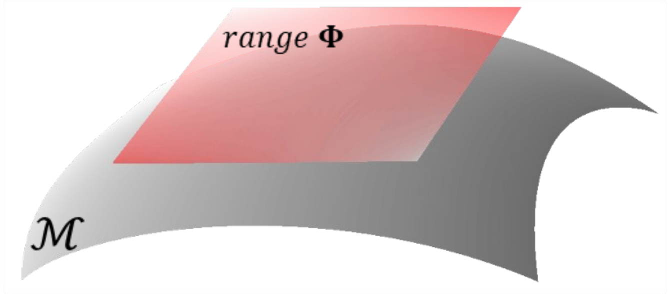


Let $\boldsymbol{u} \approx \boldsymbol{\Phi}\, \mathbf{q}$

Reduced Order Model (ROM)

$\boldsymbol{\Phi}^T \boldsymbol{r}(\boldsymbol{\Phi}\, \mathbf{q}; \boldsymbol{\mu}) = \mathbf{0}$

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



A MUCH SMALLER SYSTEM!

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

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Hyper-reduction

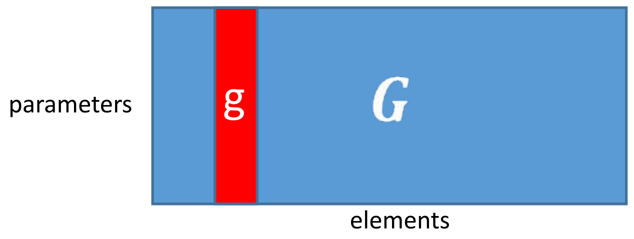
The goal is to find a **subset of elements and corresponding weights** by solving an optimization problem

$$(\boldsymbol{E},\boldsymbol{W}) = \arg\min \|\zeta\|_0$$

$$s.t. \quad \left\|\boldsymbol{G}\boldsymbol{1} - \boldsymbol{G}\zeta\right\|_2^2 \leq \epsilon\left\|\boldsymbol{G}\boldsymbol{1}\right\|_2^2$$

$$\zeta_i \geq 0$$

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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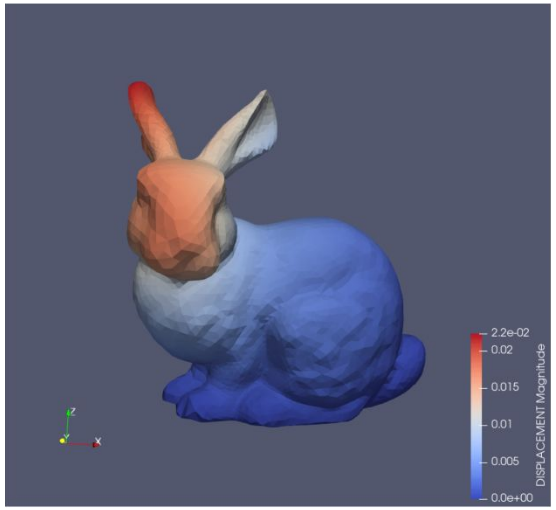
Hyper-reduction

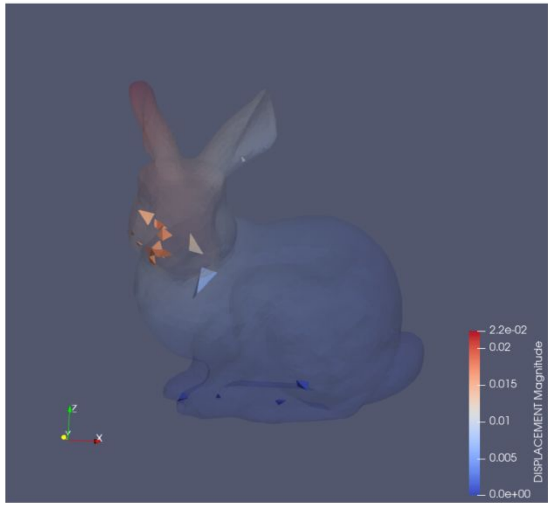
Assembly comparison FOM vs HROM:

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

FOM Simulation



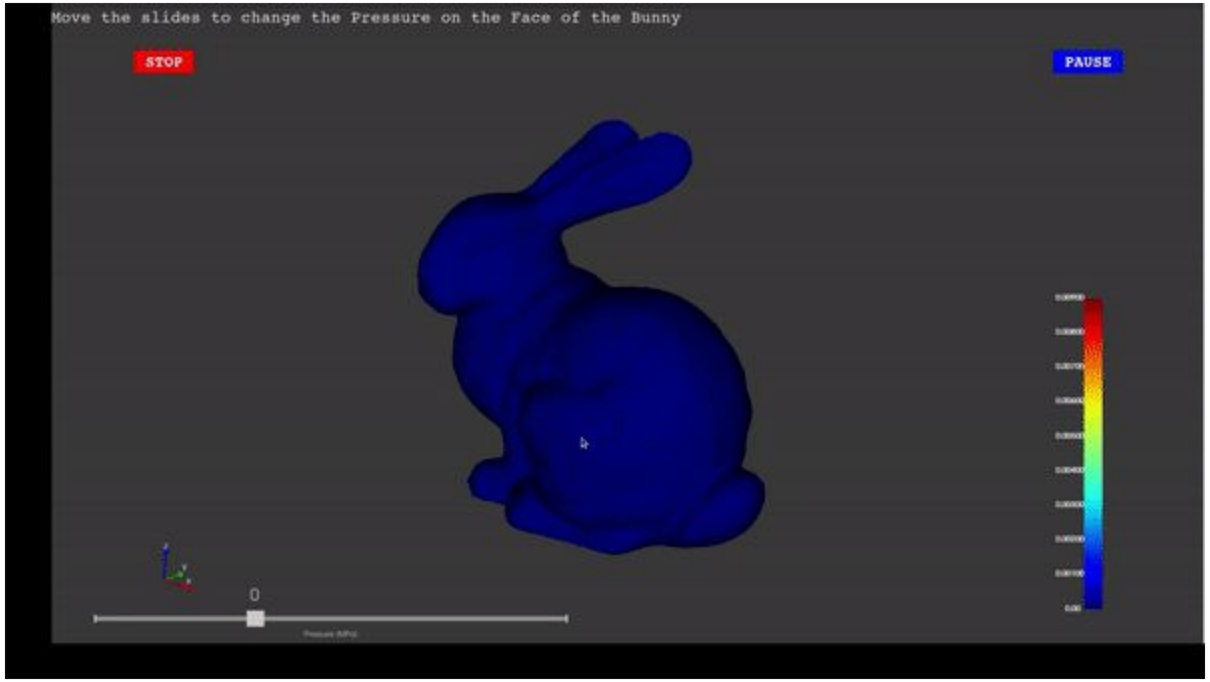
HROM Simulation



Hyper-reduction

$$\left(\sum_{e\in E} \boldsymbol{\Phi}_e^T \boldsymbol{A}_e \boldsymbol{\Phi}_{\mathbf{e}}\, \omega_e\right)\boldsymbol{q} = \sum_{e\in E} \boldsymbol{\Phi}_{\mathbf{e}}^T \boldsymbol{b}_e \omega_e$$

HROM Simulation



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POD weaknesses and strengths

- Straightforward procedure for training and inference

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

Local POD

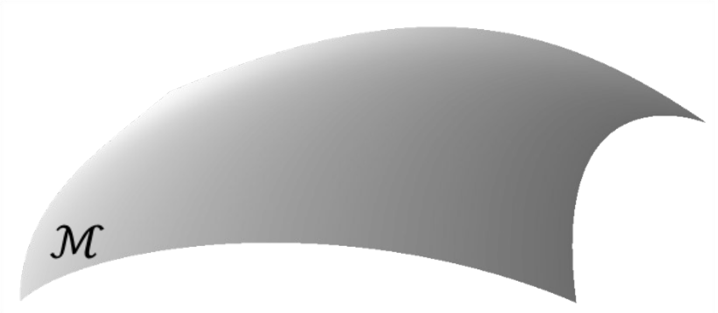
Full Order Model (FOM)

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

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

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

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

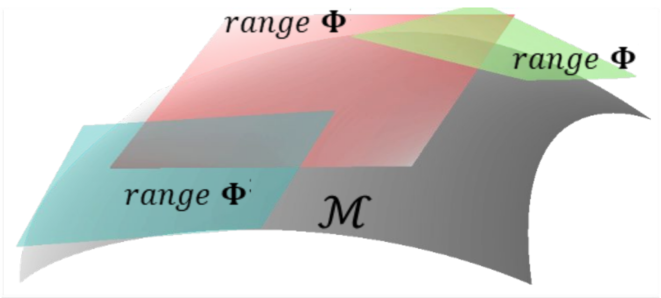


Let $\boldsymbol{u} \approx \boldsymbol{\Phi}^{\mathbf{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^{1^T} \boldsymbol{r}(\boldsymbol{\Phi}^1\, \mathbf{q}; \boldsymbol{\mu}) = \mathbf{0}$$

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



Local POD

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

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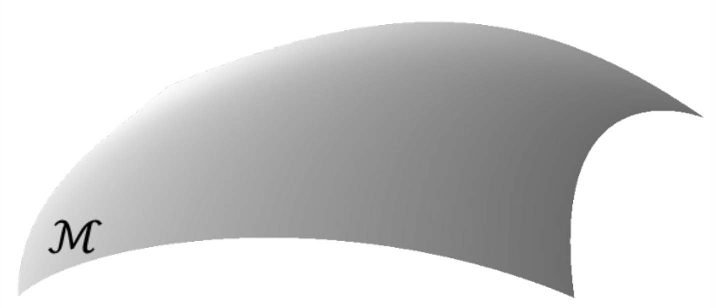
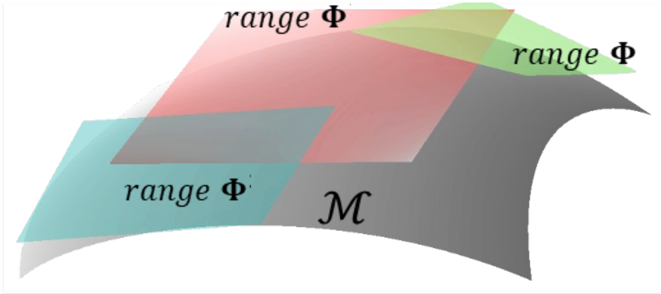


Let $\boldsymbol{u} \approx \boldsymbol{\Phi}^{\mathrm{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

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

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



Local POD

Full Order Model (FOM)

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

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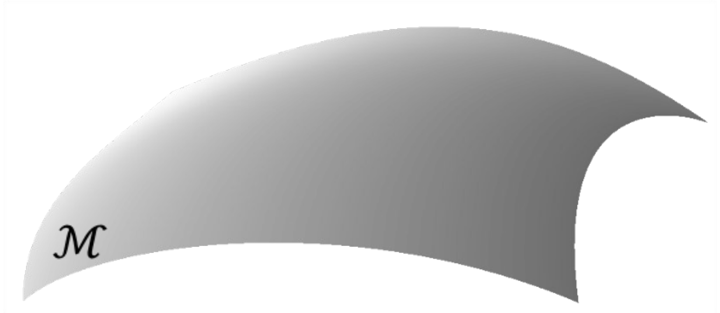
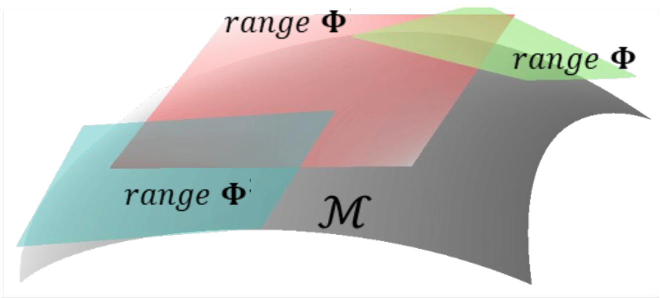


Let $\boldsymbol{u} \approx \boldsymbol{\Phi}^{\mathbf{i}}\, \mathbf{q}$

Reduced Order Model (ROM)

$$\boldsymbol{\Phi}^{3^T} \boldsymbol{r}(\boldsymbol{\Phi}^3\, \mathbf{q};\boldsymbol{\mu}) = \mathbf{0}$$

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



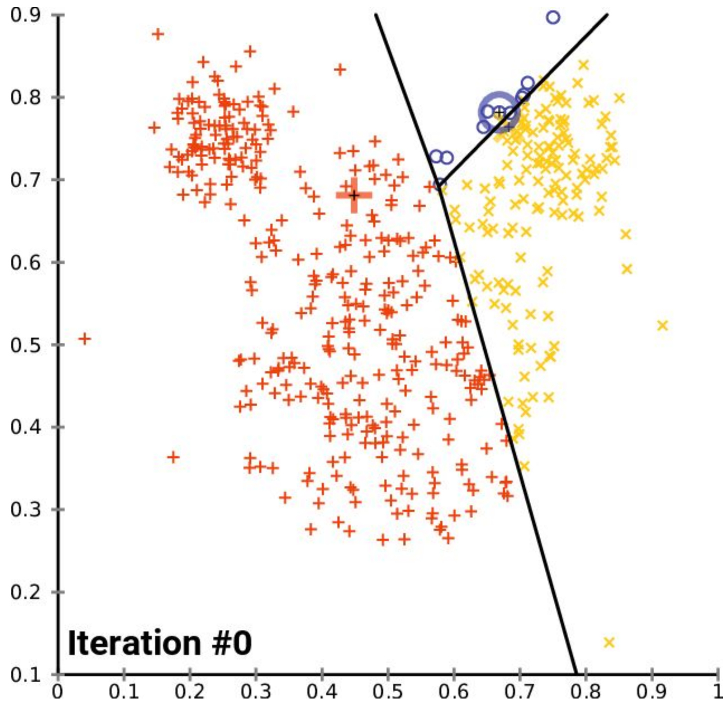
Local POD. K-means

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

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

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

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



Animation from Wikipedia

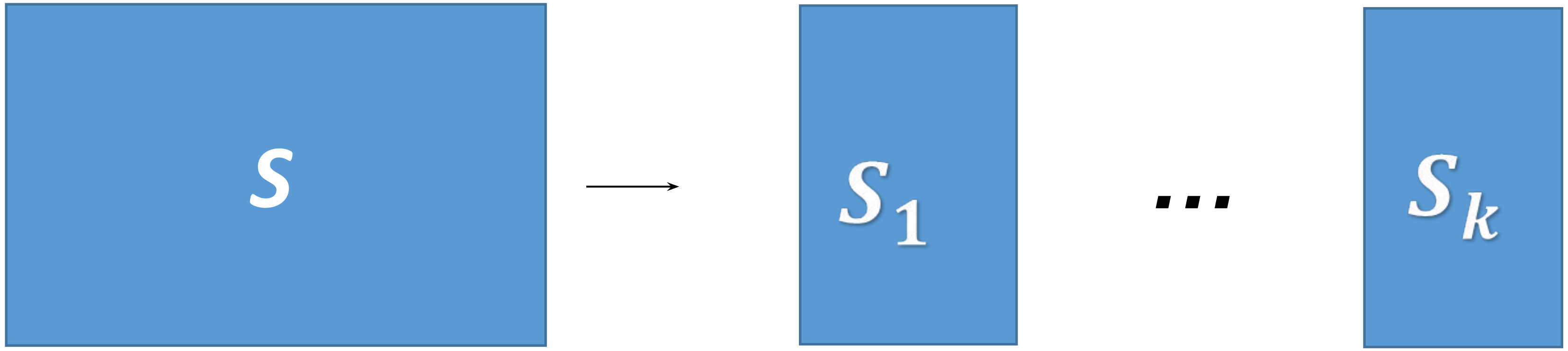
Solve via alternating minimization:

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

Local POD. Building multiple bases

- Use an unsupervised learning method to build clusters

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



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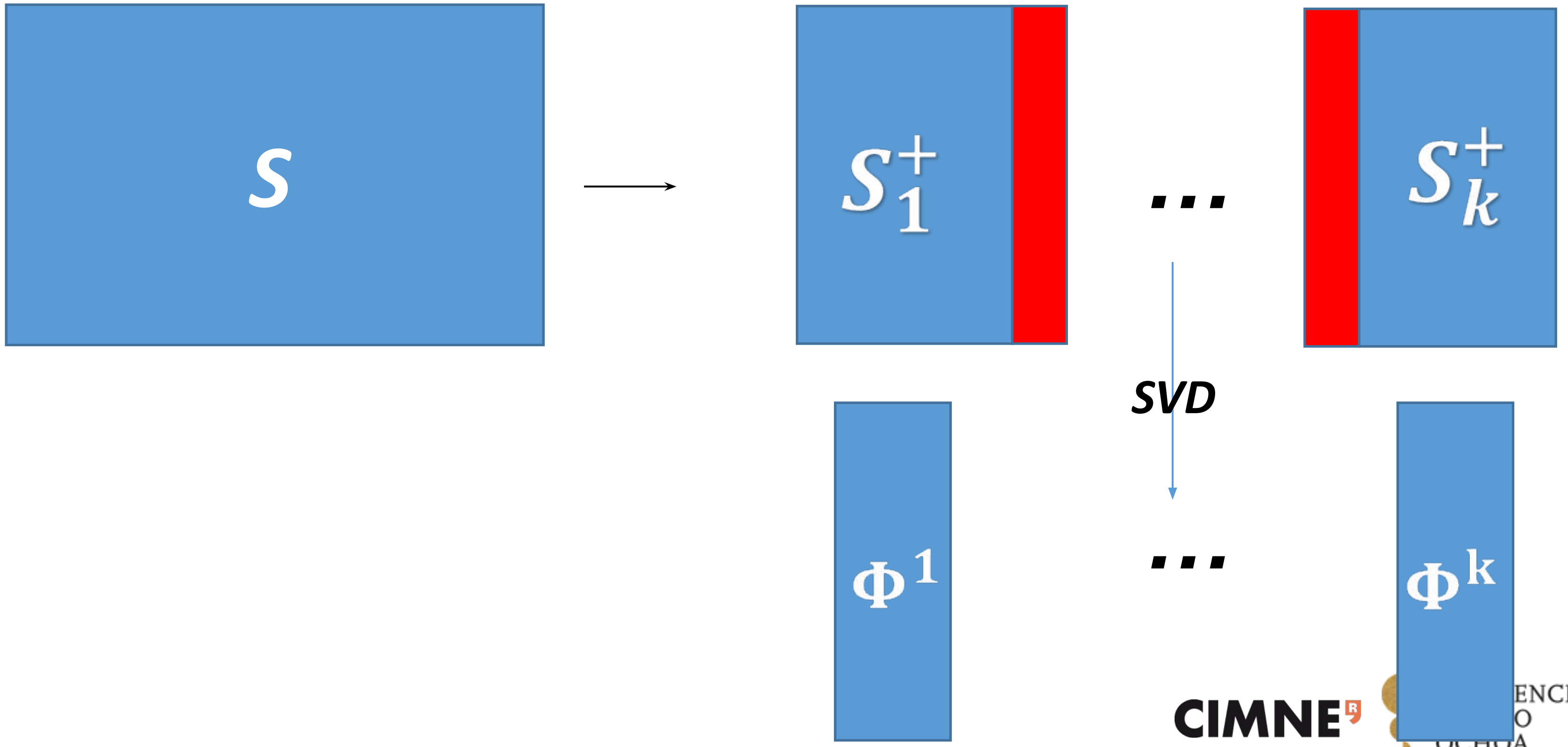
Local POD. Building multiple bases

- Use an unsupervised learning method to build clusters

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

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



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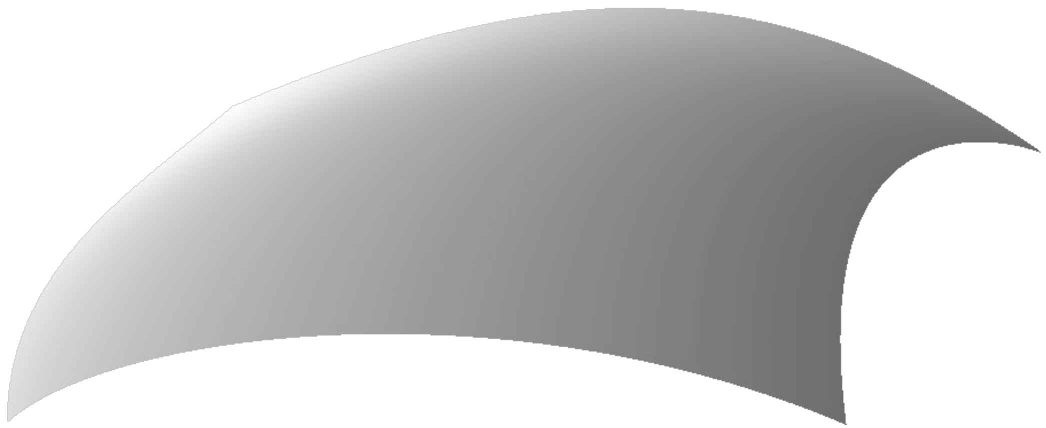
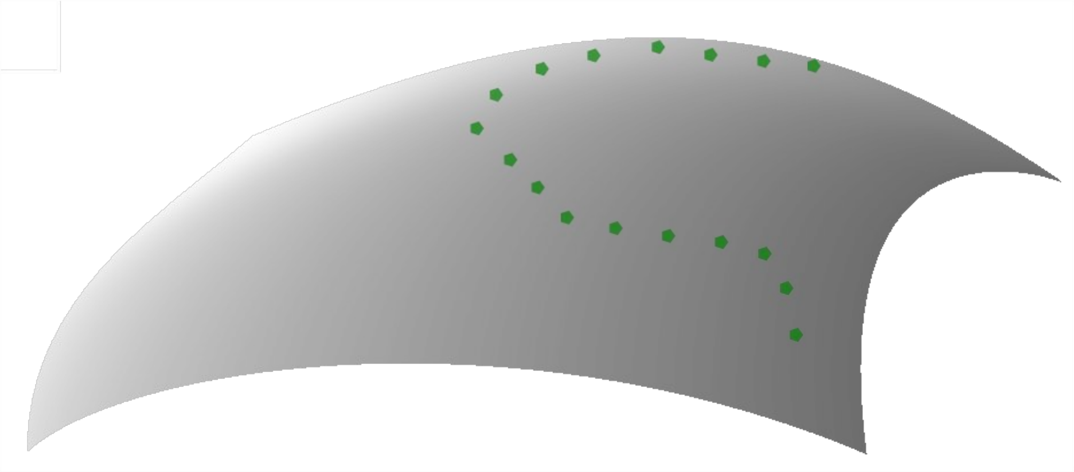
Local POD. Our overlapping proposal



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

Local POD. Our overlapping proposal



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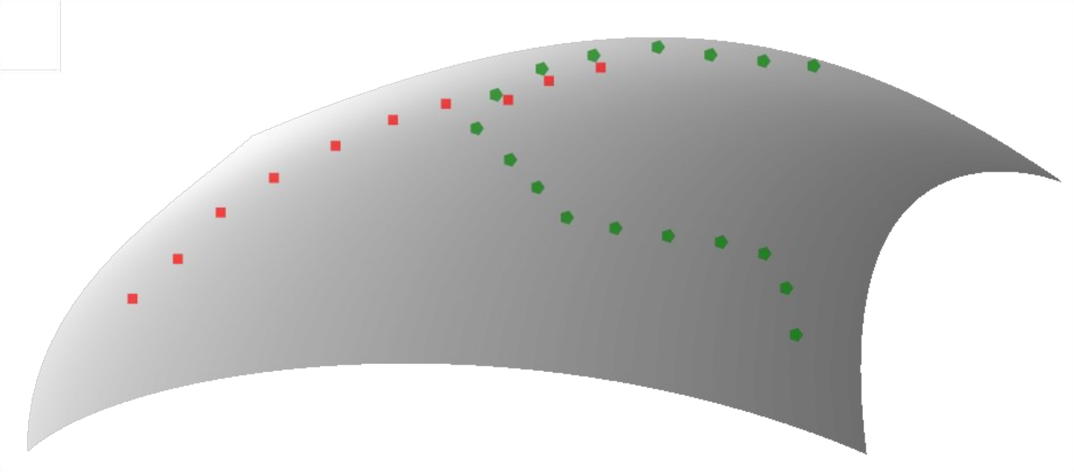

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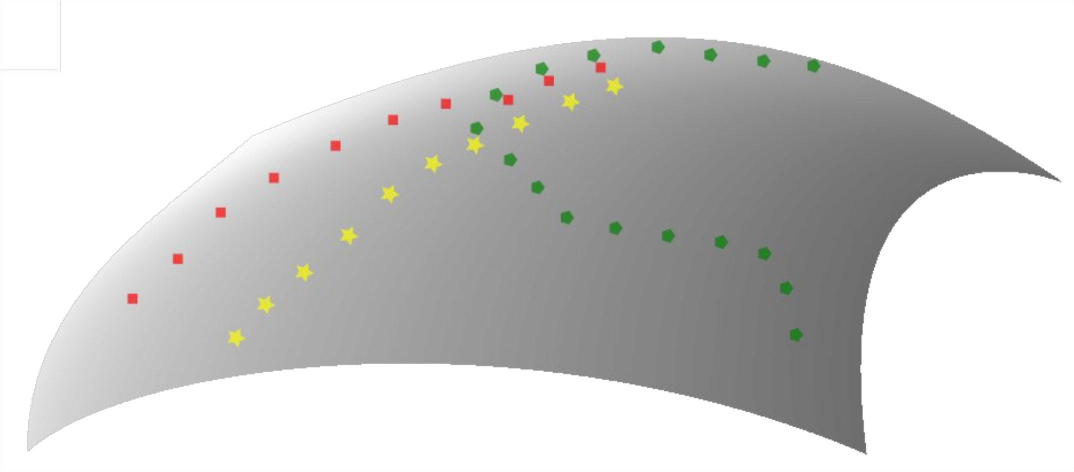

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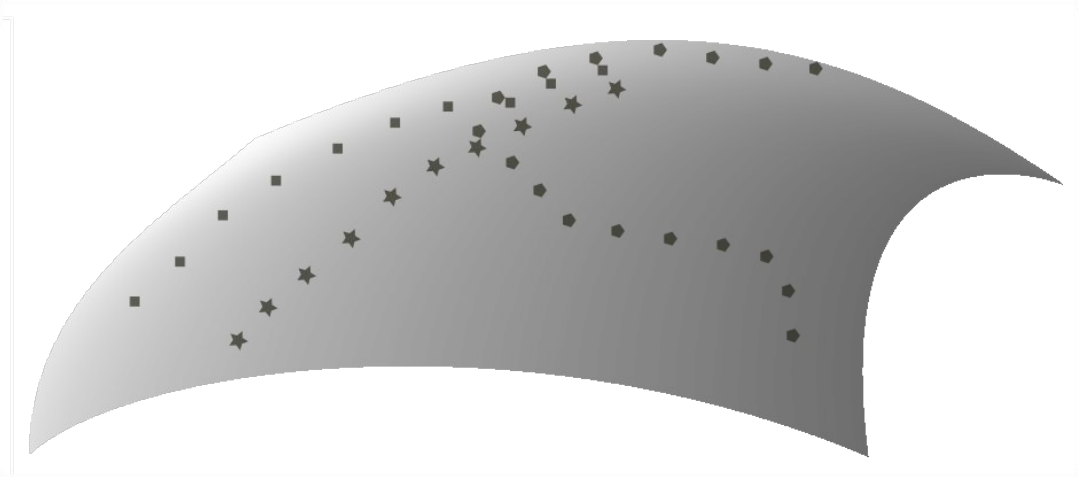

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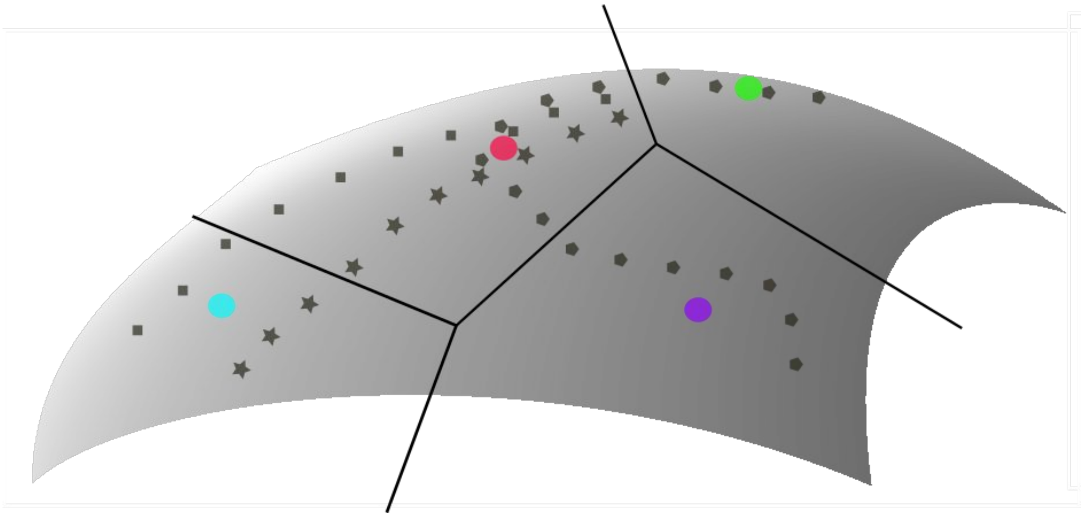

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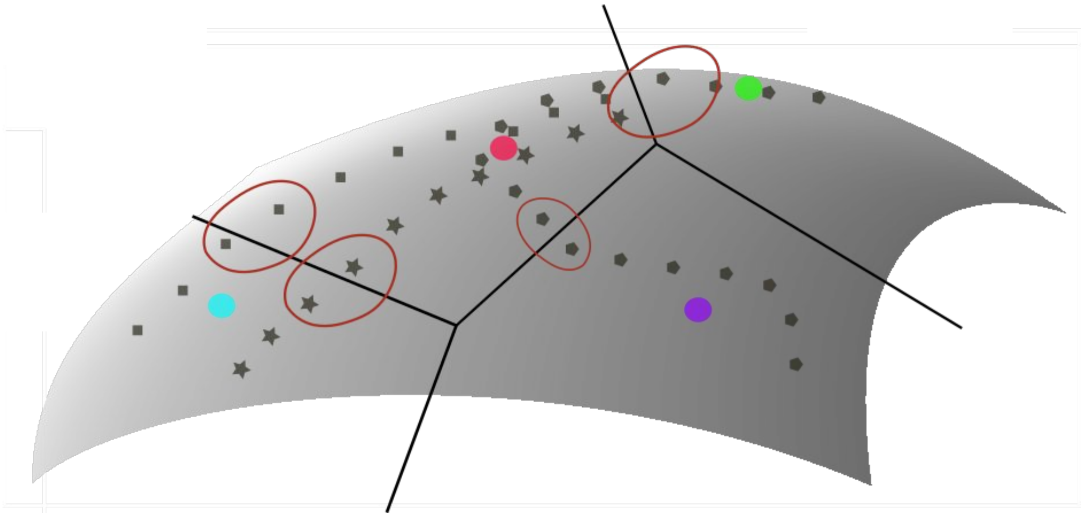

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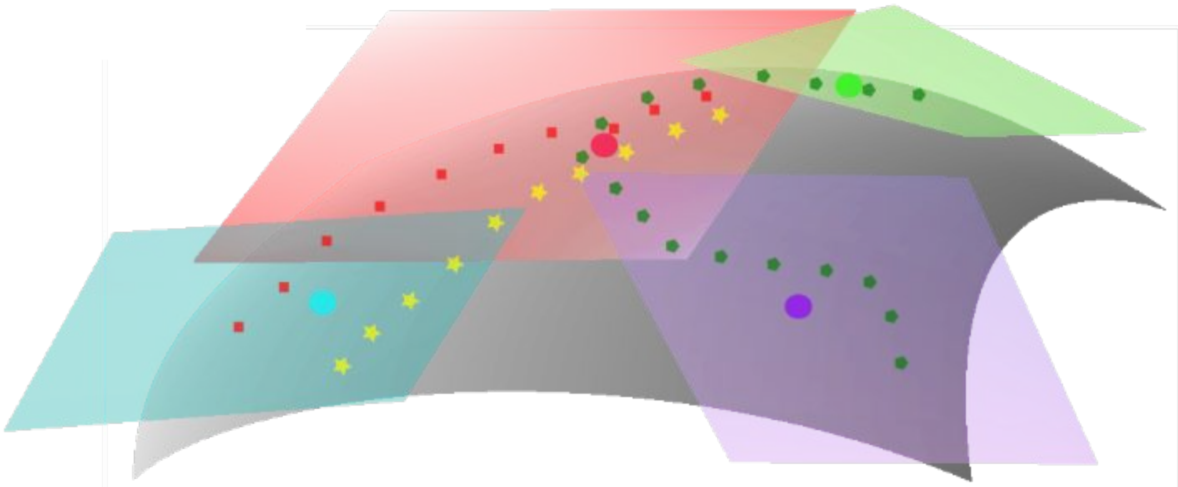

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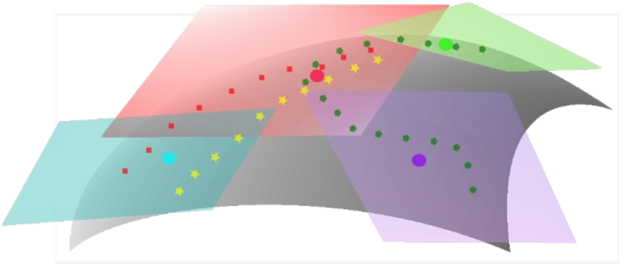

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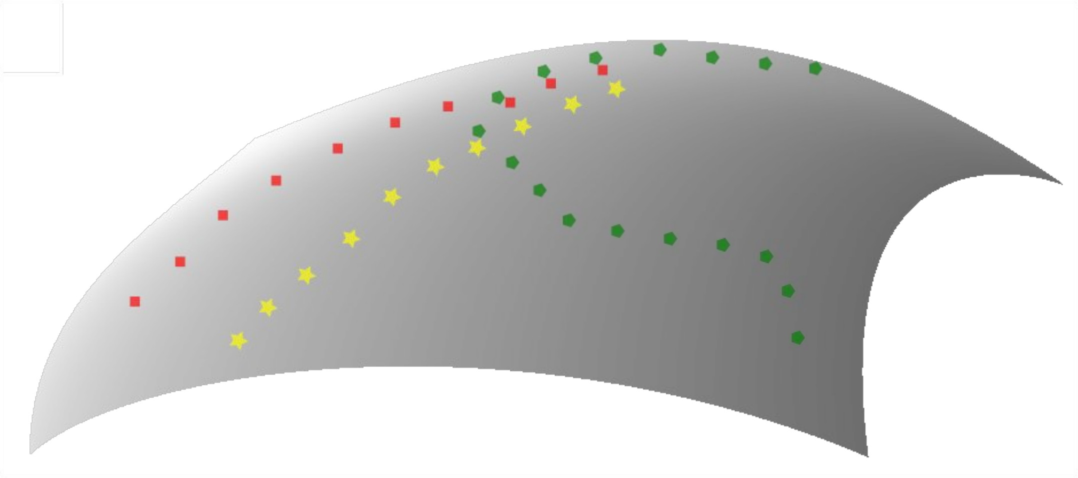
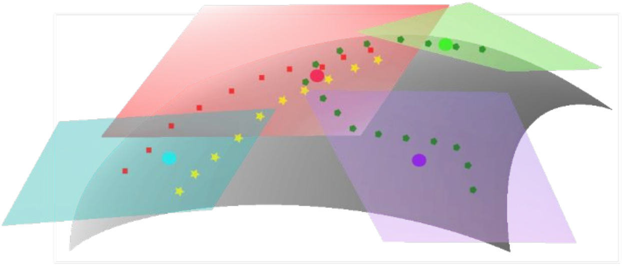


Our overlapping proposal

Local POD. Our overlapping proposal



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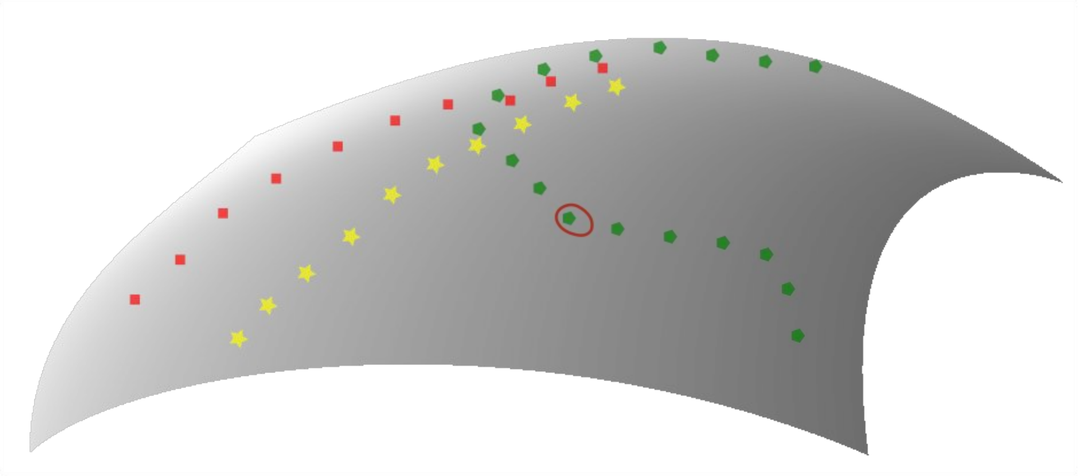

Our overlapping proposal

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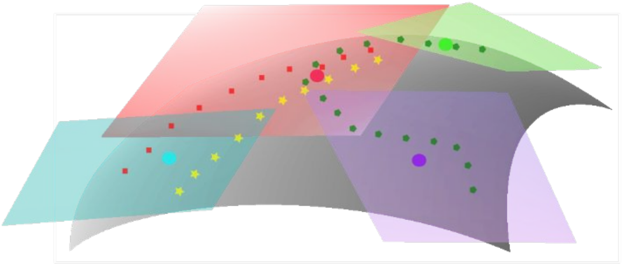
Local POD. Our overlapping proposal



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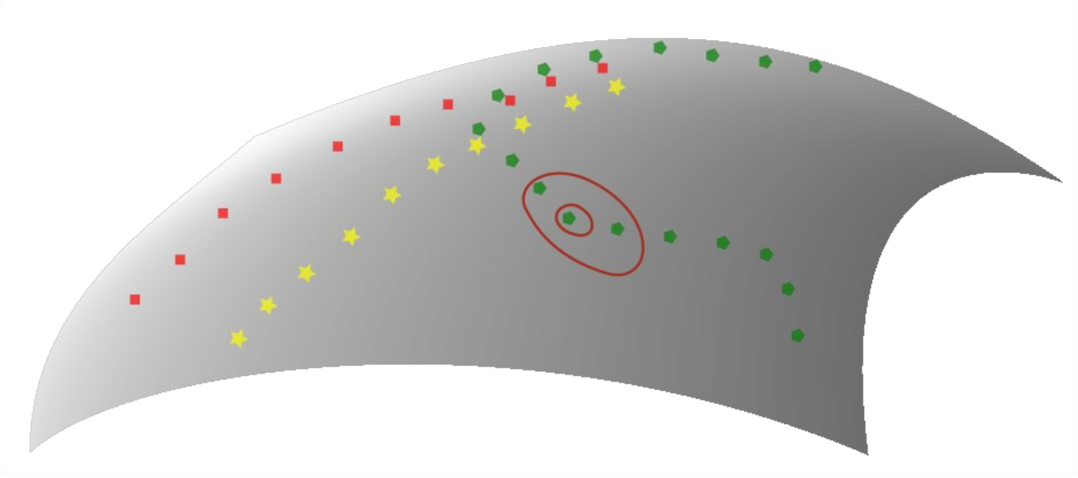
(Roweis,2000):doi.org/10.1126/science.290.5500.2323



Our overlapping proposal

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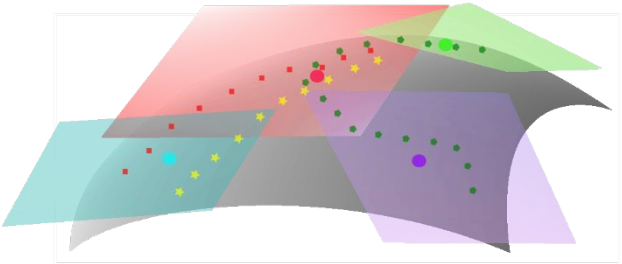

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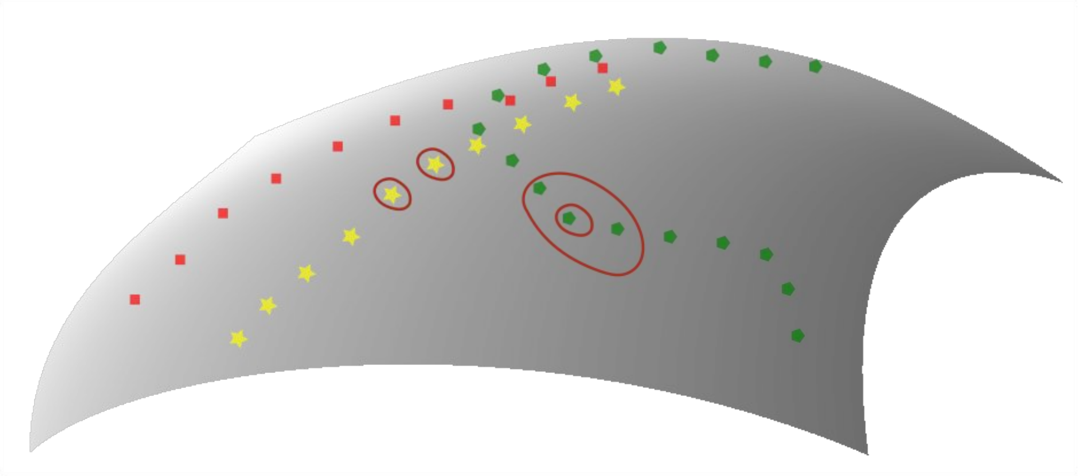

Our overlapping proposal

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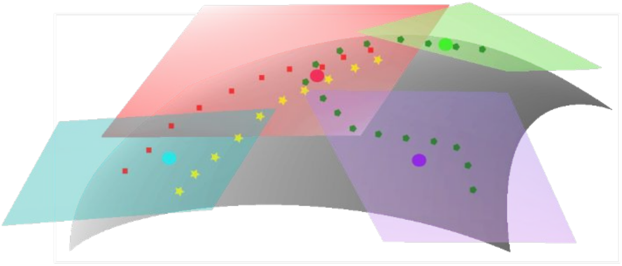

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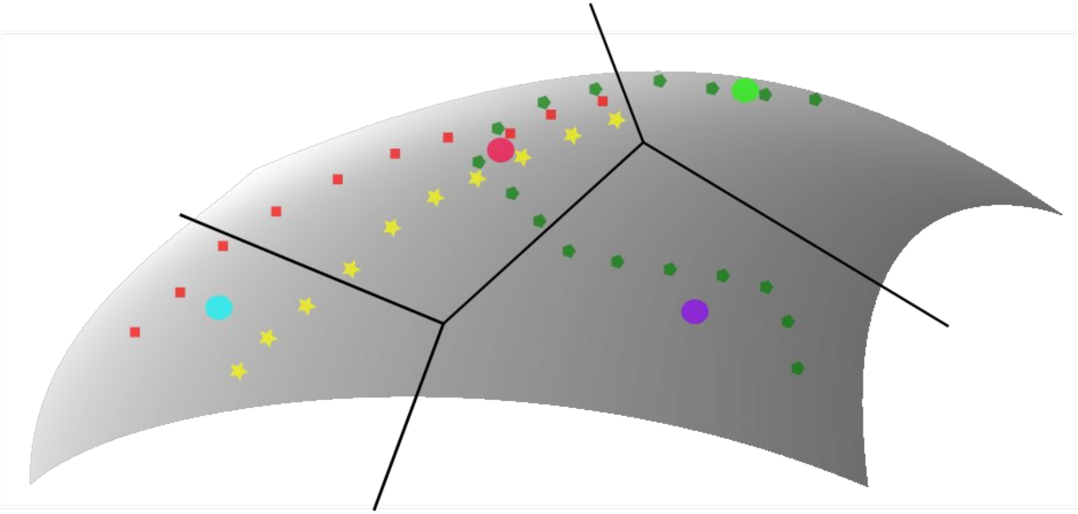

Our overlapping proposal

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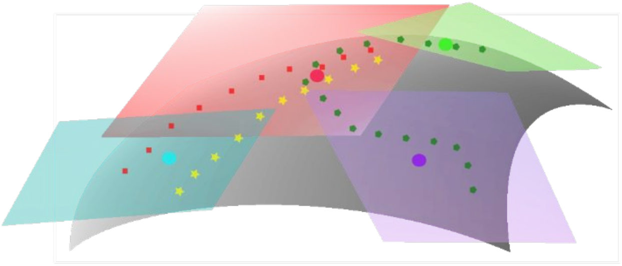

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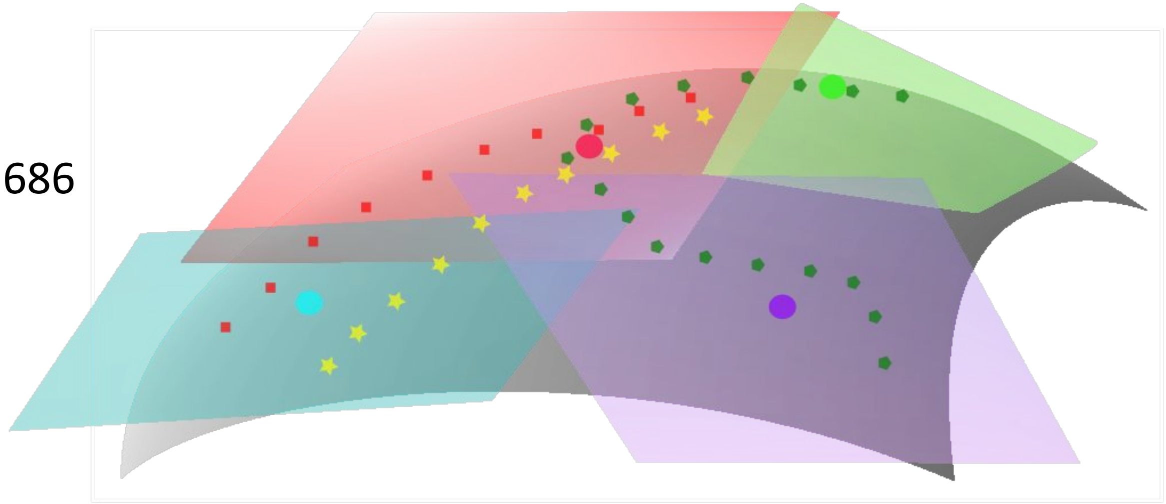

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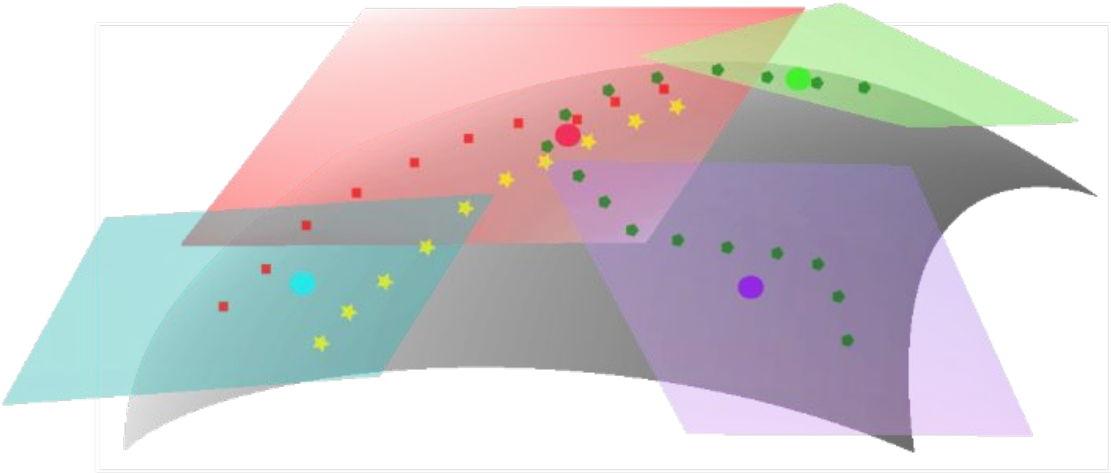

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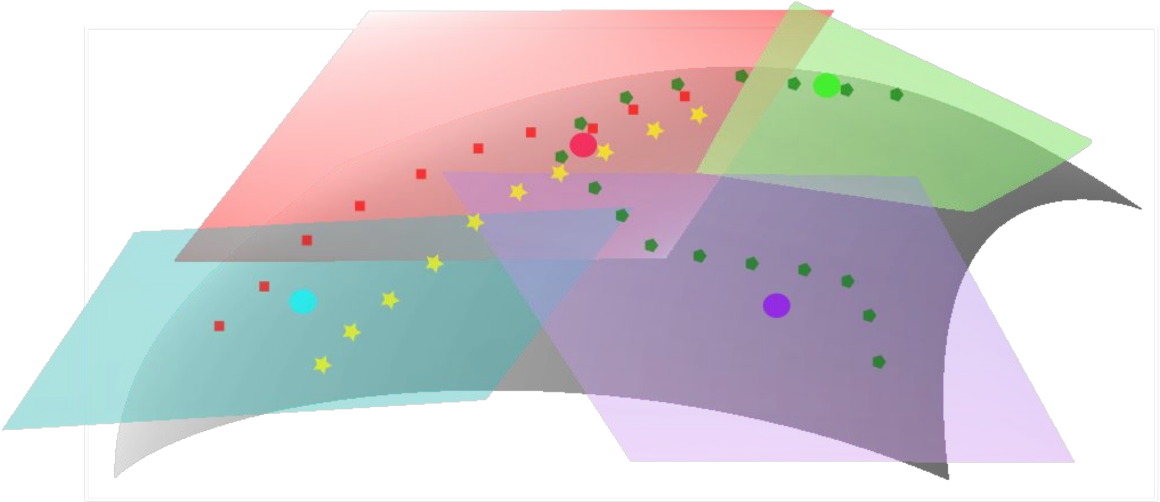

Our overlapping proposal

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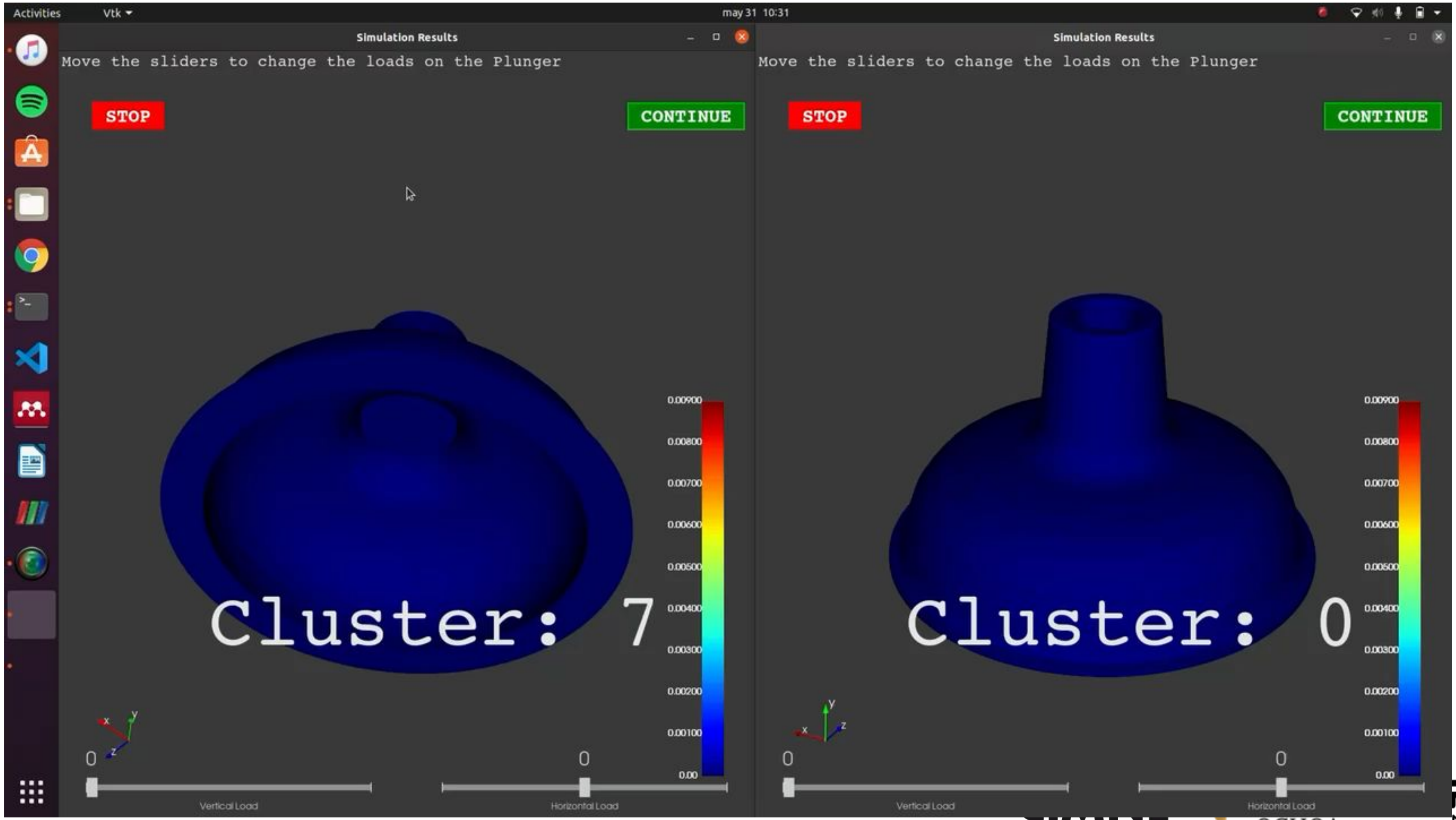
Local POD. Example 1

(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

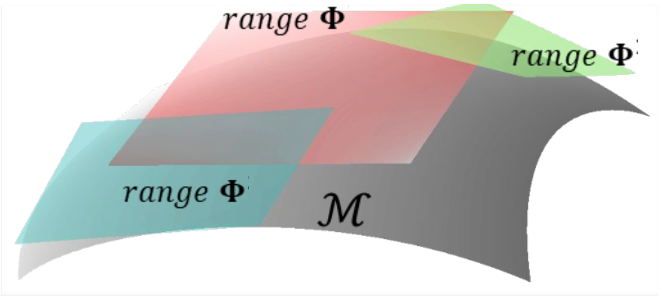
1. Get Non-overlapping clusters $\boldsymbol{S_i} = \boldsymbol{kmeans}(\boldsymbol{S})$
2. Add necessary overlapping $\boldsymbol{S_i^+} = \boldsymbol{overlap}(\boldsymbol{S_i})$

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

Local POD. Hyper-reduction

Reduced Order Model (ROM)

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



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

G_3

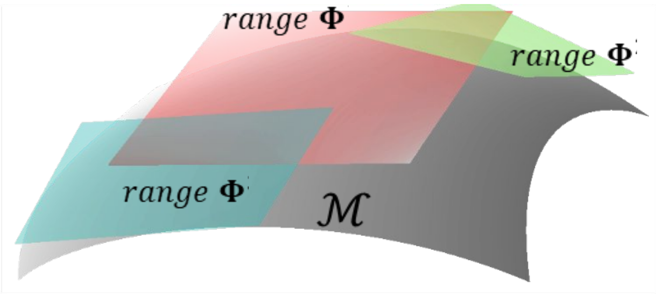
G_1

G_2

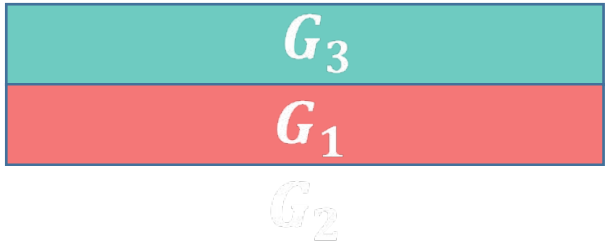
Local POD. Hyper-reduction

Reduced Order Model (ROM)

$$\Phi^{1^T} r(\Phi^1 \mathbf{q}; \mu) = 0$$



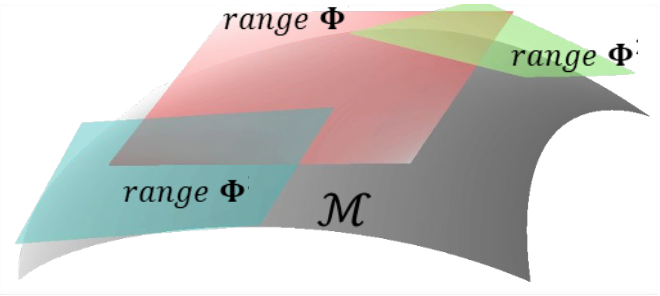
$$G = G(\Phi, R)$$



Local POD. Hyper-reduction

Reduced Order Model (ROM)

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



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

$$G_3$$

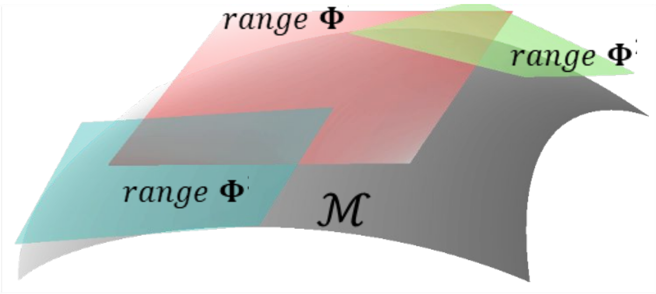
$$G_1$$

$$G_2$$

Local POD. Hyper-reduction

Reduced Order Model (ROM)

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



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

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

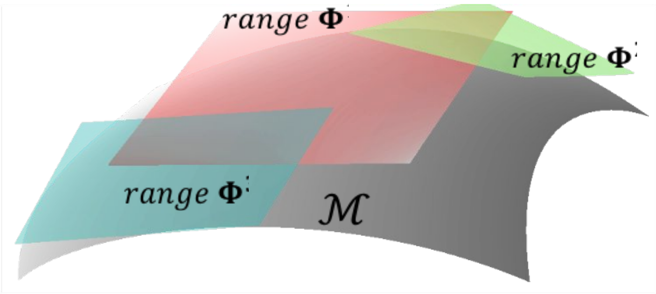
$$s.t. \quad \omega_i > 0$$

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

Local POD. Improved hyper-reduction

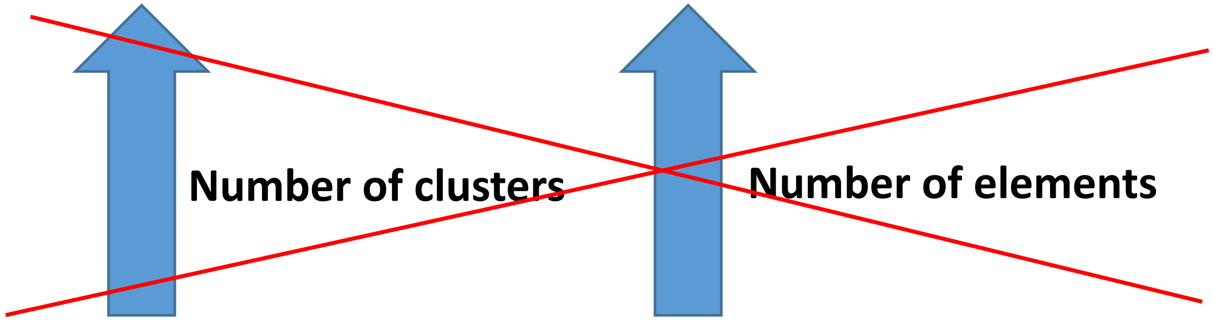
Reduced Order Model (ROM)

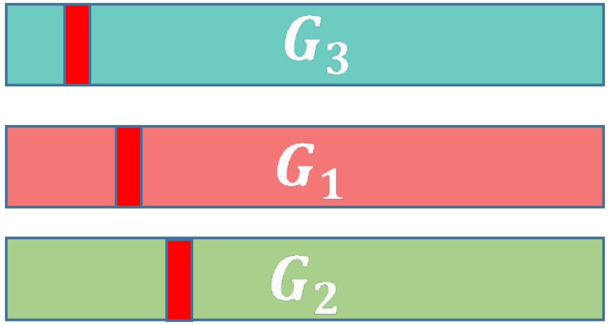
$$\Phi^{2^T} r(\Phi^2 \mathbf{q}; \mu) = \mathbf{0}$$



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

Expectation:



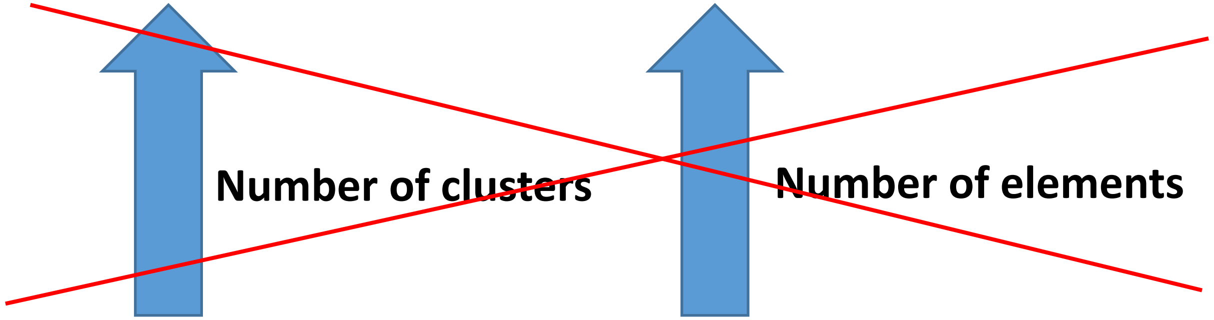


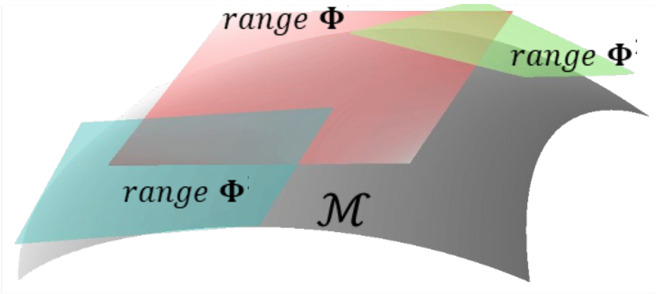
Local POD. Improved hyper-reduction

Reduced Order Model (ROM)

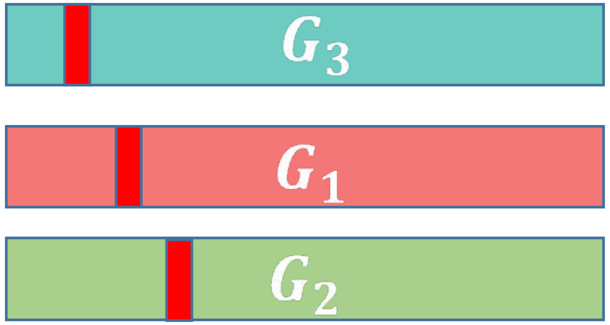
$$\Phi^{2^T} r(\Phi^2 \mathbf{q}; \mu) = \mathbf{0}$$

Expectation:





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



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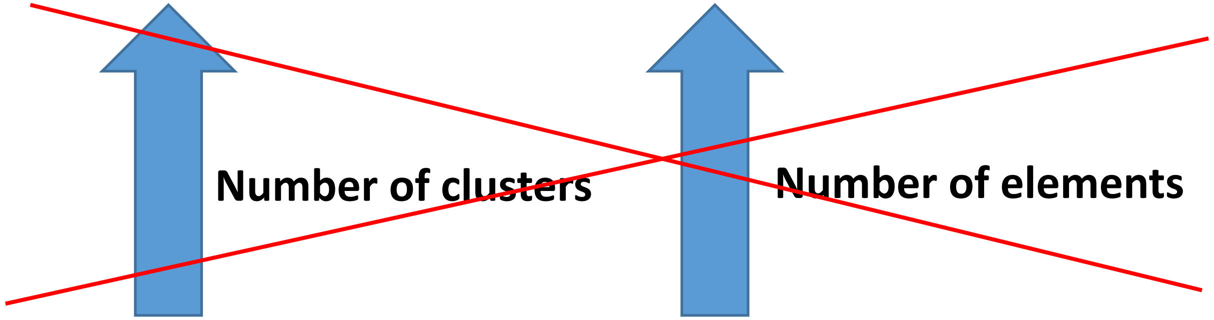
Local POD. Improved hyper-reduction

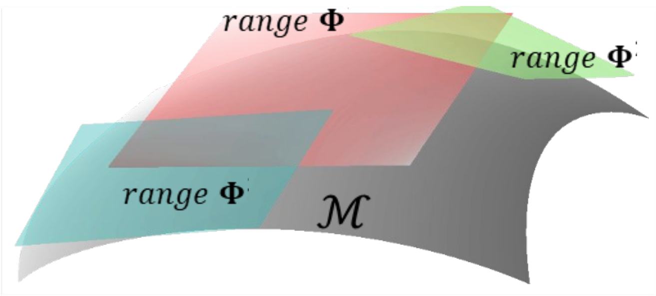
Reduced Order Model (ROM)

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

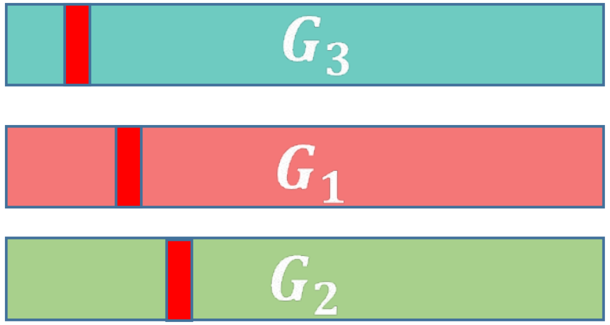
Expectation:



In reality:



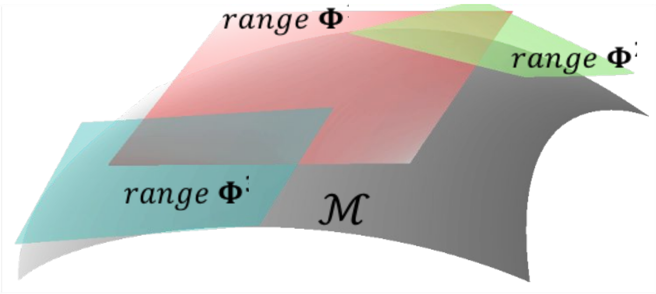
$$G = G(\Phi, R)$$



Local POD. Improved hyper-reduction

Reduced Order Model (ROM)

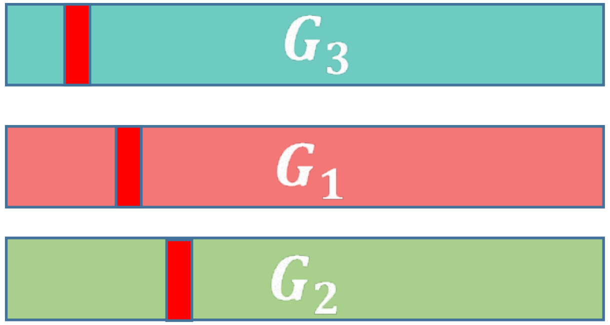
$$\Phi^{2^T} r(\Phi^2 \mathbf{q}; \boldsymbol{\mu}) = \mathbf{0}$$



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

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

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



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

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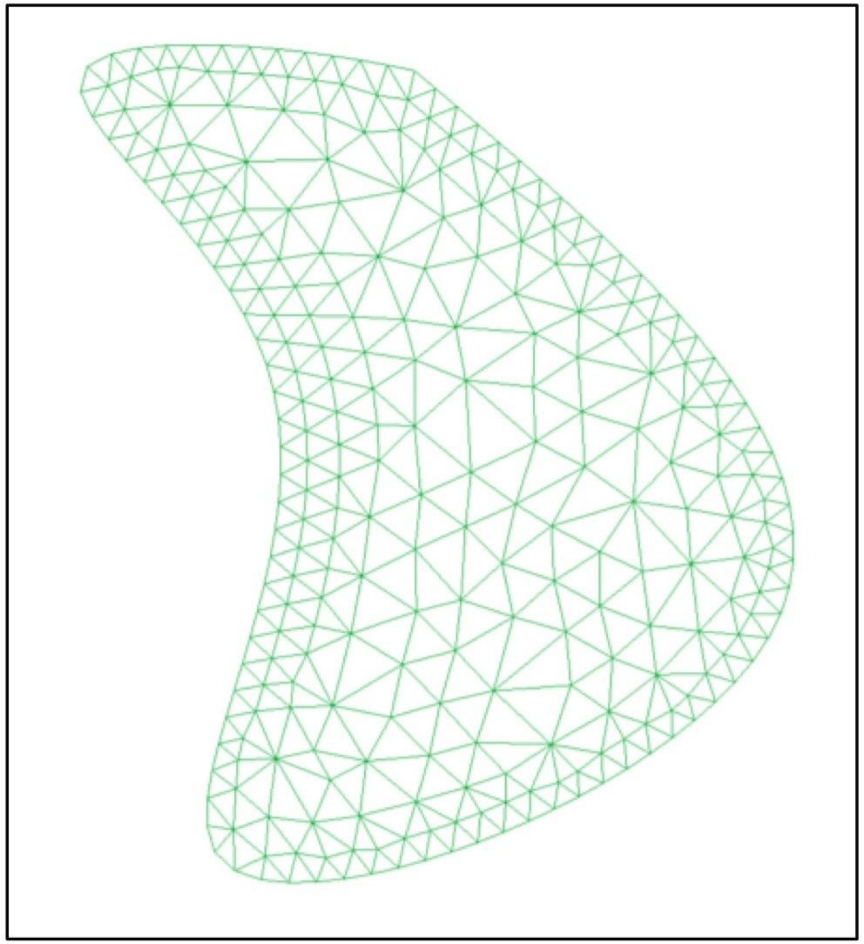
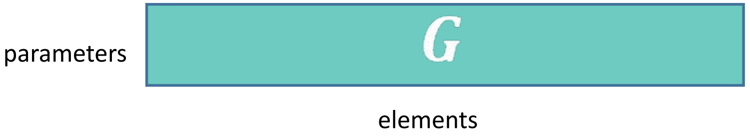
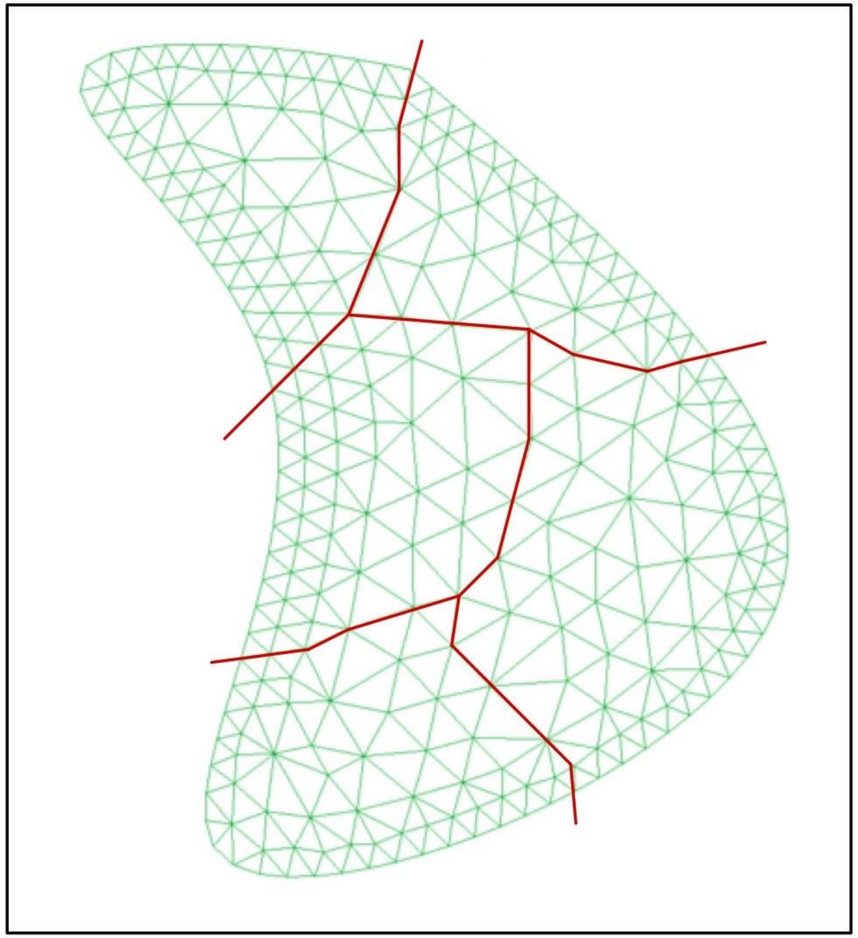
Local POD. Parallelisation of ECM



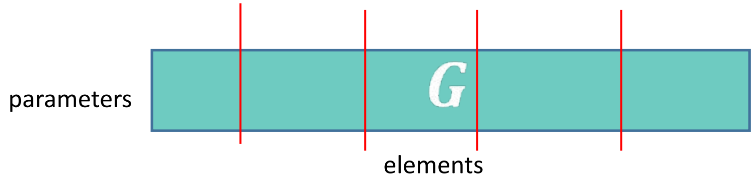
$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi}, \boldsymbol{R})$$



Local POD. Parallelisation of ECM



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



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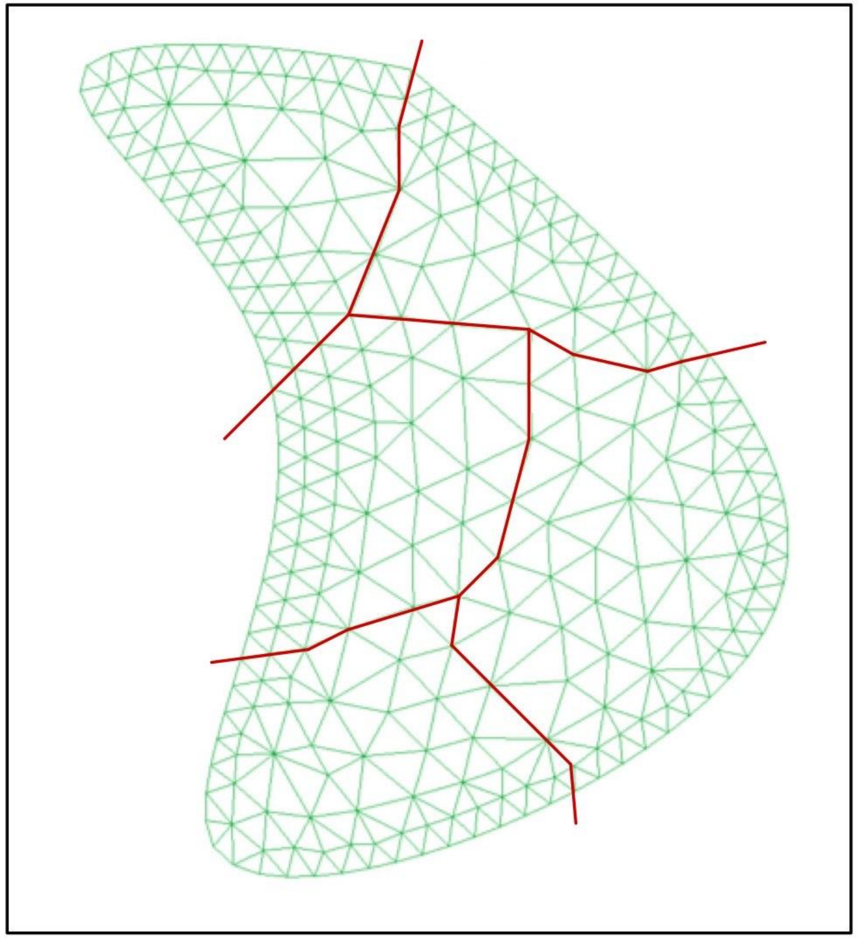
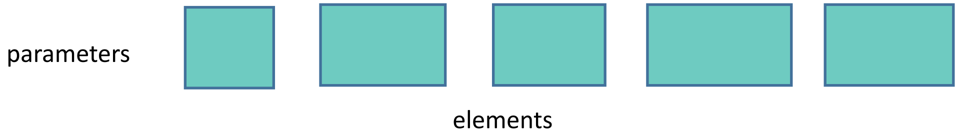
Local POD. Parallelisation of ECM

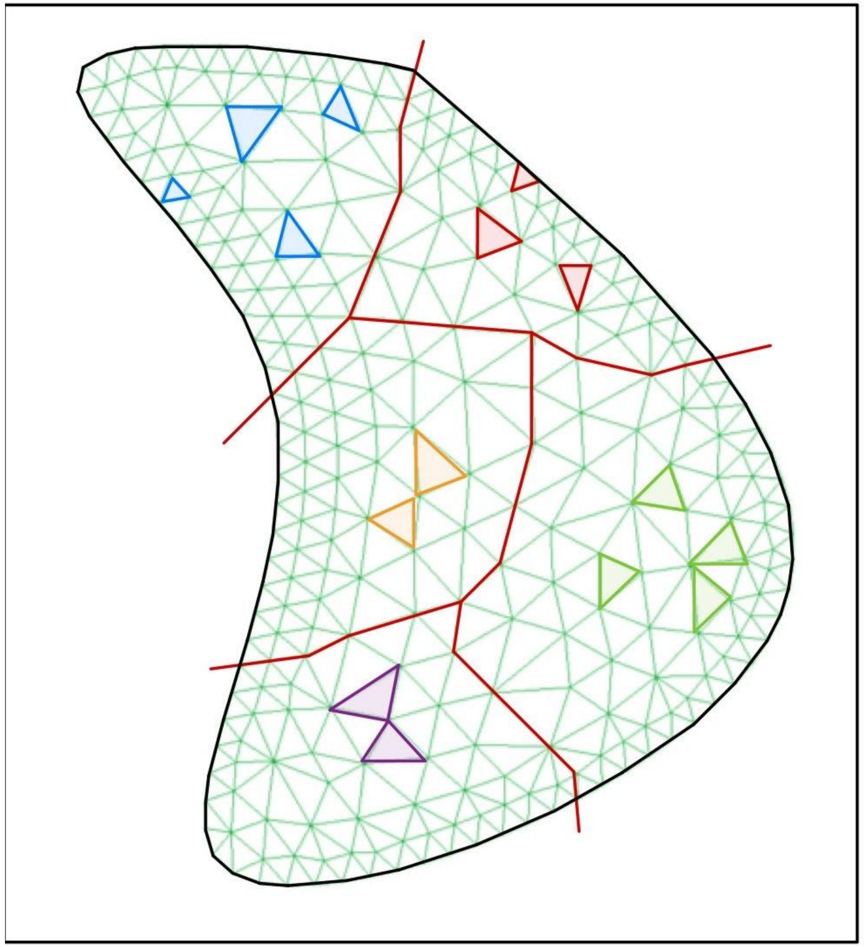


$$(\boldsymbol{E},\boldsymbol{W}) = ECM(\boldsymbol{G})$$

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

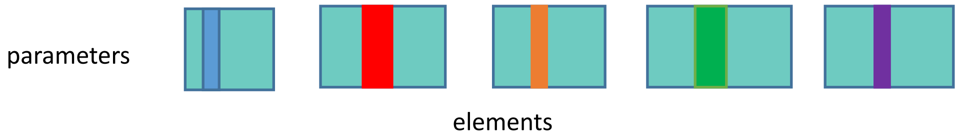


Local POD. Parallelisation of ECM

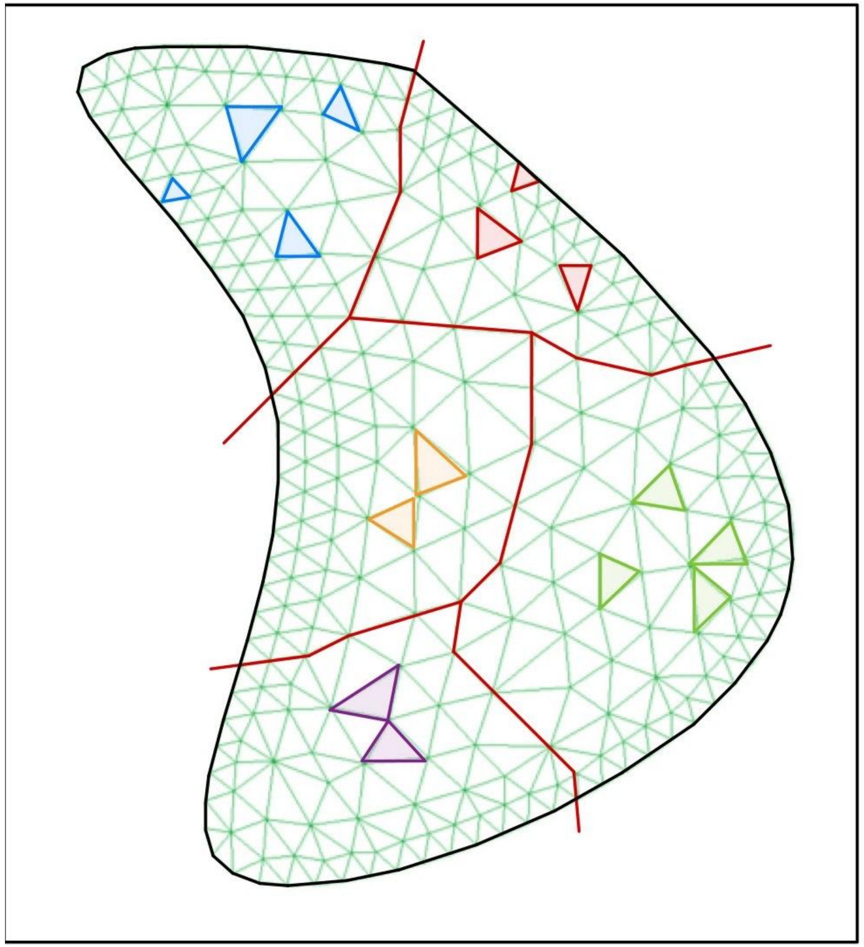


$$(\boldsymbol{E}, \boldsymbol{W}) = ECM(\boldsymbol{G})$$

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

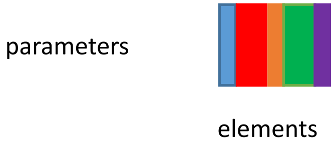


Local POD. Parallelisation of ECM



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

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



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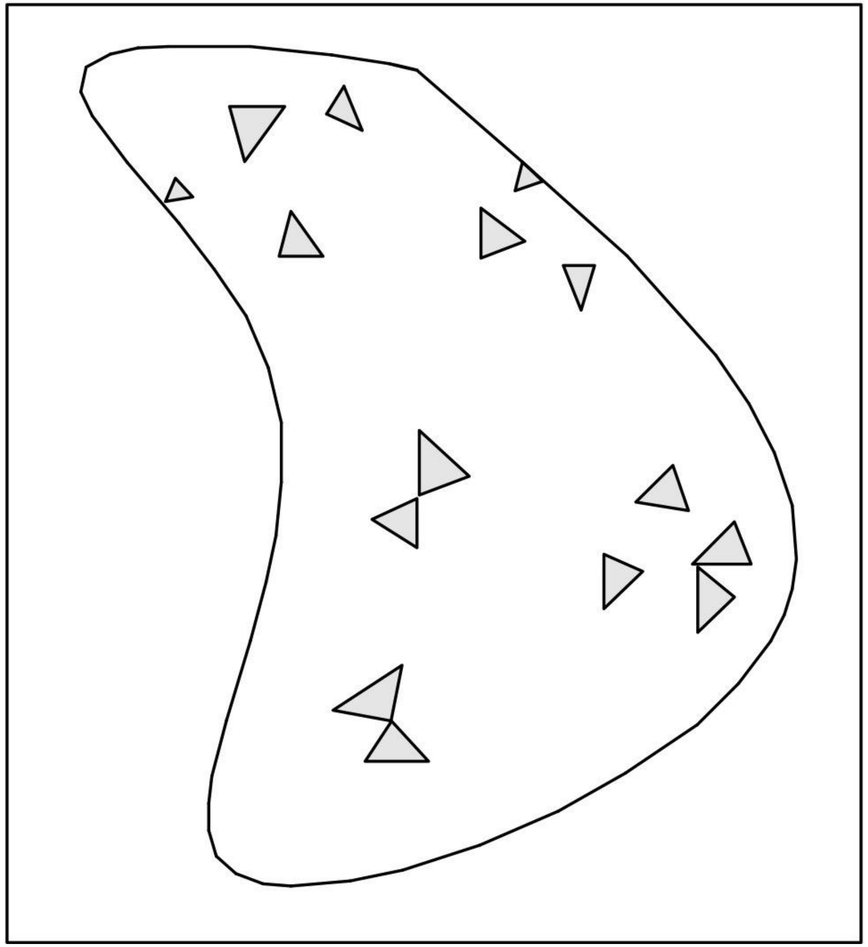
Local POD. Parallelisation of ECM



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

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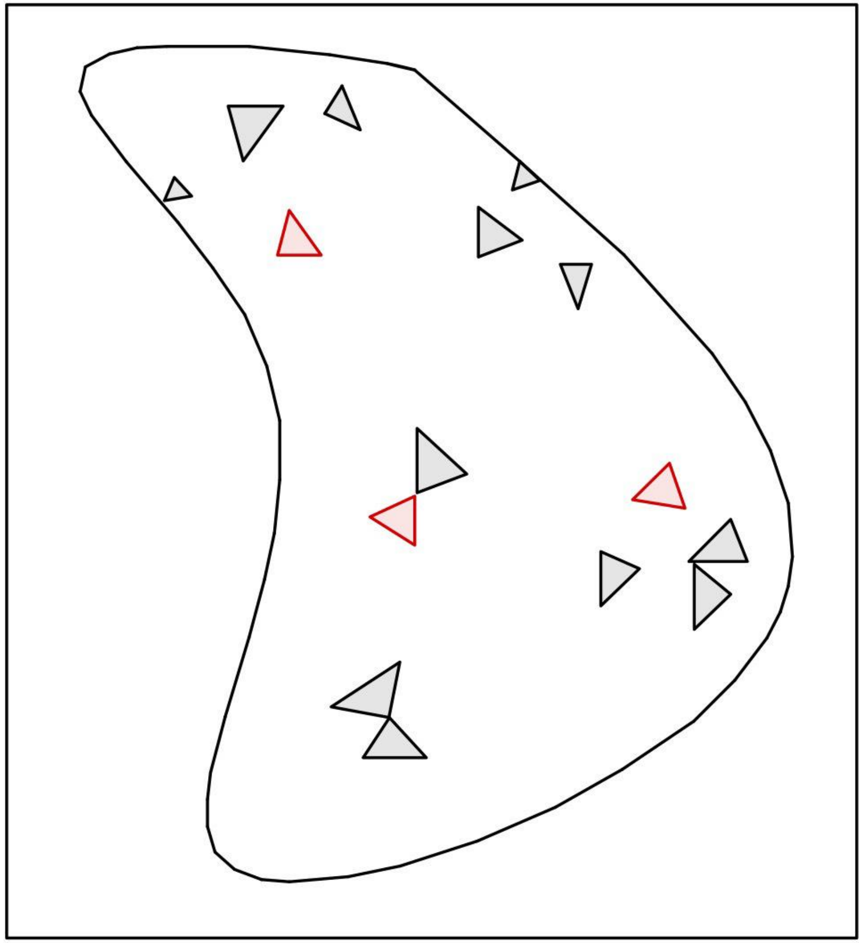
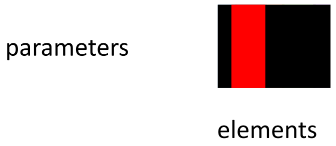
Local POD. Parallelisation of ECM

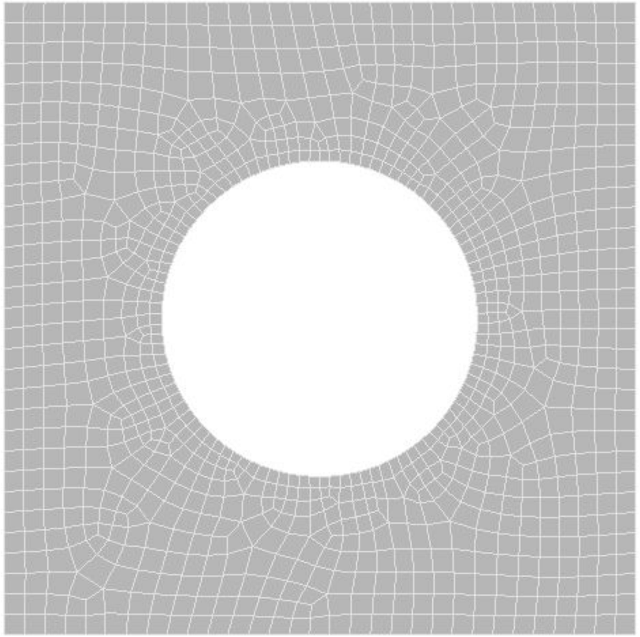


$$(\boldsymbol{E}, \boldsymbol{W}) = ECM(\boldsymbol{G})$$

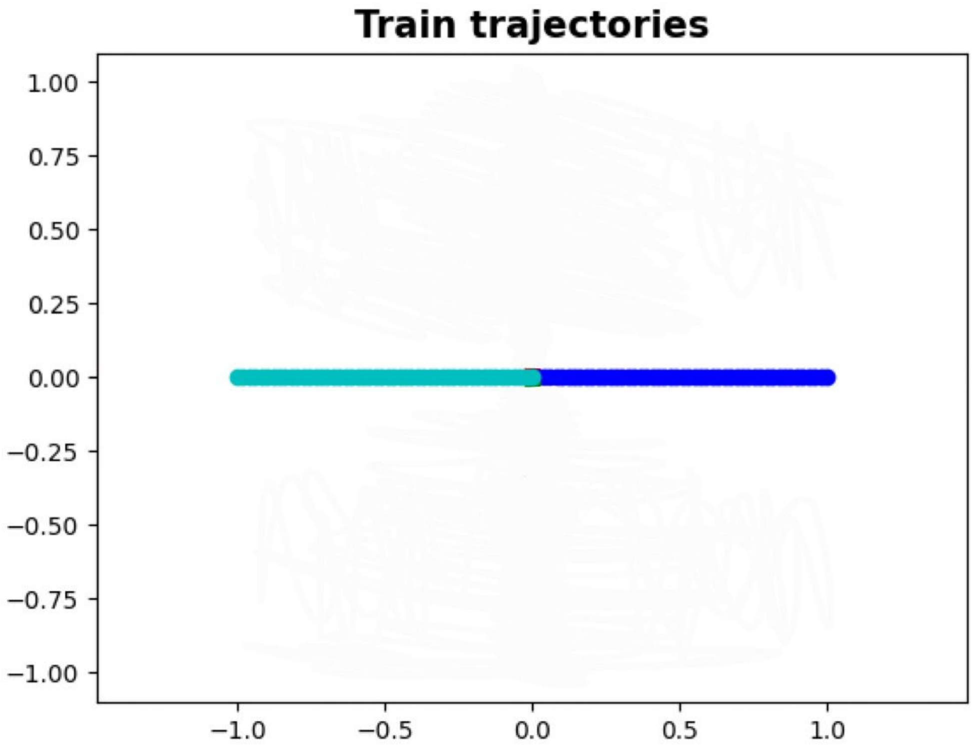
$$\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{\Phi}, \boldsymbol{R})$$



Local POD. Example 2



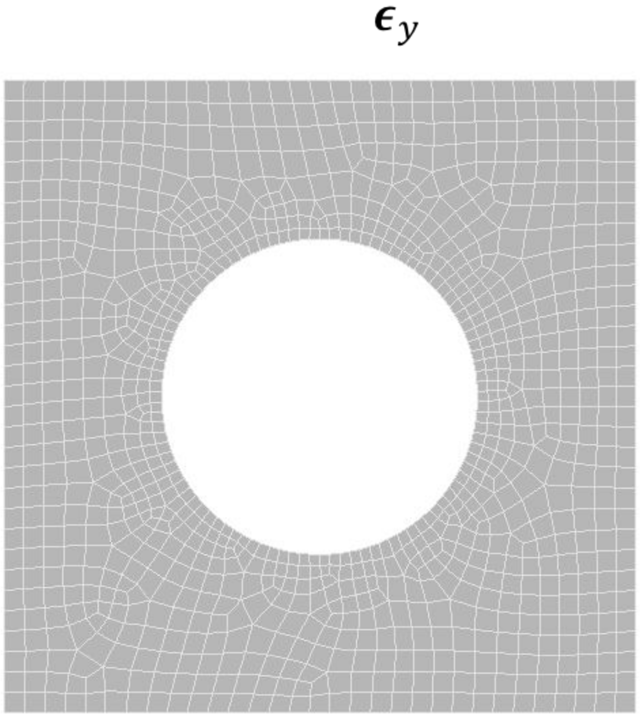
ϵ_x

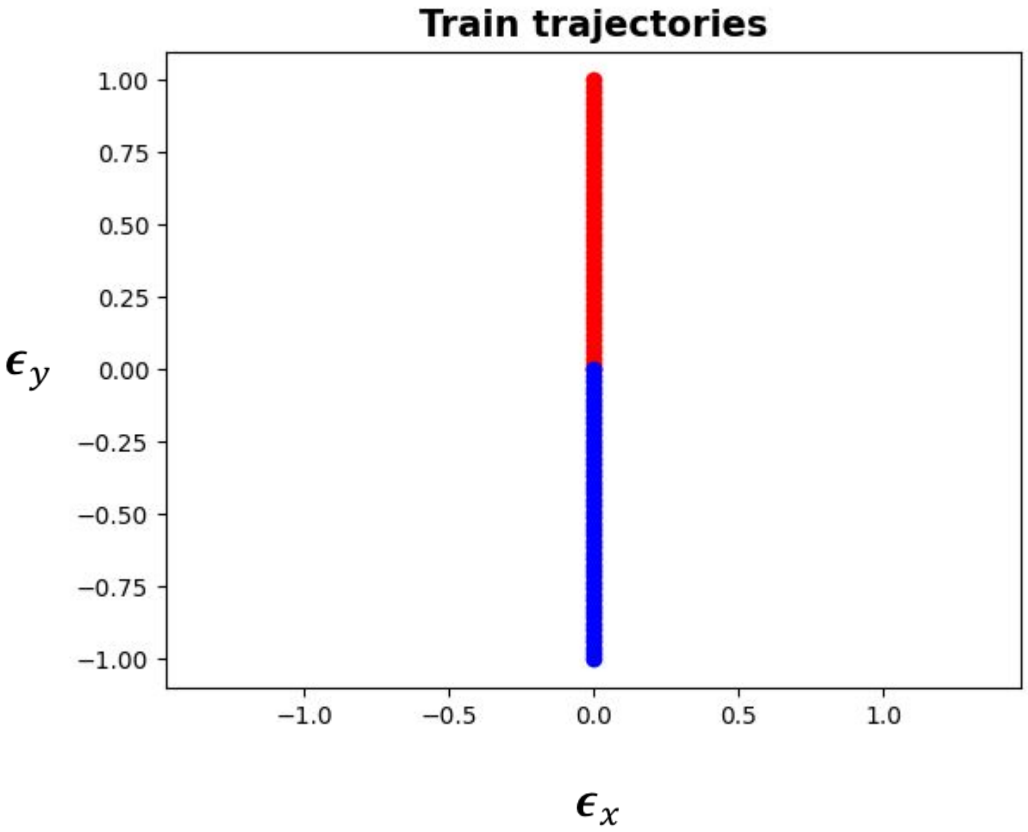


ϵ_y

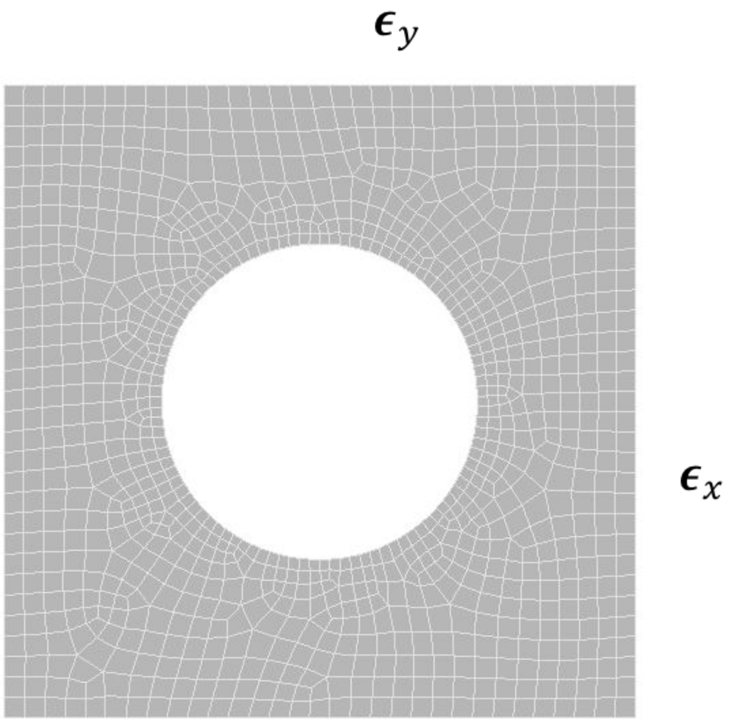
ϵ_x

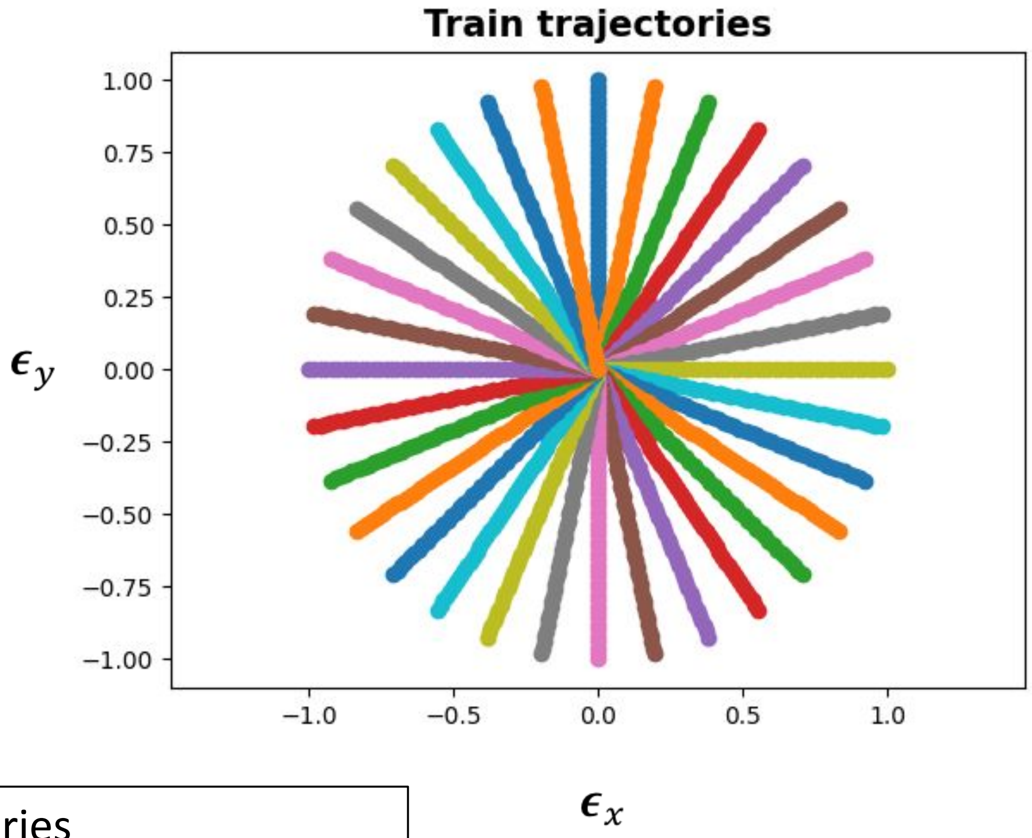
Local POD. Example 2





Local POD. Example 2





32 trajectories
50 snapshots per trajectory
1600 snapshots

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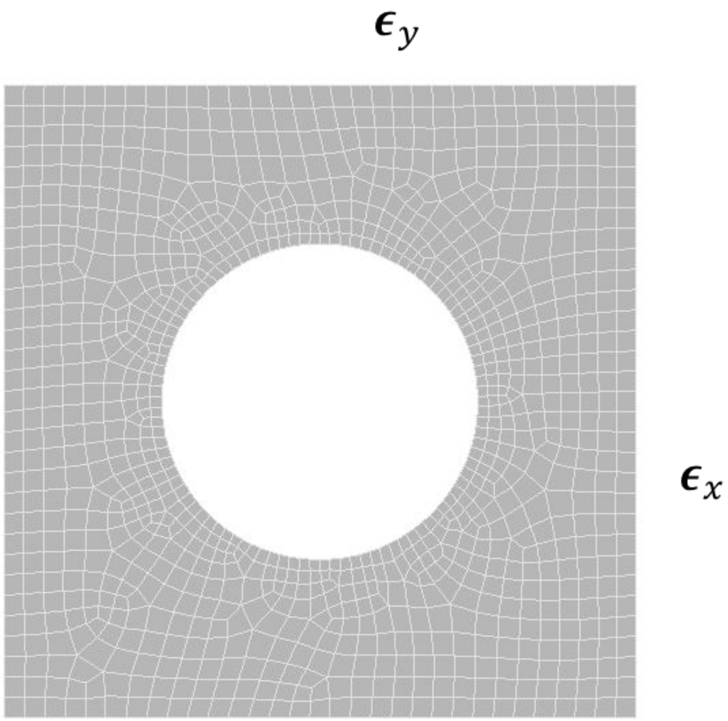
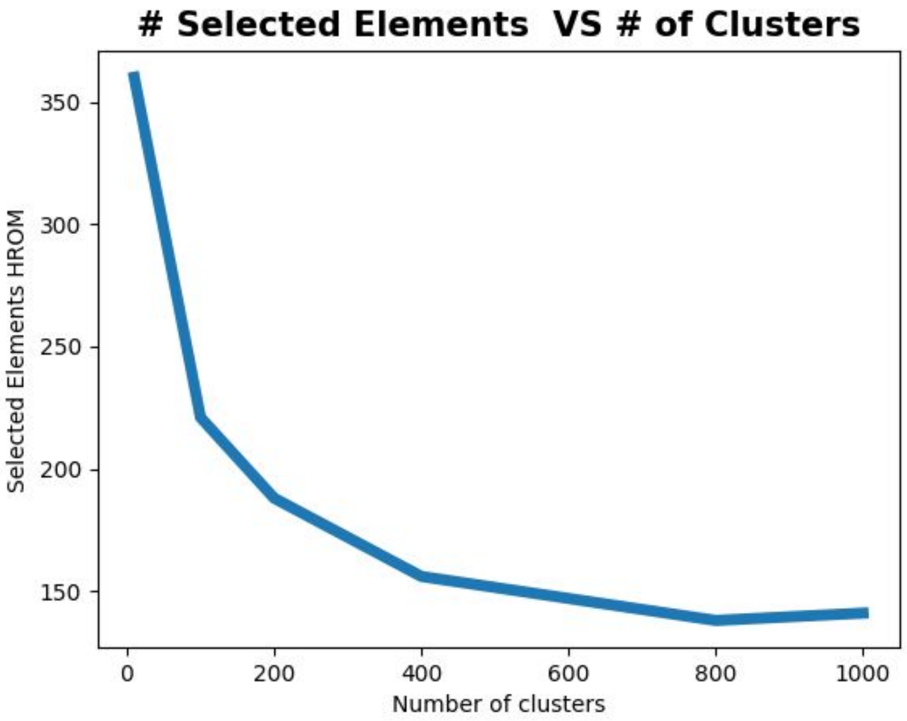
Local POD. Example 2





32 trajectories
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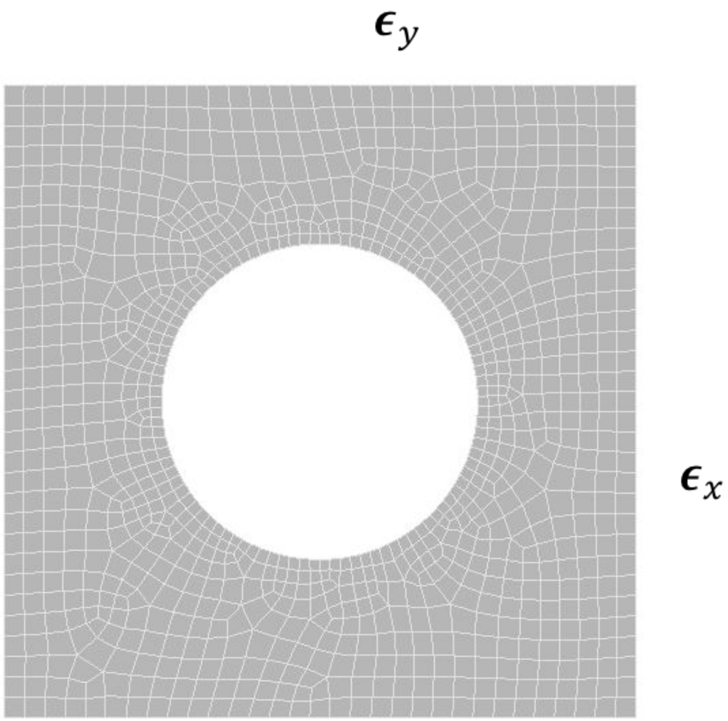
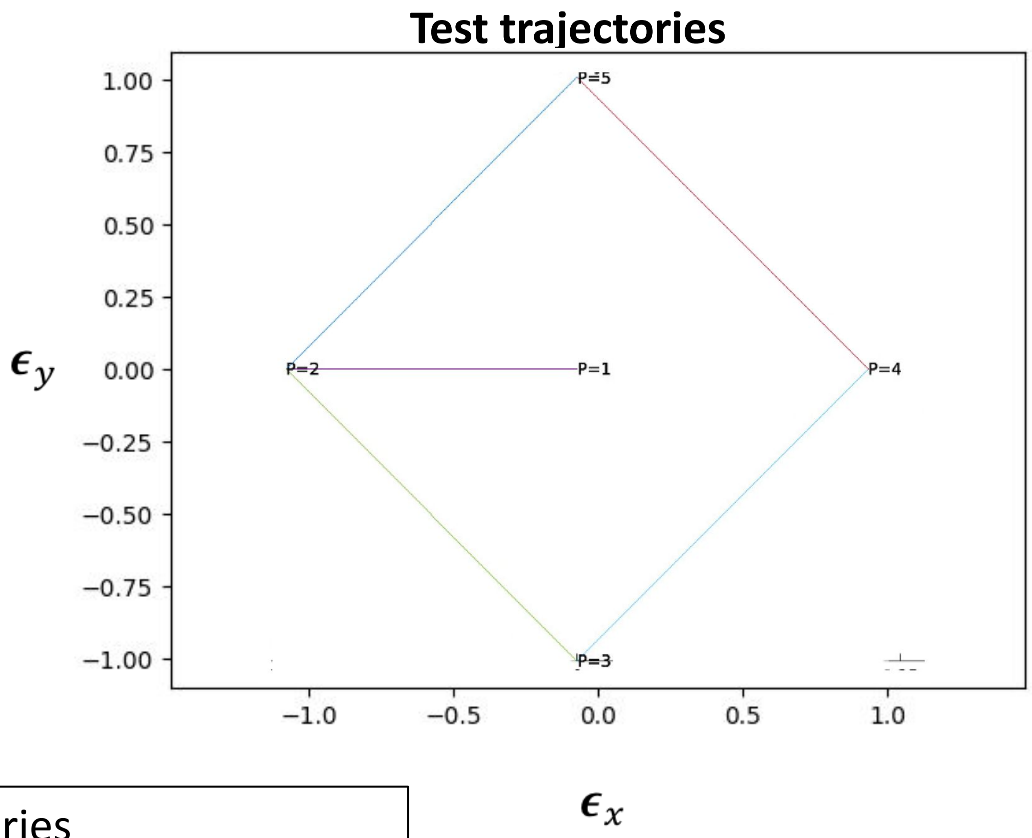
CIMNE EXCELENCIA SEVERO OCHOA KRATOS MULTI-PHYSICS

Local POD. Example 2

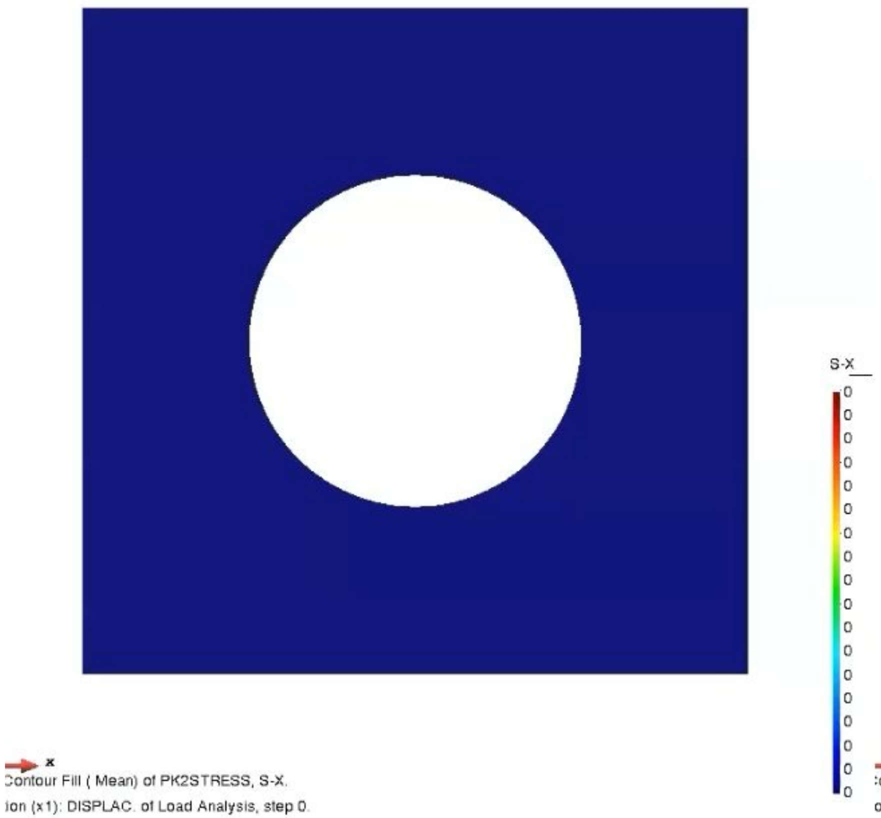




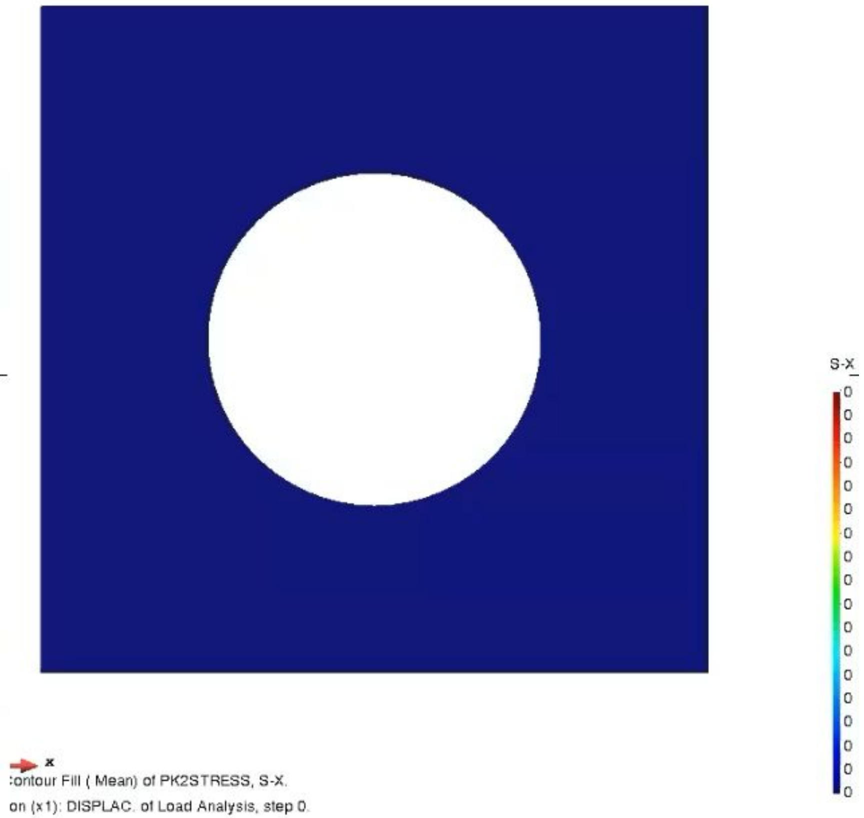
32 trajectories
50 snapshots per trajectory
1600 snapshots

Local POD. Example 2

FOM



HROM



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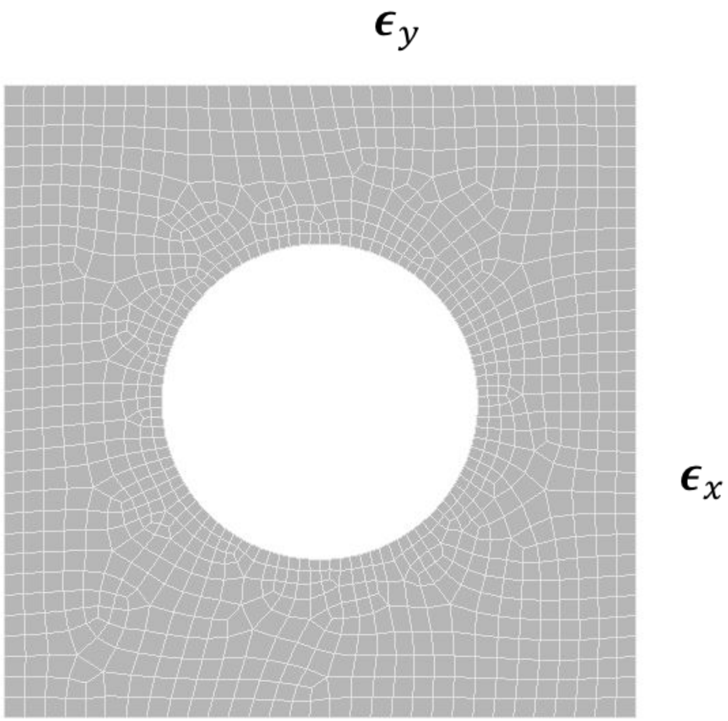
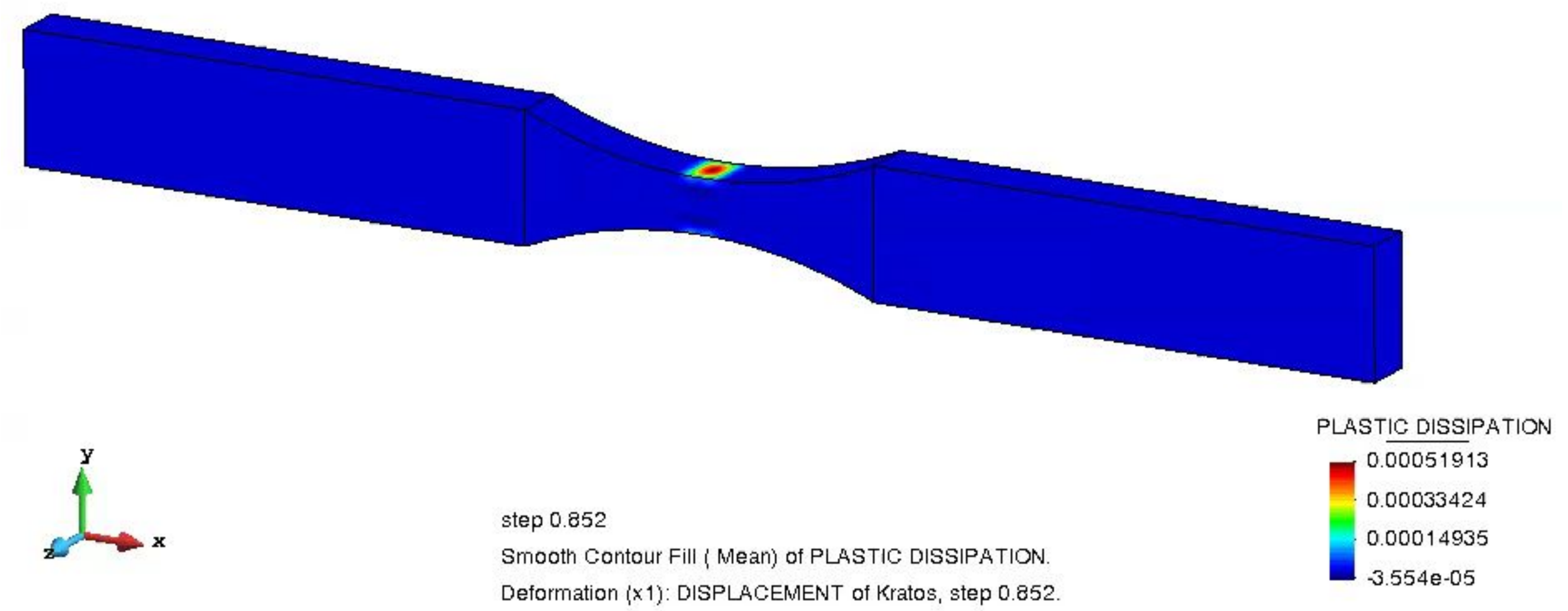
Local POD. Example 2



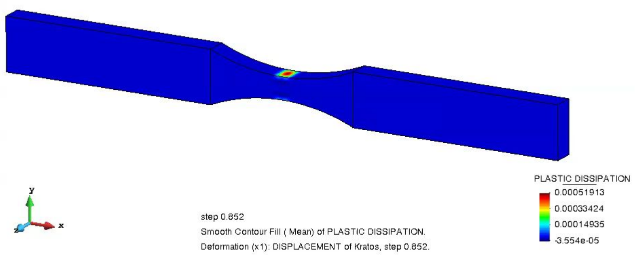
10X less elements required compared with a single basis

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

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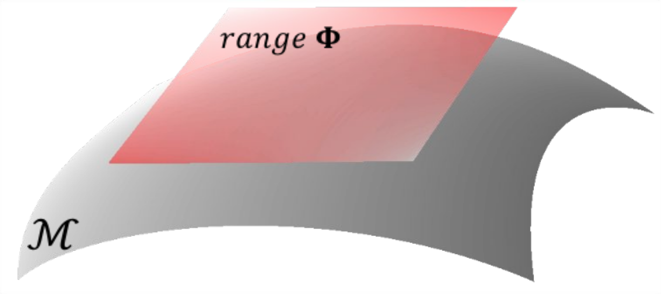
Local POD. Strengths and weaknesses

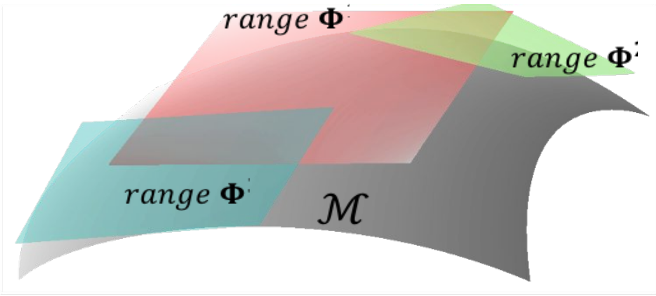
- Reasonable overhead in training and negligible in inference
- Smaller bases and elements sets, therefore faster ROMs

- Easy to overfit to training trajectories

General conclusions

- The Local POD was presented
  - Advantages using our robust overlapping and hyper-reduction
- Future work:
  - application of method to multiple escenarios
  - combination of Local POD with DL





THANK YOU

GRATEFUL TO:

EdgeTwins HPC

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 946009

Link to Kratos github site

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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.