Model Order Reduction for Multidisciplinary Design Optimization in Higher-Dimensional Parameter Spaces

Gabriele Boncoraglio

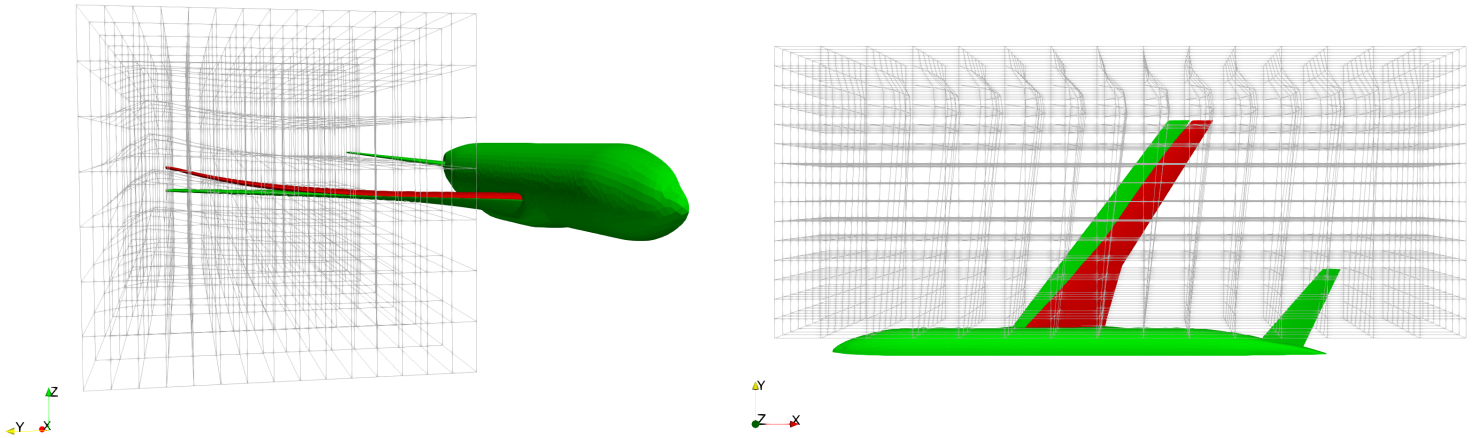
Farhat Research Group
Stanford University

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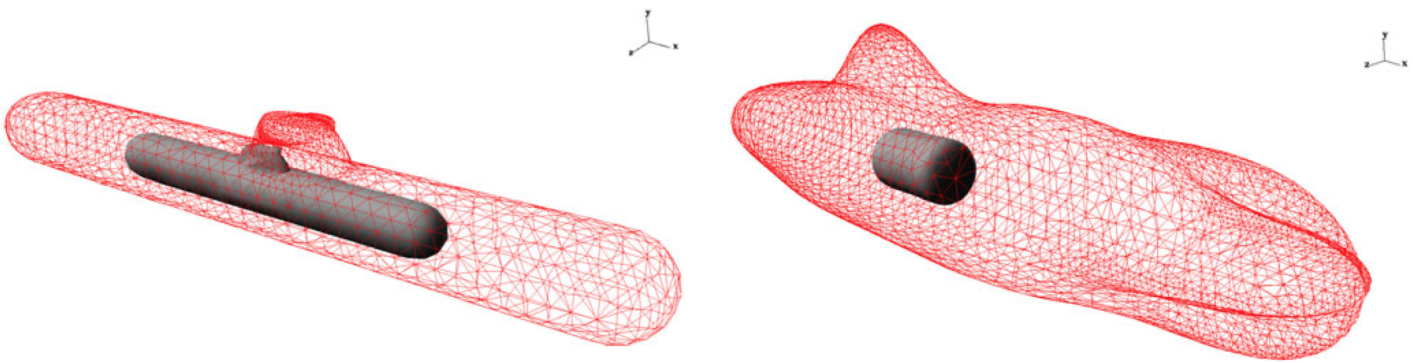


- Optimal design problems



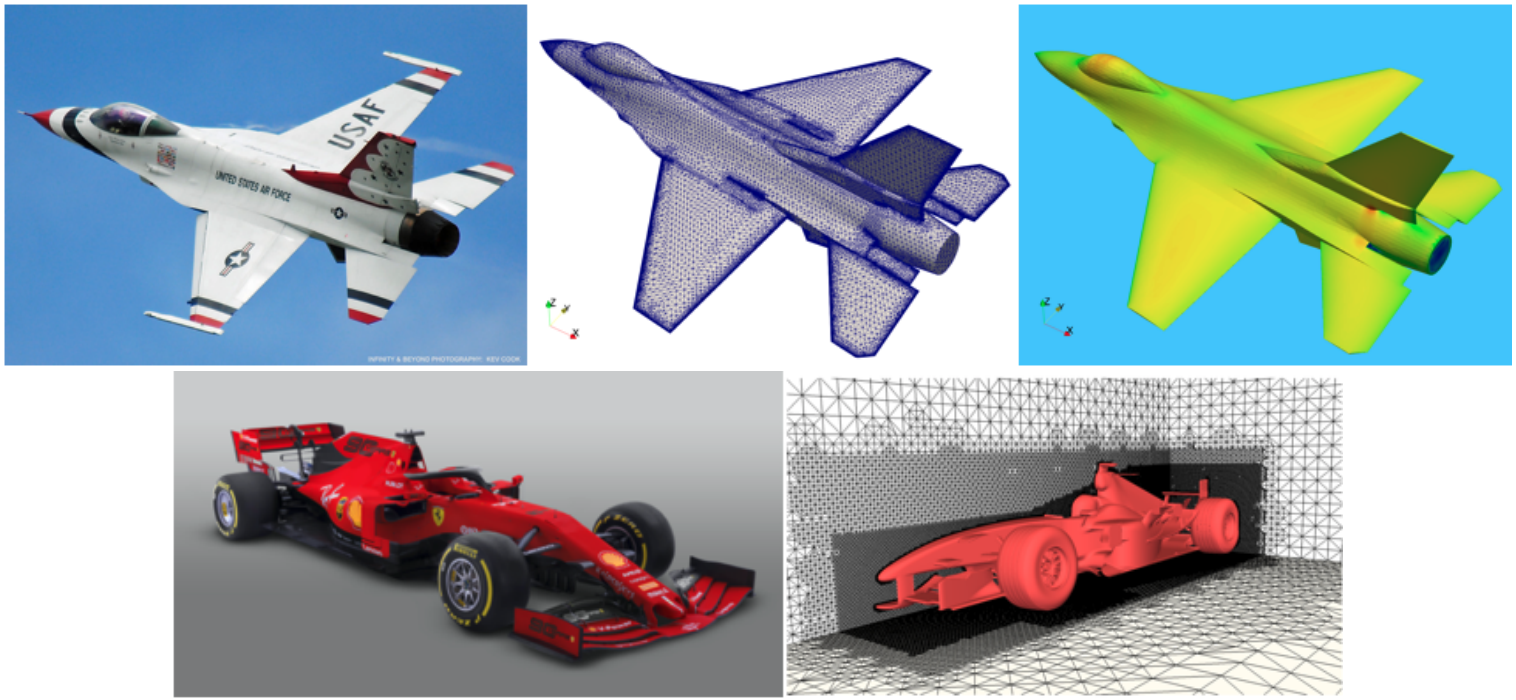
Aerodynamic shape design problem

- Inverse problems



Inverse obstacle acoustic scattering problem

In **computational physics**, the state of the numerical solution of PDEs has reached impressive levels of maturity



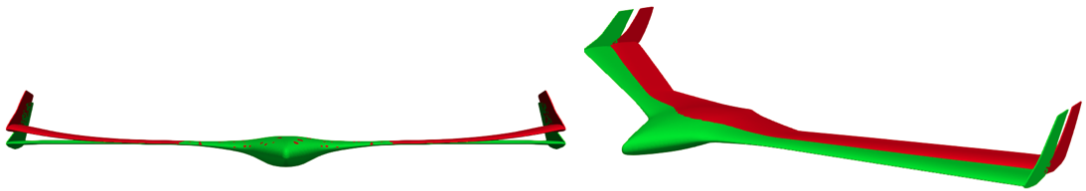
- **High-dimensional simulations** require significant computational resources
- **Repeated** queries of such simulations, as required by the solution of a PDE-constrained optimization problem, may be **prohibitively time-consuming**

$$\min_{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{N_{\boldsymbol{\mu}}}, \mathbf{w} \in \mathbb{R}^{N_{\mathbf{w}}}} \quad f_i(\mathbf{w}; \boldsymbol{\mu}), \qquad i = 1, \cdots, n_f$$

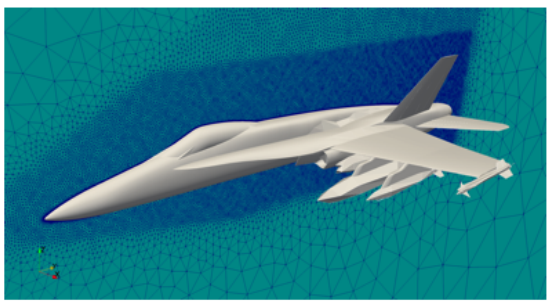
$$\text{subject to} \quad c_j(\mathbf{w}; \boldsymbol{\mu}) \geqslant 0, \quad j = 1, \cdots, n_c$$

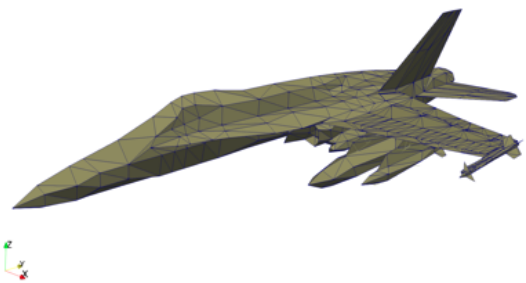
$$\mathbf{R}(\mathbf{w}; \boldsymbol{\mu}) = \mathbf{0}$$

- $\mathbf{R} : \mathbb{R}^{N_{\mathbf{w}}} \times \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}^{N_{\mathbf{w}}}$ — discretized PDE
- $f_i : \mathbb{R}^{N_{\mathbf{w}}} \times \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}$ — i-th objective function
- $c_j : \mathbb{R}^{N_{\mathbf{w}}} \times \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}$ — j-th algebraic constraint
- $\mathbf{w} \in \mathbb{R}^{N_{\mathbf{w}}}$ — PDE state vector
- $\boldsymbol{\mu} \in \mathbb{R}^{N_{\boldsymbol{\mu}}}$ — optimization parameters







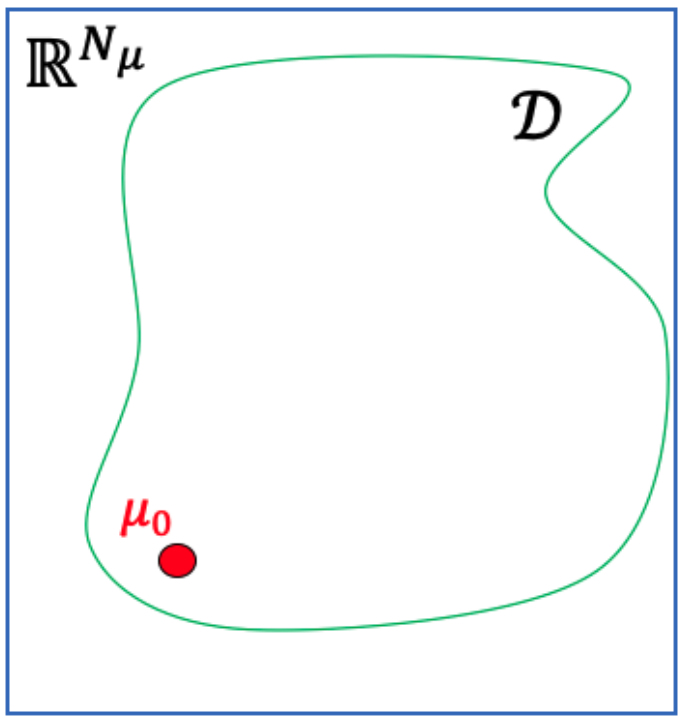


$$\begin{aligned} \min_{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{N_{\boldsymbol{\mu}}}} \quad & f_i(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}), && i = 1, \cdots, n_f \\ \text{subject to} \quad & c_j(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}) \geqslant 0, && j = 1, \cdots, n_c \end{aligned}$$

- The components of $\boldsymbol{\mu}$ are the only optimization parameters
- **Several CPU-intensive solutions** of the aforementioned PDEs

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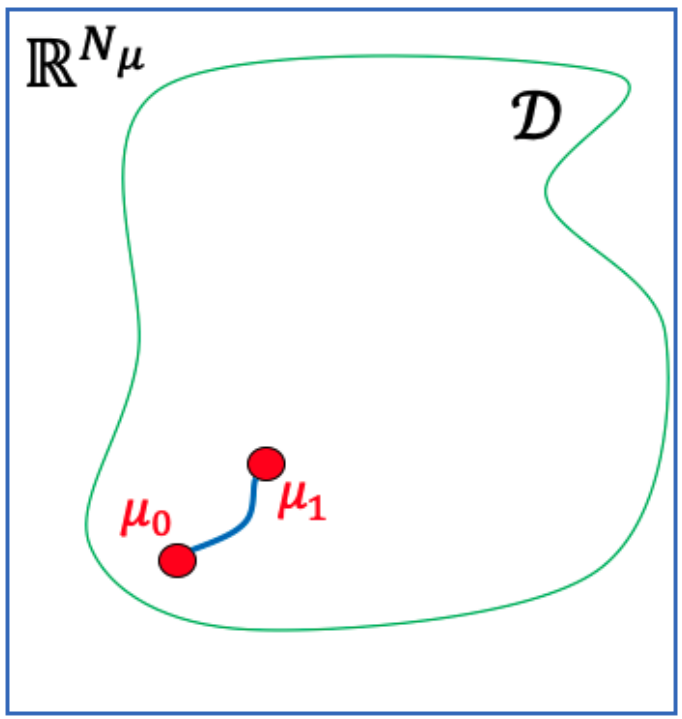
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$$\boldsymbol{\mu}_0 \quad \rightarrow \quad \mathbf{R}(\mathbf{w}; \boldsymbol{\mu}_0) = \mathbf{0} \quad \rightarrow \quad \mathbf{w}_0 = \mathbf{w}(\boldsymbol{\mu}_0) \quad \rightarrow \quad \begin{cases} f_i(\mathbf{w}_0; \boldsymbol{\mu}_0) \\ c_j(\mathbf{w}_0; \boldsymbol{\mu}_0) \end{cases}$$

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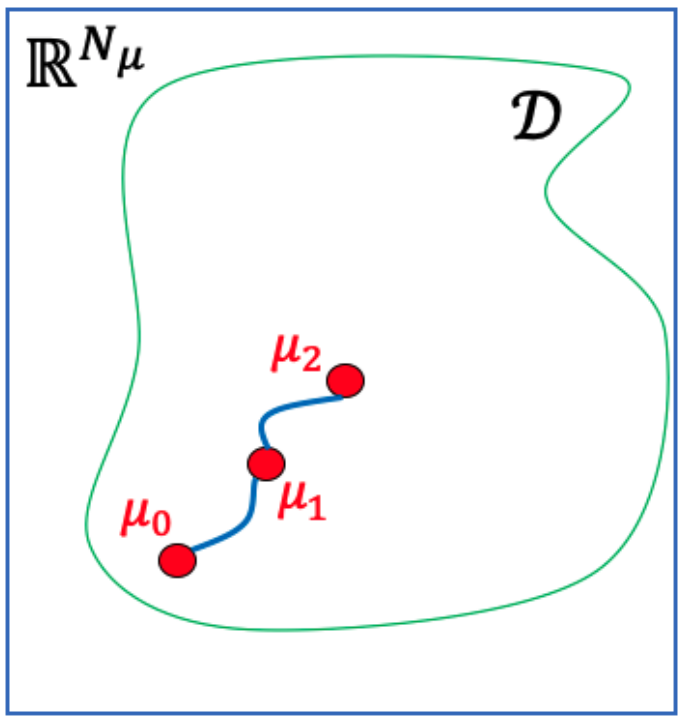
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$$\boldsymbol{\mu}_1 \quad \rightarrow \quad \mathbf{R}(\mathbf{w}, \boldsymbol{\mu}_1) = \mathbf{0} \quad \rightarrow \quad \mathbf{w}_1 = \mathbf{w}(\boldsymbol{\mu}_1) \quad \rightarrow \quad \begin{cases} f_i(\mathbf{w}_1; \boldsymbol{\mu}_1) \\ c_j(\mathbf{w}_1; \boldsymbol{\mu}_1) \end{cases}$$

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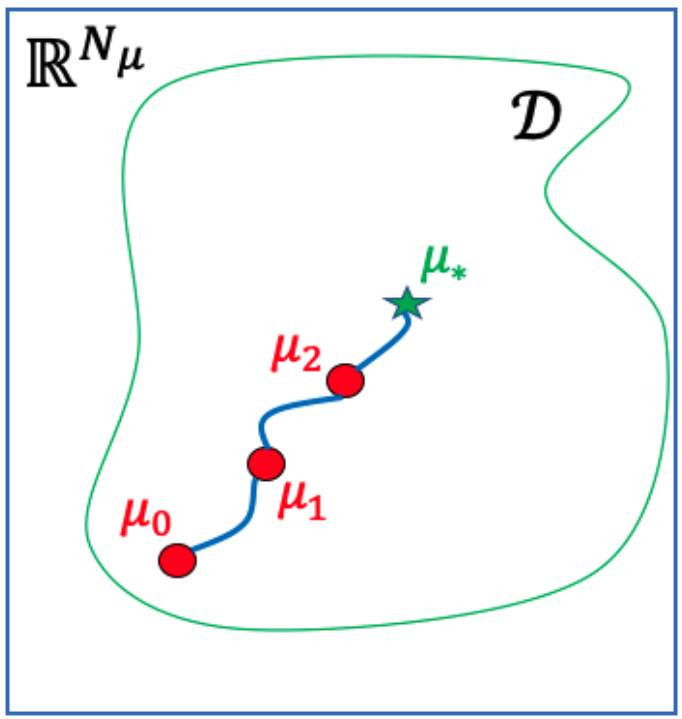


$$\boldsymbol{\mu}_2 \quad \rightarrow \quad \mathbf{R}(\mathbf{w}, \boldsymbol{\mu}_2) = \mathbf{0} \quad \rightarrow \quad \mathbf{w}_2 = \mathbf{w}(\boldsymbol{\mu}_2) \quad \rightarrow \quad \begin{cases} f_i(\mathbf{w}_2; \boldsymbol{\mu}_2) \\ c_j(\mathbf{w}_2; \boldsymbol{\mu}_2) \end{cases}$$

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$$\boldsymbol{\mu}_* \quad \rightarrow \quad \mathbf{R}(\mathbf{w}; \boldsymbol{\mu}_*) = \mathbf{0} \quad \rightarrow \quad \mathbf{w}_* = \mathbf{w}(\boldsymbol{\mu}_*) \quad \rightarrow \quad \begin{cases} f_i(\mathbf{w}_*; \boldsymbol{\mu}_*) \\ c_j(\mathbf{w}_*; \boldsymbol{\mu}_*) \end{cases}$$

- Model reduction ansatz: state vector lies in a low-dimensional affine subspace

$$\mathbf{w} \approx \mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}}\mathbf{w}_r$$

  - $\mathbf{V}_{\mathbf{w}} = \left[\mathbf{v}_1, \cdots, \mathbf{v}_{N_{\mathbf{w}_r}}\right] \in \mathbb{R}^{N_{\mathbf{w}} \times N_{\mathbf{w}_r}}$ is the ROB ($N_{\mathbf{w}} \gg N_{\mathbf{w}_r}$)
  - $\mathbf{w}_r \in \mathbb{R}^{N_{\mathbf{w}_r}}$ are the generalized coordinates of $\mathbf{w}$

- Substitute into $\mathbf{R}(\mathbf{w}; \boldsymbol{\mu}) = \mathbf{0}$ and project onto columnspace of a basis $\mathbf{W}_{\mathbf{w}} \in \mathbb{R}^{N_{\mathbf{w}} \times N_{\mathbf{w}_r}}$ to obtain a square system, i.e., the projection-based reduced-order model (PROM)

$$\mathbf{r}(\mathbf{w}_r; \boldsymbol{\mu}) = \mathbf{W}_{\mathbf{w}}^{\top}\mathbf{R}(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}}\mathbf{w}_r; \boldsymbol{\mu}) = \mathbf{0}$$

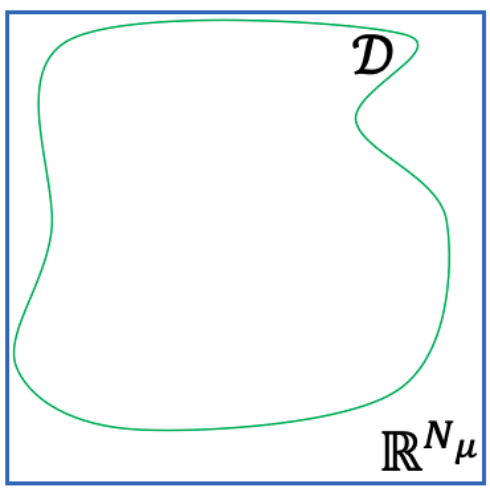
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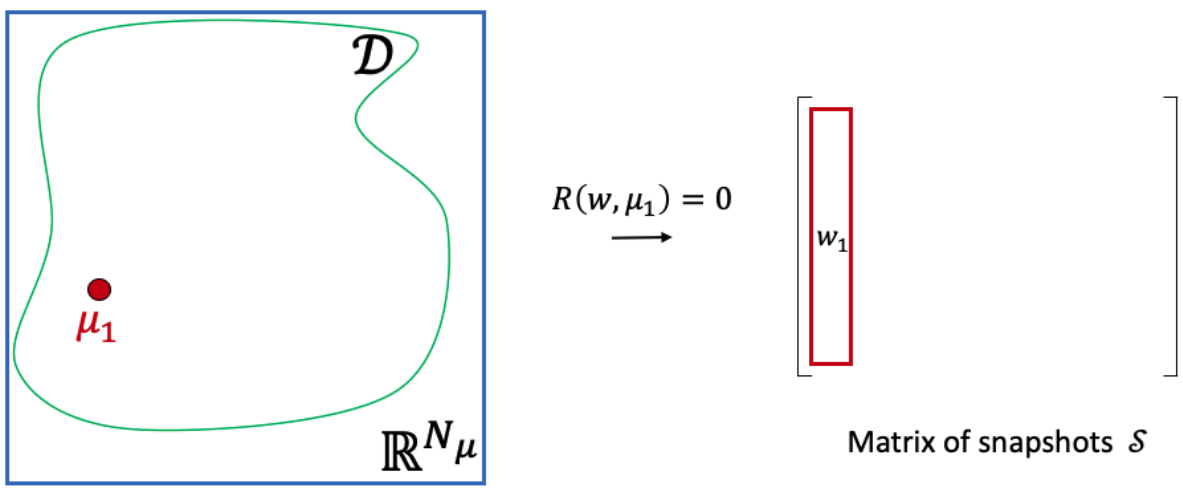
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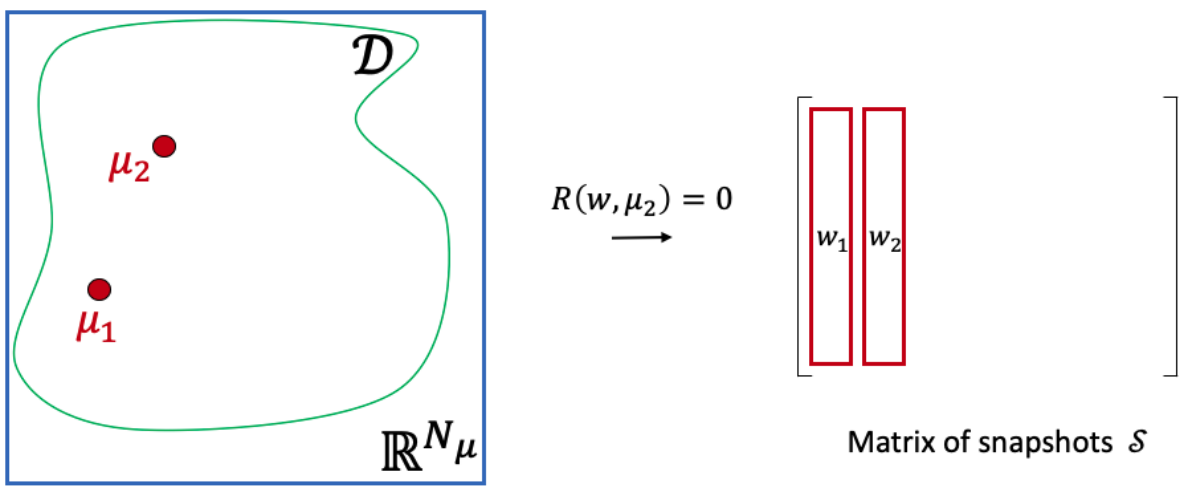
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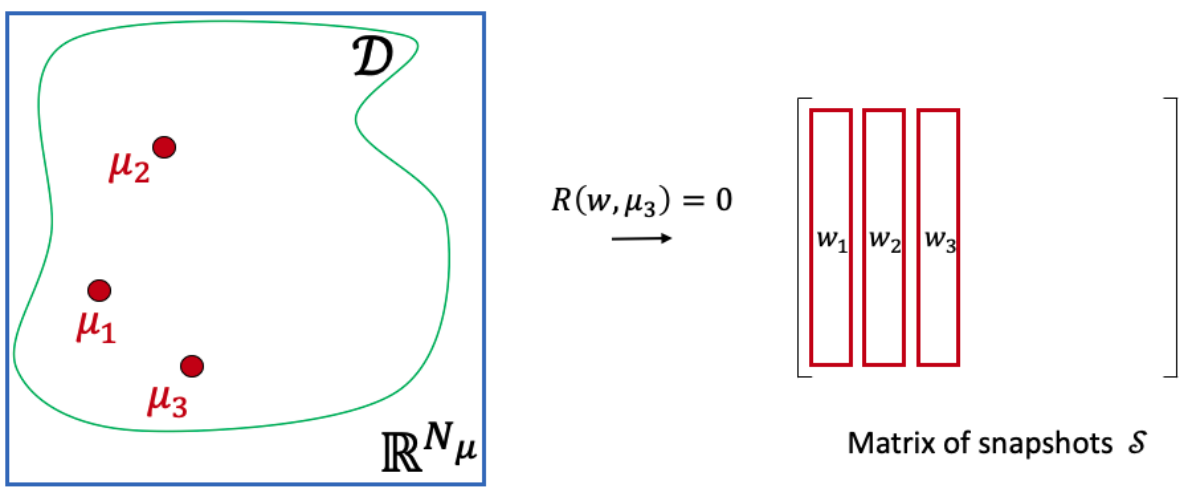
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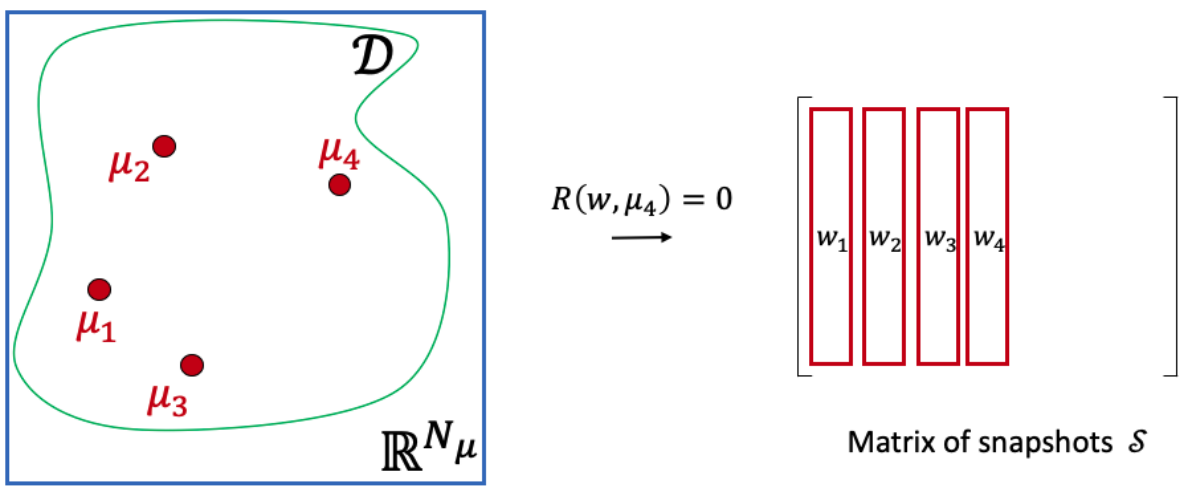
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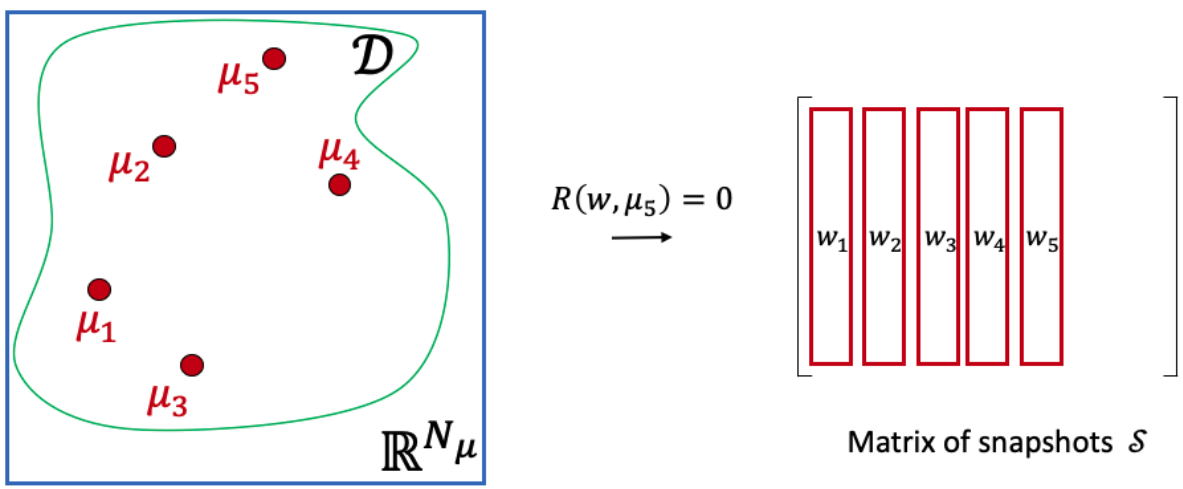
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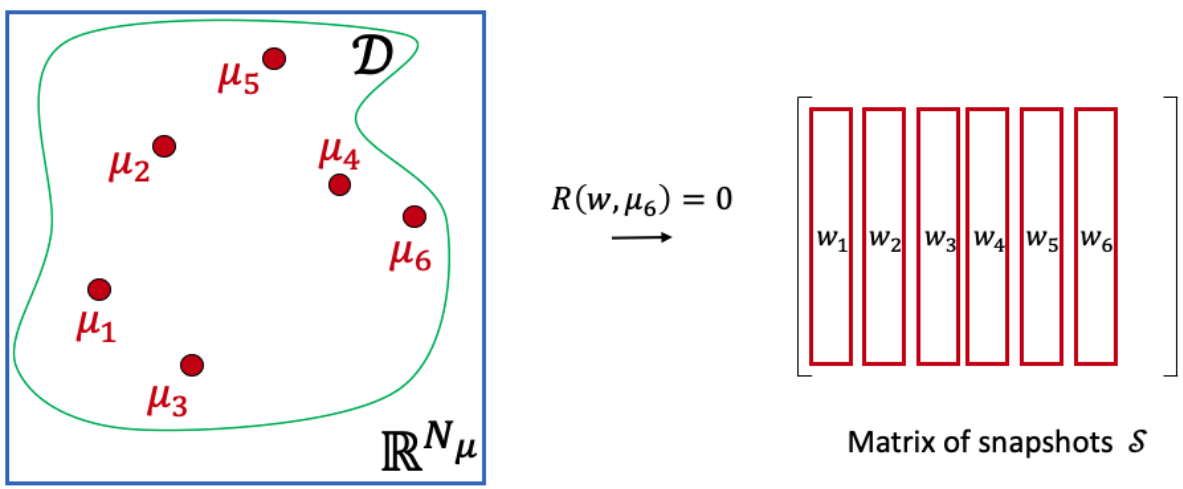
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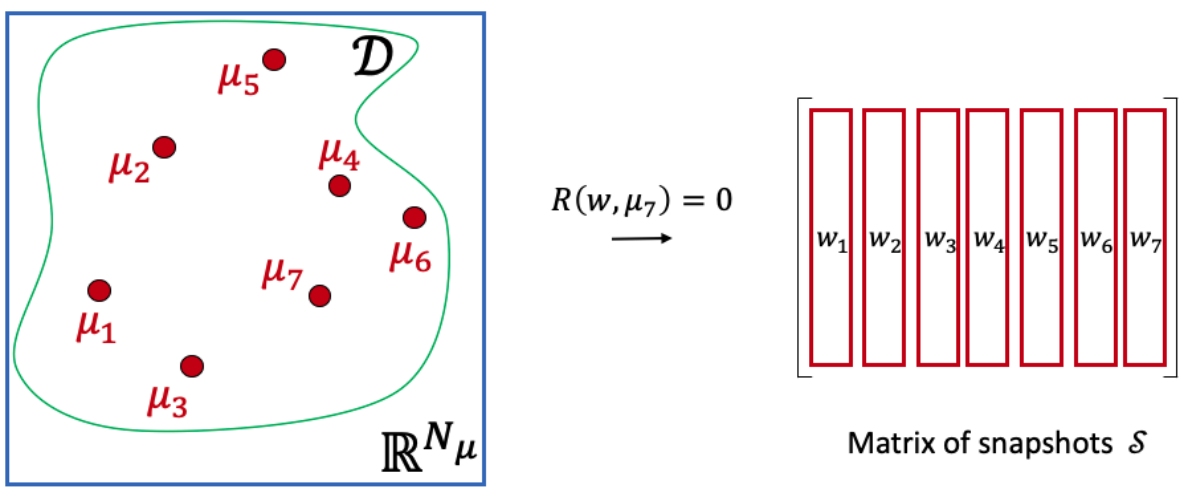
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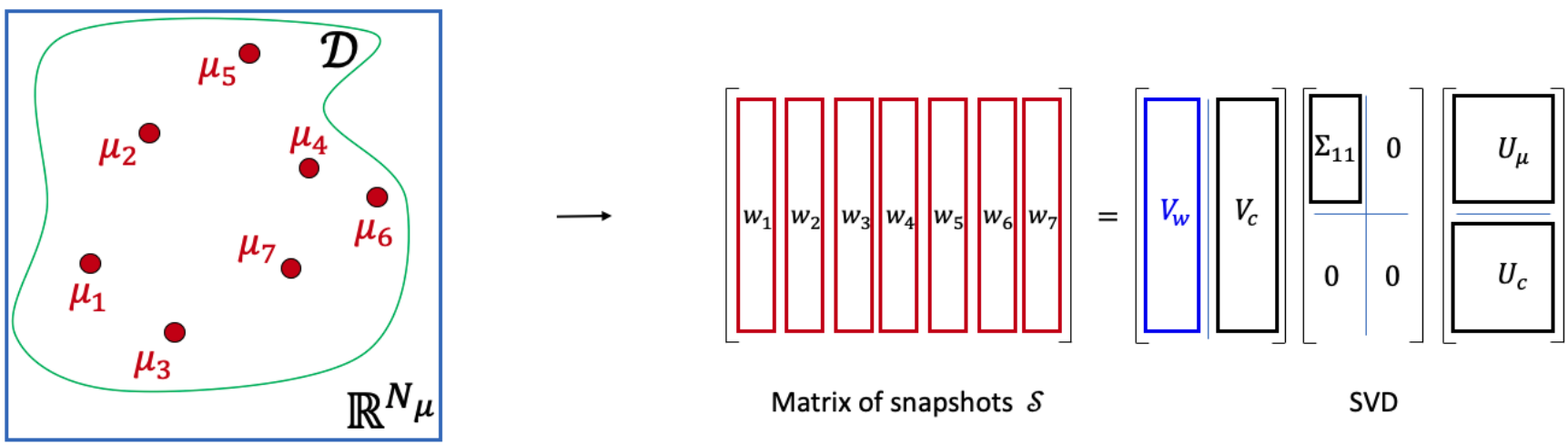
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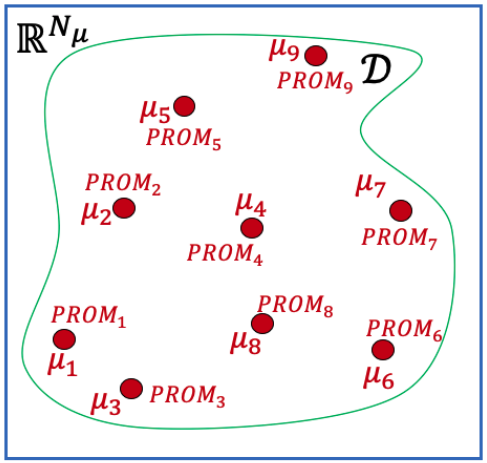
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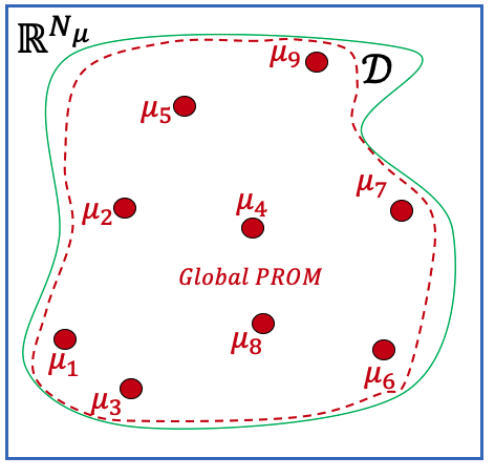
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- Different PROMs for different types of parametric PDEs

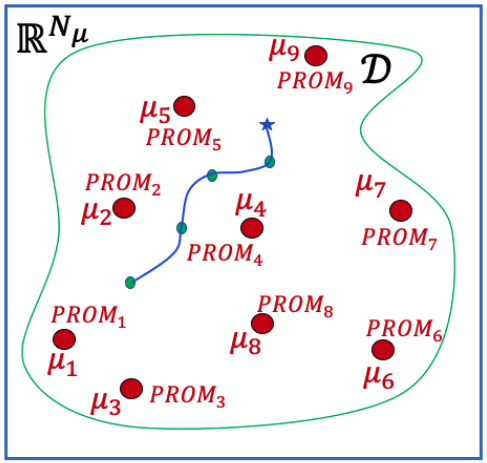


Database $\mathcal{DB}$ of local linear PROMs

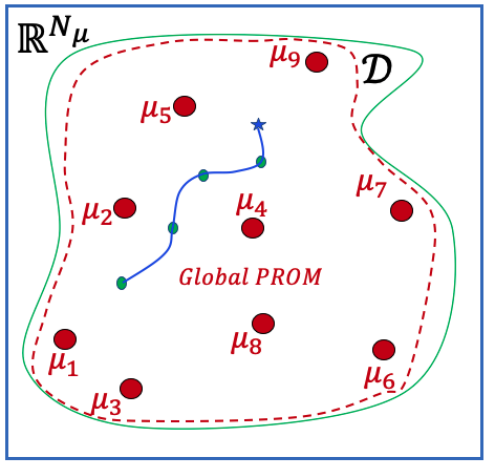


Global nonlinear PROMs

- Different PROMs for different types of parametric PDEs

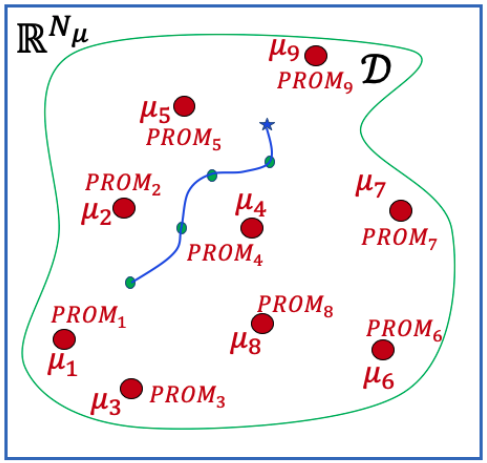


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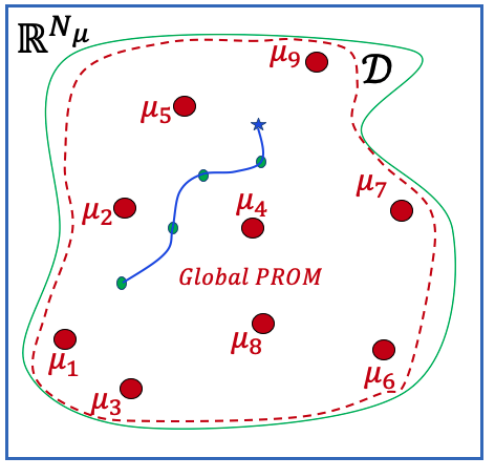


Global nonlinear PROMs

- Different PROMs for different types of parametric PDEs



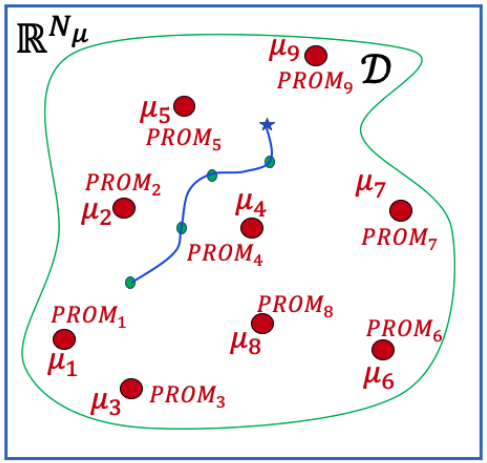
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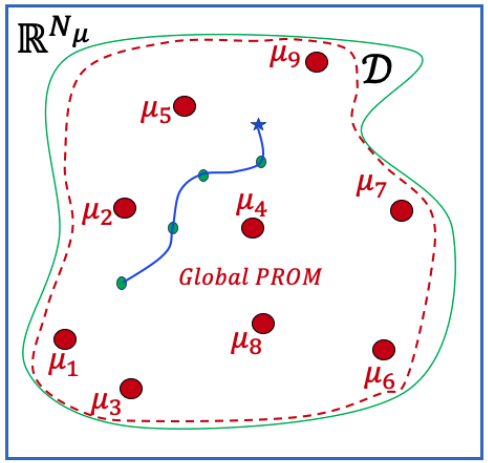
Global nonlinear PROMs

- Proposed approach
  - solve the optimization problem in a **lower-dimensional** active design space $\mathcal{D}_A$
  - use the concept of a piecewise-global rather than global model

- Different PROMs for different types of parametric PDEs

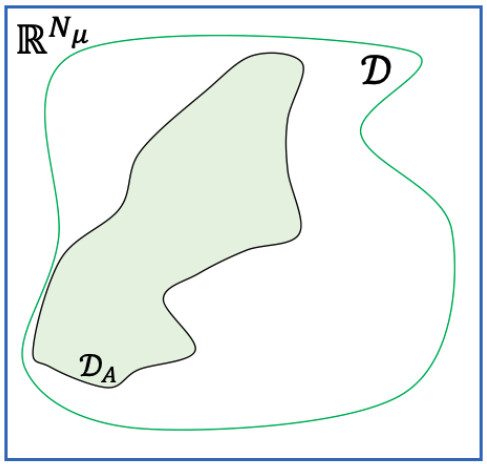


Database $\mathcal{DB}$ of local linear PROMs

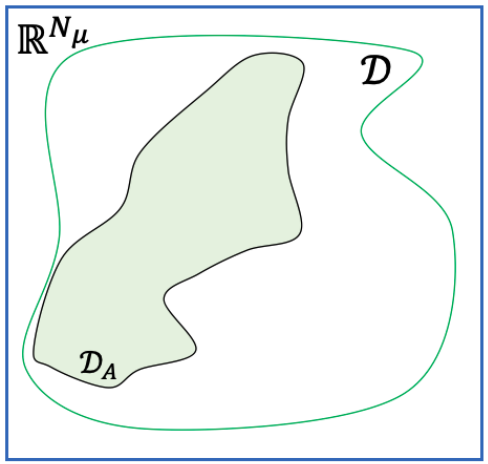


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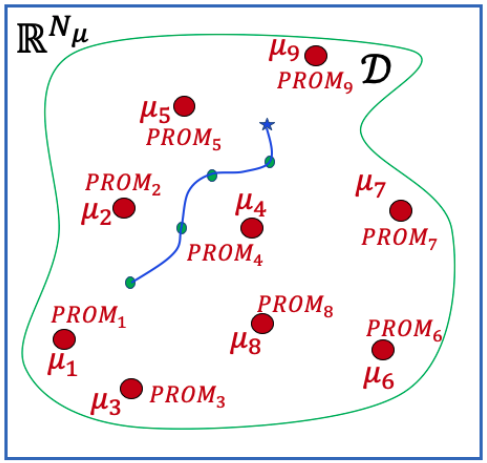


Database $\mathcal{DB}$ of local linear PROMs

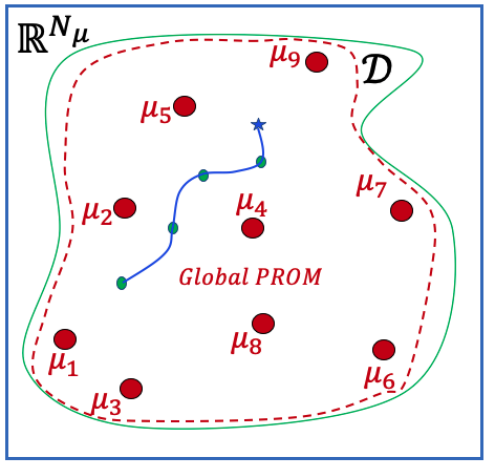


Global nonlinear PROMs

- Different PROMs for different types of parametric PDEs

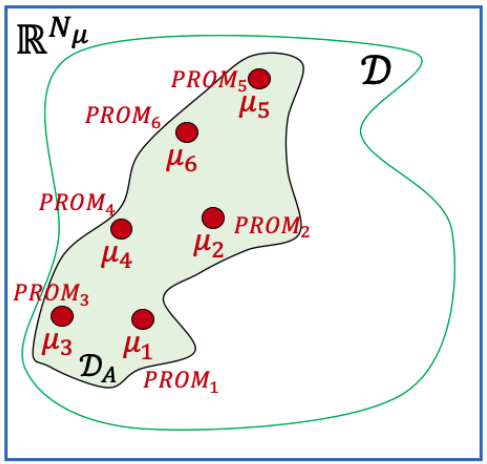


Database $\mathcal{DB}$ of local linear PROMs

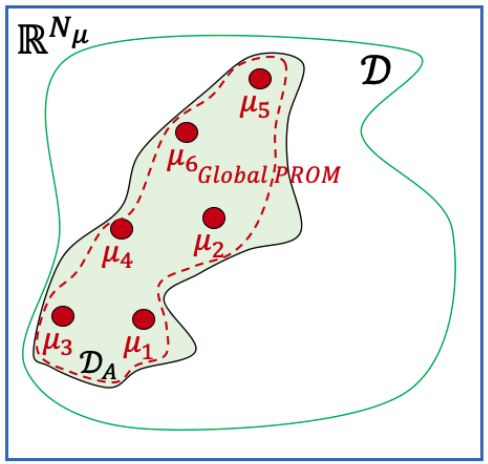


Global nonlinear PROMs

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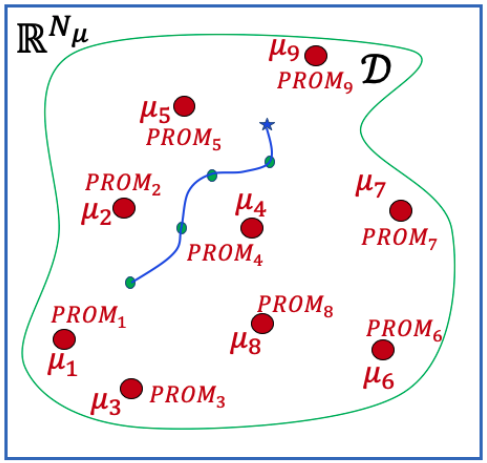


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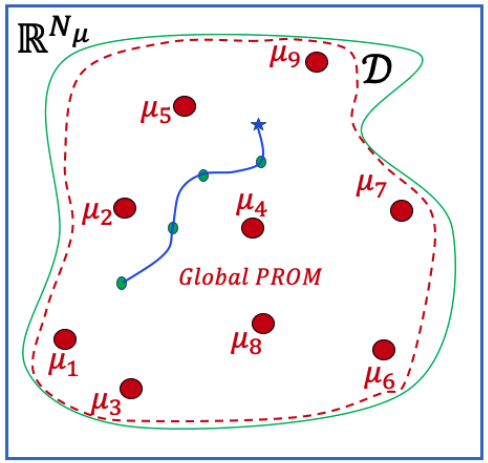


Global nonlinear PROMs

- Different PROMs for different types of parametric PDEs

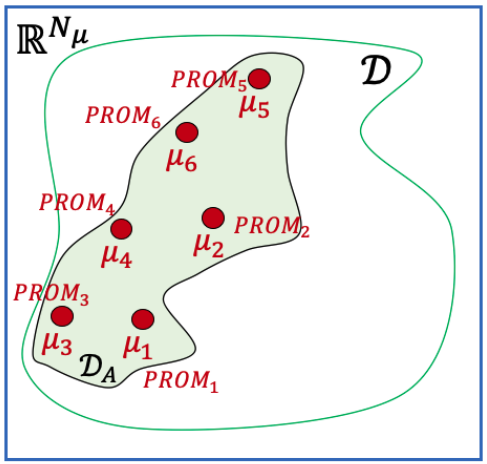


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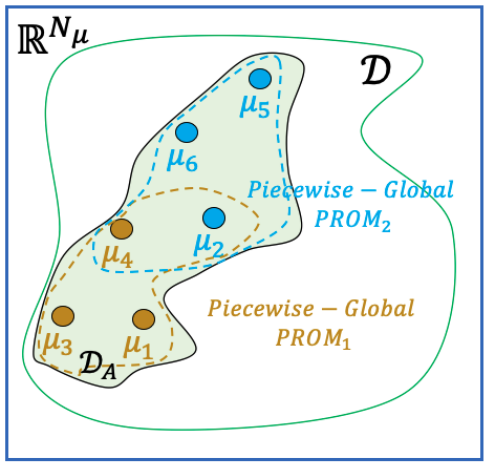


Global nonlinear PROMs

- Proposed approach
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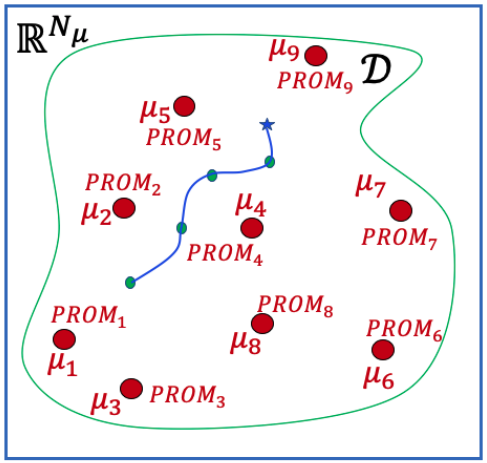


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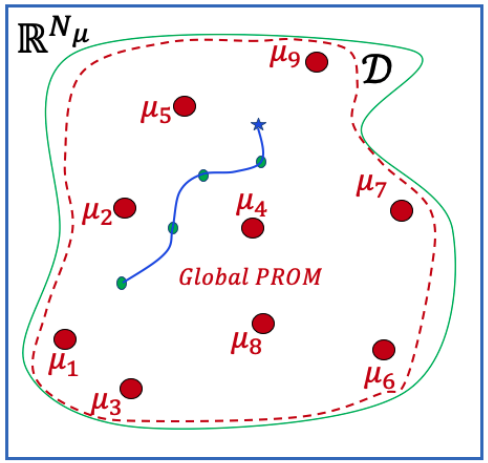


Piecewise-Global nonlinear PROMs

- Different PROMs for different types of parametric PDEs

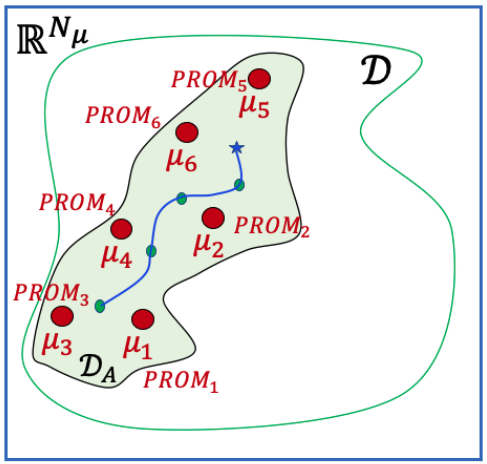


Database $\mathcal{DB}$ of local linear PROMs

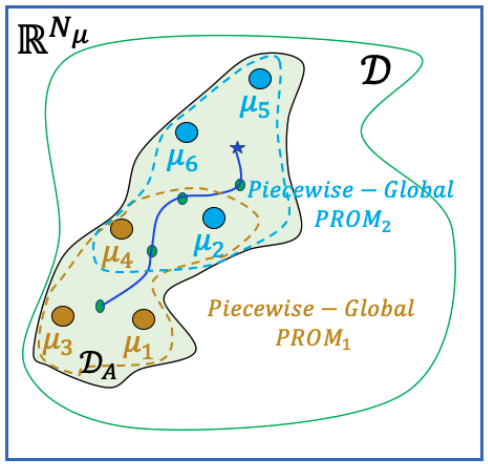


Global nonlinear PROMs

- Proposed approach
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Database $\mathcal{DB}$ of local linear PROMs



Piecewise-Global nonlinear PROMs

Parametric linear PDE

$$\mathbf{R}(\mathbf{w}(\boldsymbol{\mu});\boldsymbol{\mu}) = \mathbf{A}(\boldsymbol{\mu})\,\dot{\mathbf{w}}(\boldsymbol{\mu}) + \mathbf{B}(\boldsymbol{\mu})\,\mathbf{w}(\boldsymbol{\mu}) - \mathbf{c}(\boldsymbol{\mu}) = \mathbf{0}$$

where $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{N_{\mathbf{w}} \times N_{\mathbf{w}}}$ and $\mathbf{c}, \mathbf{w} \in \mathbb{R}^{N_{\mathbf{w}}}$

- Galerkin ($\mathbf{W}_{\mathbf{w}} = \mathbf{V}_{\mathbf{w}}$) or Petrov-Galerkin ($\mathbf{W}_{\mathbf{w}} \neq \mathbf{V}_{\mathbf{w}}$) PROM

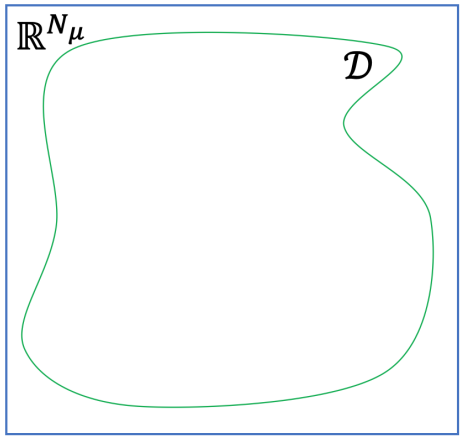
$$\mathbf{r}(\mathbf{w}_r(\boldsymbol{\mu});\boldsymbol{\mu}) = \left(\mathbf{W}_{\mathbf{w}}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{V}_{\mathbf{w}}\right)\,\dot{\mathbf{w}}_r(\boldsymbol{\mu}) + \left(\mathbf{W}_{\mathbf{w}}^T\mathbf{B}(\boldsymbol{\mu})\mathbf{V}_{\mathbf{w}}\right)\,\mathbf{w}_r(\boldsymbol{\mu}) - \mathbf{W}_{\mathbf{w}}^T\mathbf{c}(\boldsymbol{\mu}) = \mathbf{0}$$

- For a specific $\boldsymbol{\mu}$, the parametric, linear PROM is described by

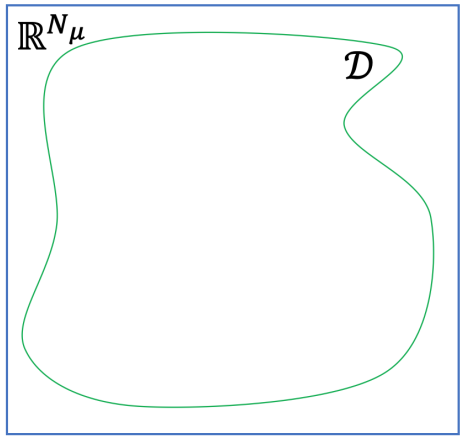
$$\mathcal{T}_r(\boldsymbol{\mu}) = \{\mathbf{A}_r(\boldsymbol{\mu}), \mathbf{B}_r(\boldsymbol{\mu}), \mathbf{c}_r(\boldsymbol{\mu})\} = \left\{\mathbf{W}_{\mathbf{w}}^T\mathbf{A}(\boldsymbol{\mu})\mathbf{V}_{\mathbf{w}}, \mathbf{W}_{\mathbf{w}}^T\mathbf{B}(\boldsymbol{\mu})\mathbf{V}_{\mathbf{w}}, \mathbf{W}_{\mathbf{w}}^T\mathbf{c}(\boldsymbol{\mu})\right\}$$

with $\mathbf{A}_r, \mathbf{B}_r \in \mathbb{R}^{N_{\mathbf{w}_r} \times N_{\mathbf{w}_r}}$ and $\mathbf{c}_r, \mathbf{w}_r \in \mathbb{R}^{N_{\mathbf{w}_r}}$

1. Build a database $\mathcal{DB} = \{\mathcal{T}_r(\boldsymbol{\mu}_j)\}_{j=1}^{N_{\mathcal{DB}}}$ by **sampling** $\mathcal{D}$

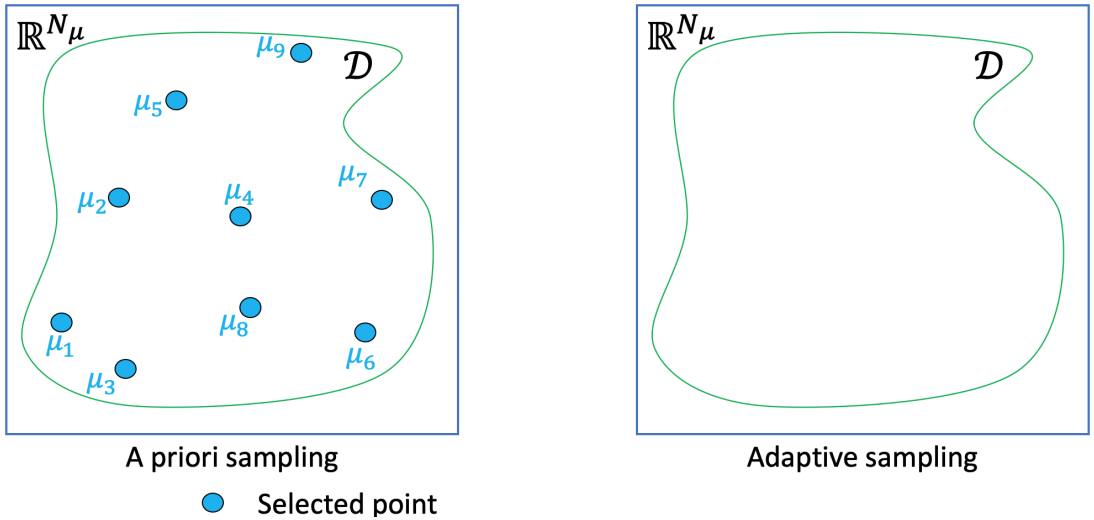


A priori sampling

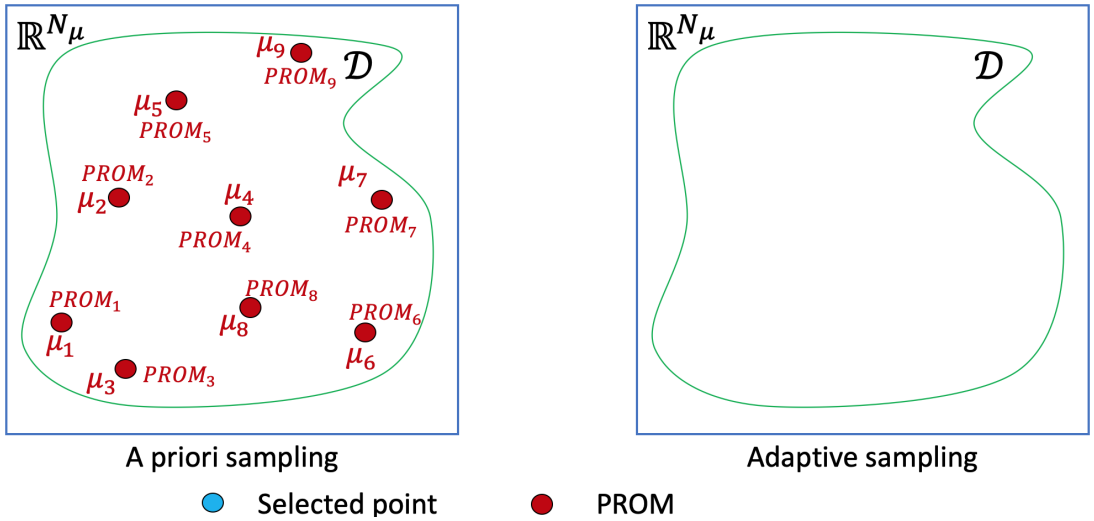


Adaptive sampling

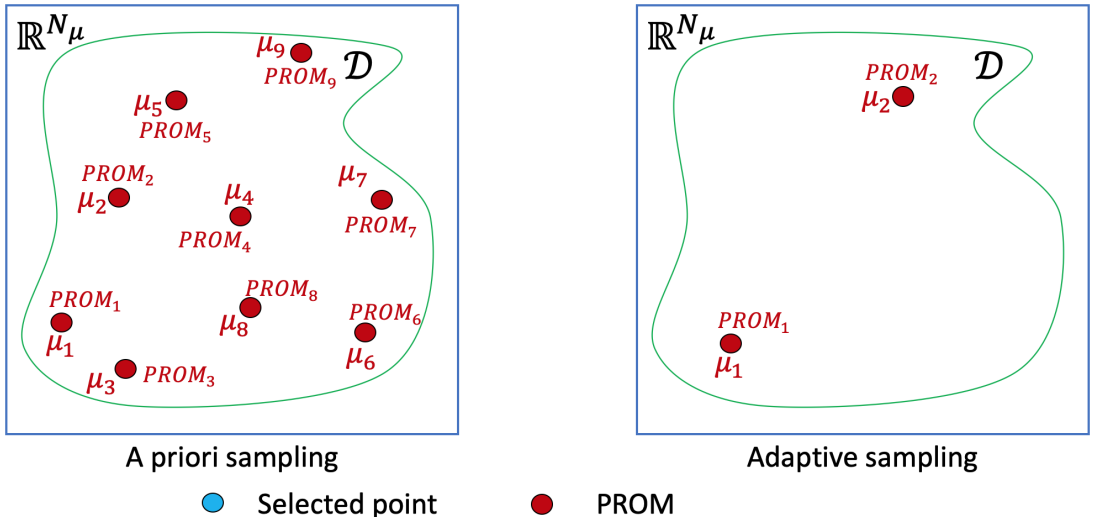
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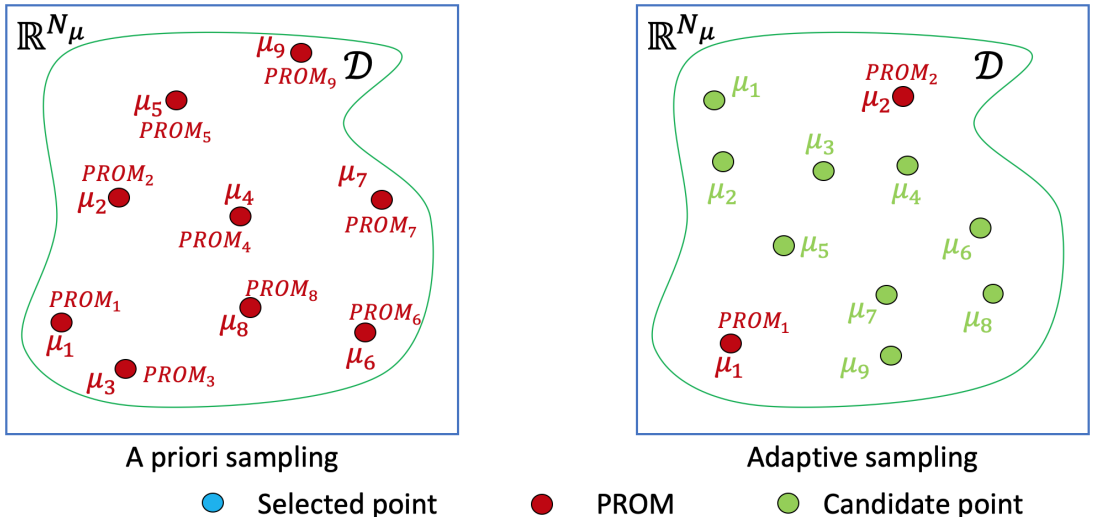
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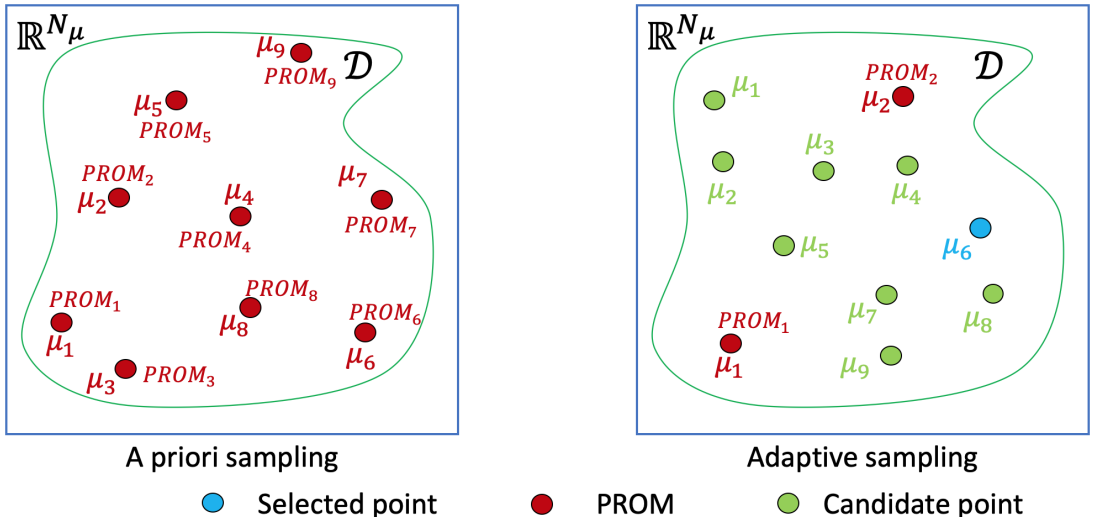
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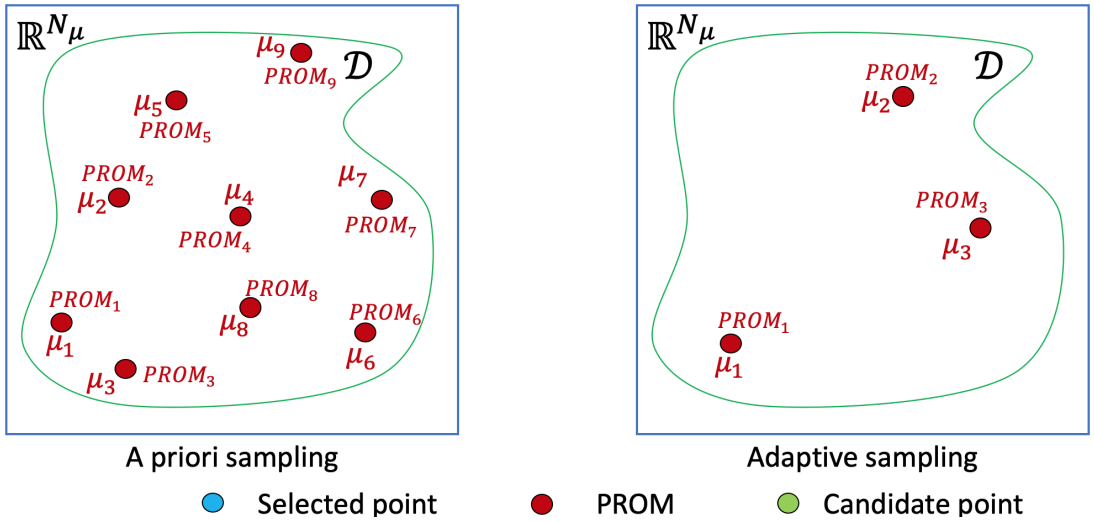
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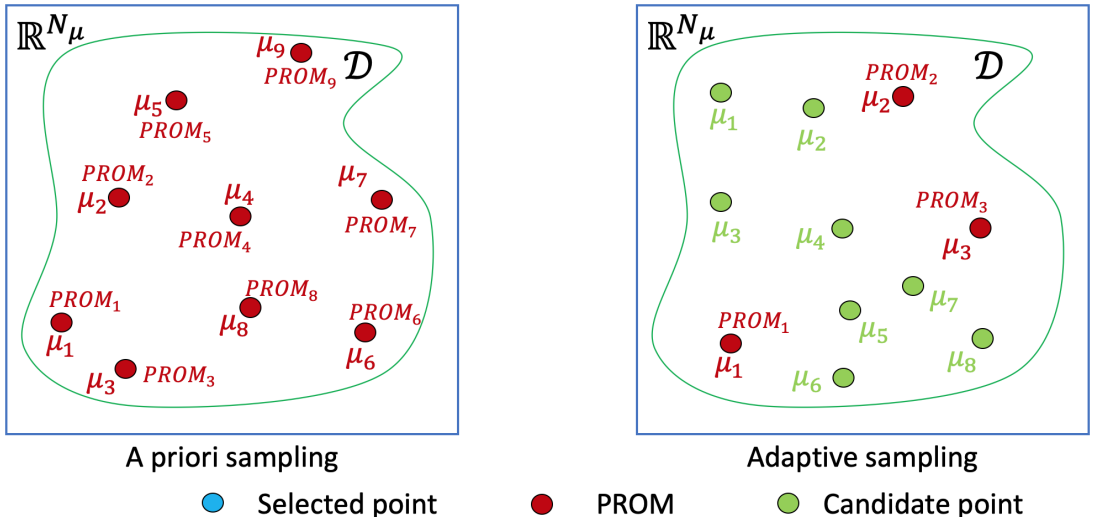
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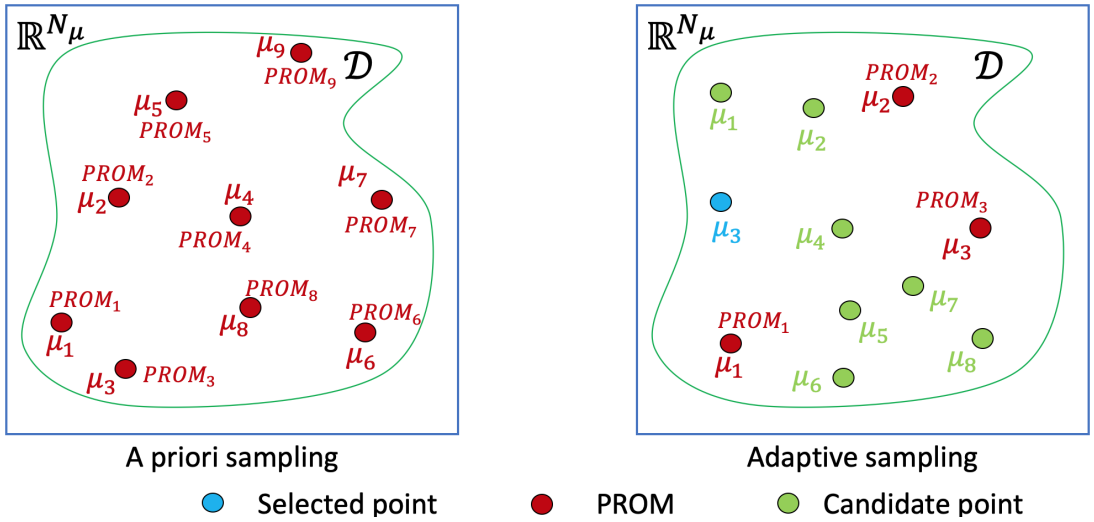
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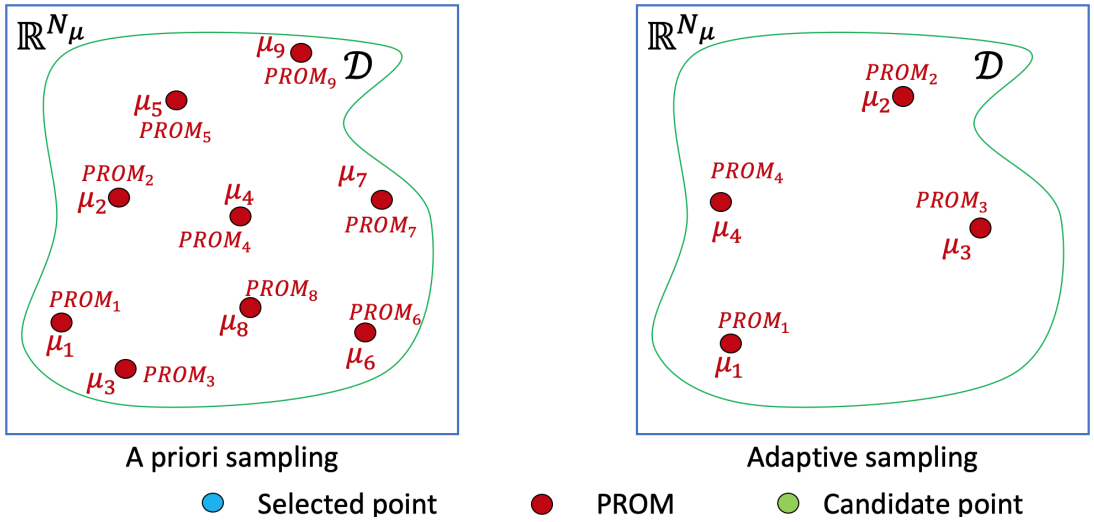
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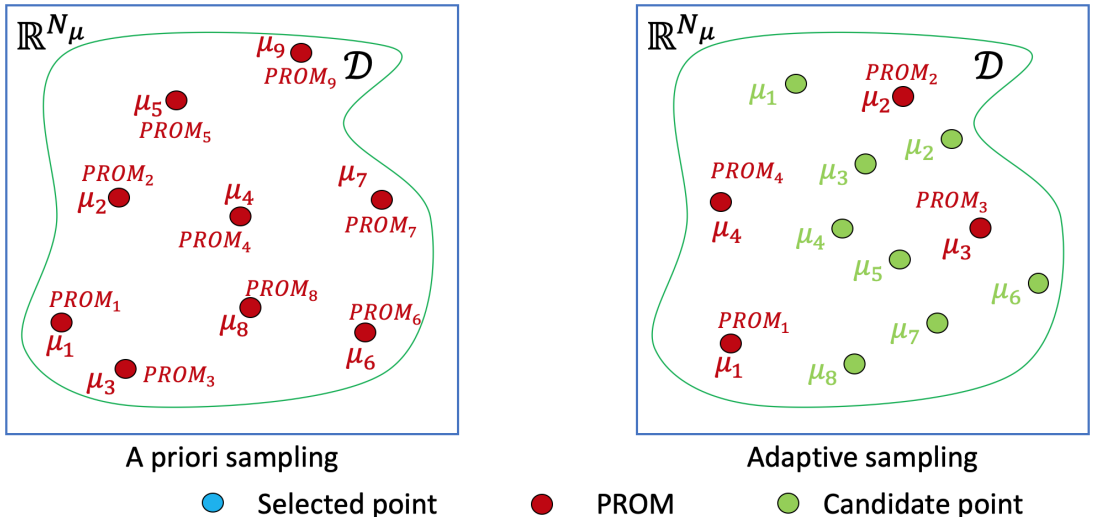
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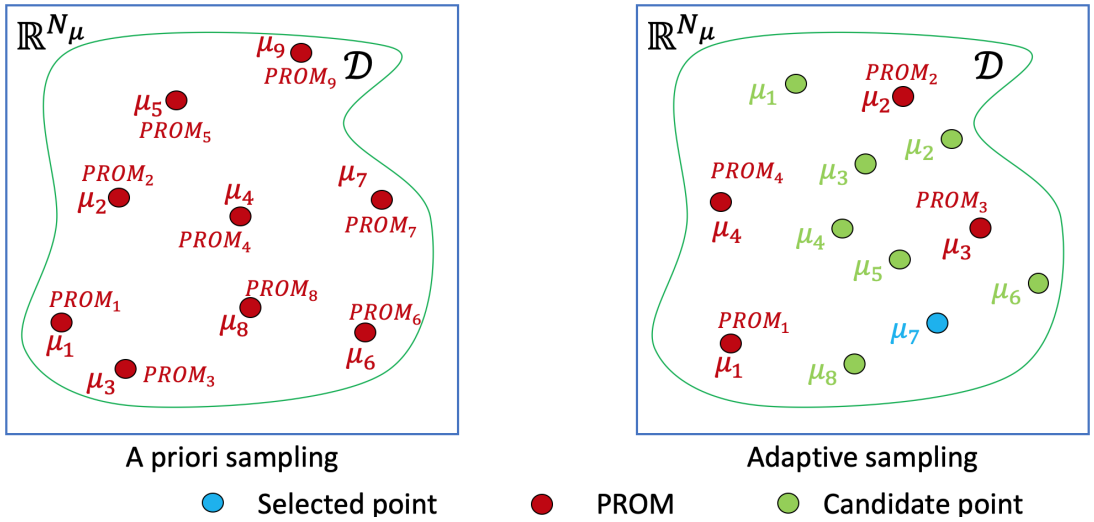
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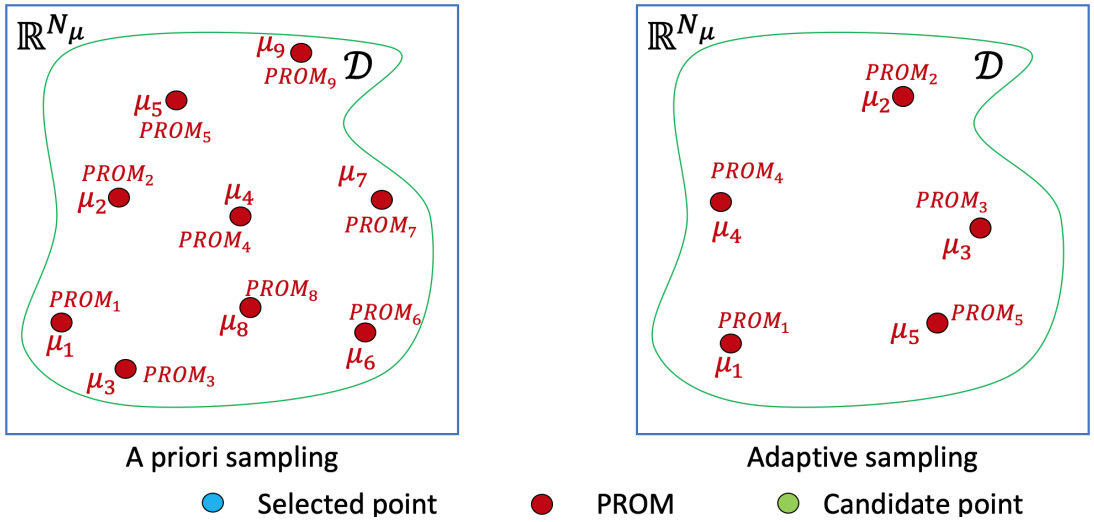
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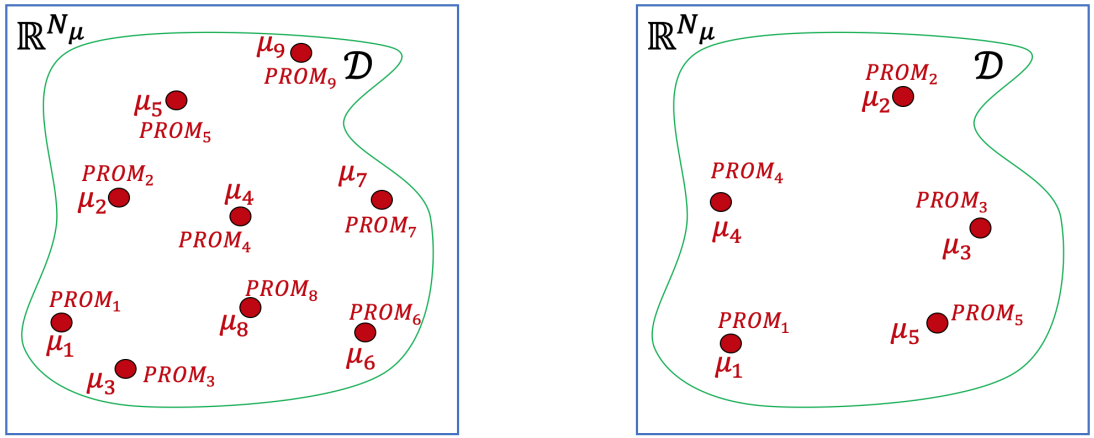
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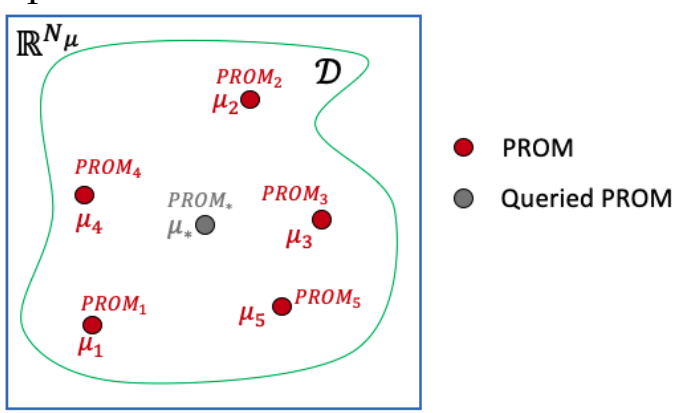
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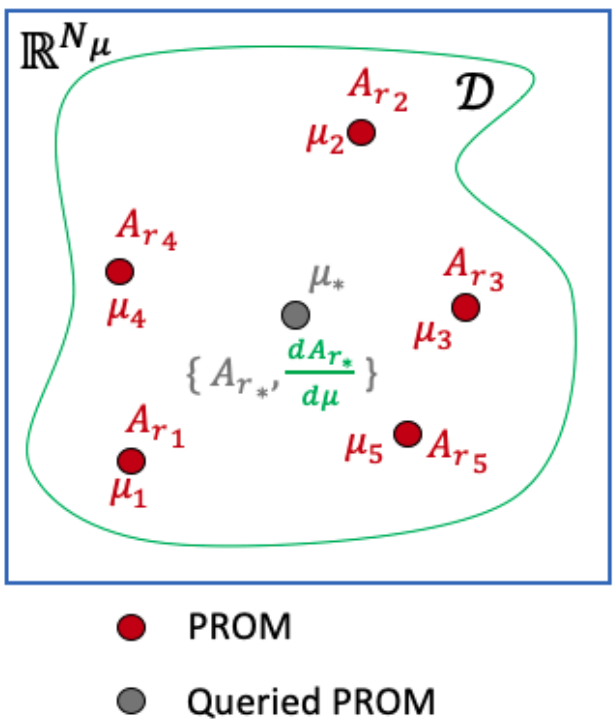
2. At any unsampled parameter point $\boldsymbol{\mu}_\star \in \mathcal{D}$ queried by the optimization procedure, reconstruct

$$\mathcal{T}_r(\boldsymbol{\mu}_\star) = \left\{ \mathbf{A}_r(\boldsymbol{\mu}_\star), \mathbf{B}_r(\boldsymbol{\mu}_\star), \mathbf{c}_r(\boldsymbol{\mu}_\star), \frac{d\mathbf{A}_r}{d\boldsymbol{\mu}}(\boldsymbol{\mu}_\star), \frac{d\mathbf{B}_r}{d\boldsymbol{\mu}}(\boldsymbol{\mu}_\star), \frac{d\mathbf{c}_r}{d\boldsymbol{\mu}}(\boldsymbol{\mu}_\star) \right\}$$

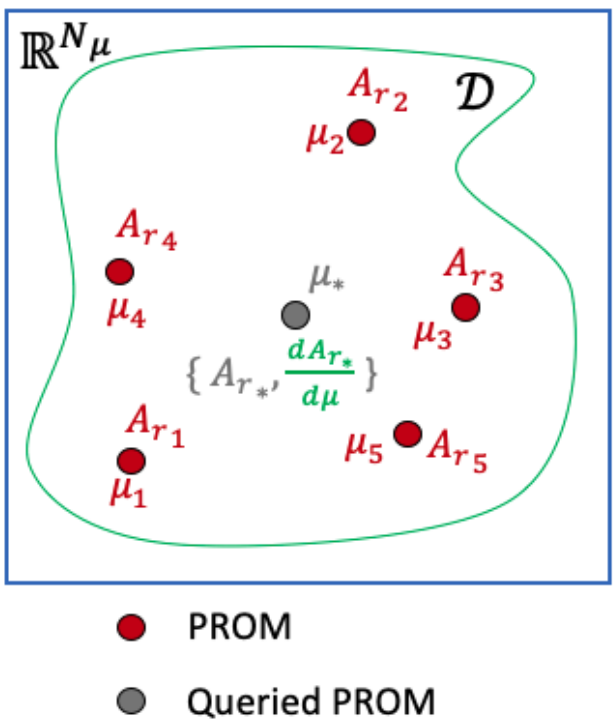
in real-time using interpolation on matrix manifolds

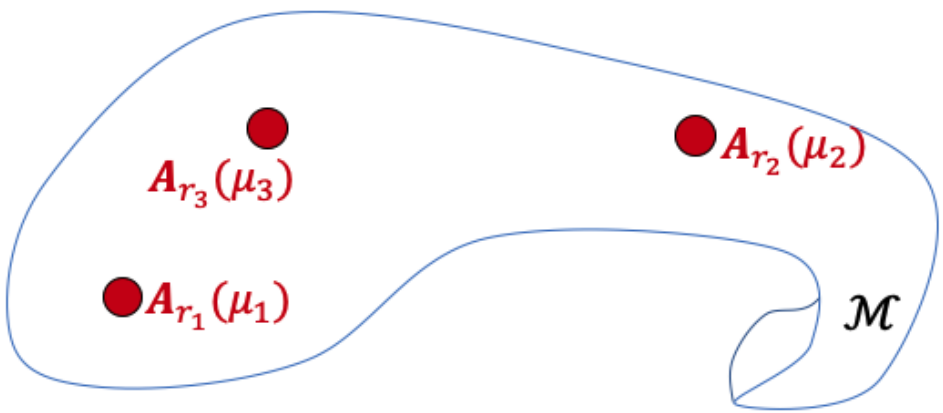


At a queried point $\boldsymbol{\mu}_\star \in \mathcal{D}$ reconstruct $\left\{ \mathbf{A}_r(\boldsymbol{\mu}_\star), \dfrac{d\mathbf{A}_r}{d\boldsymbol{\mu}}(\boldsymbol{\mu}_\star) \right\}$ using **interpolation** on matrix manifolds

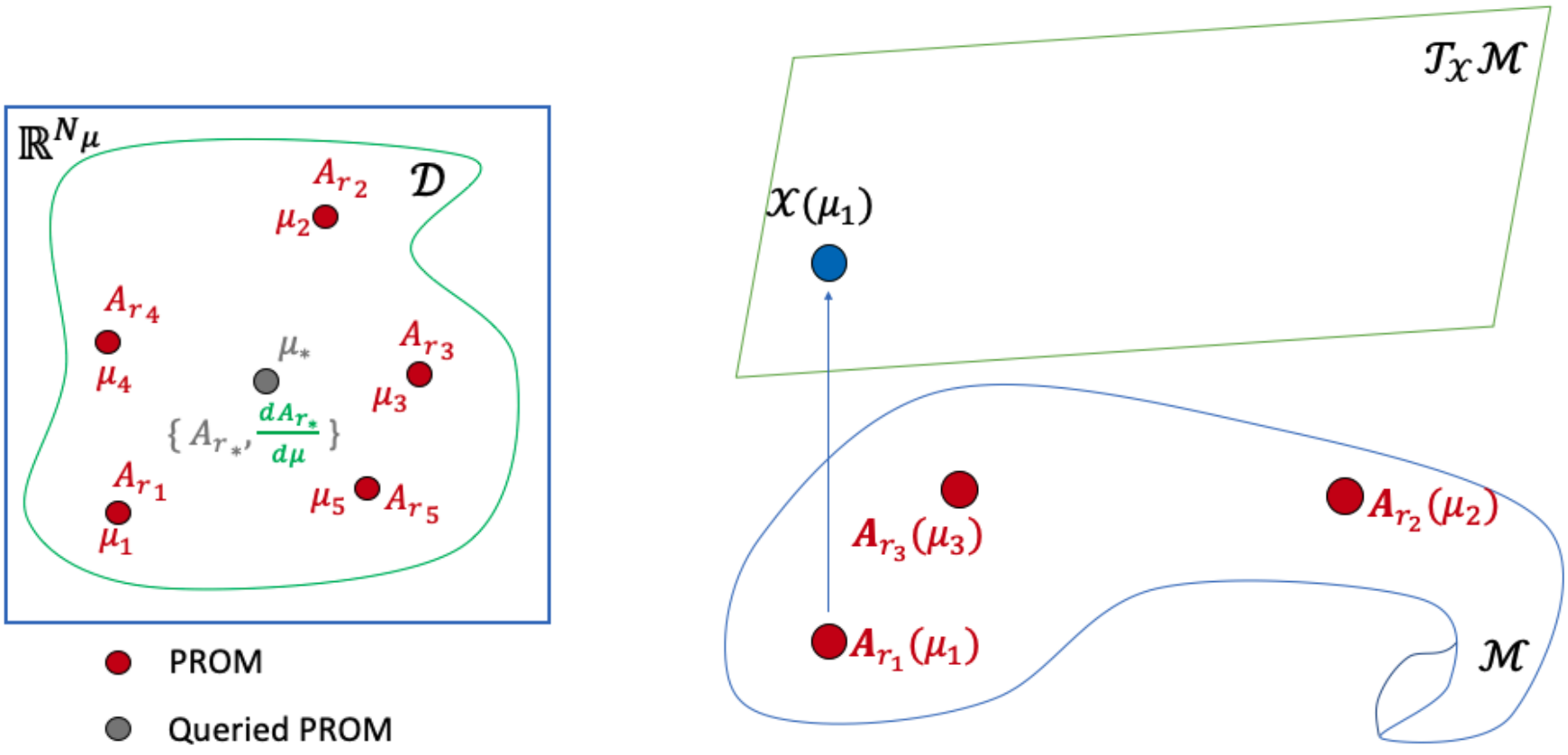


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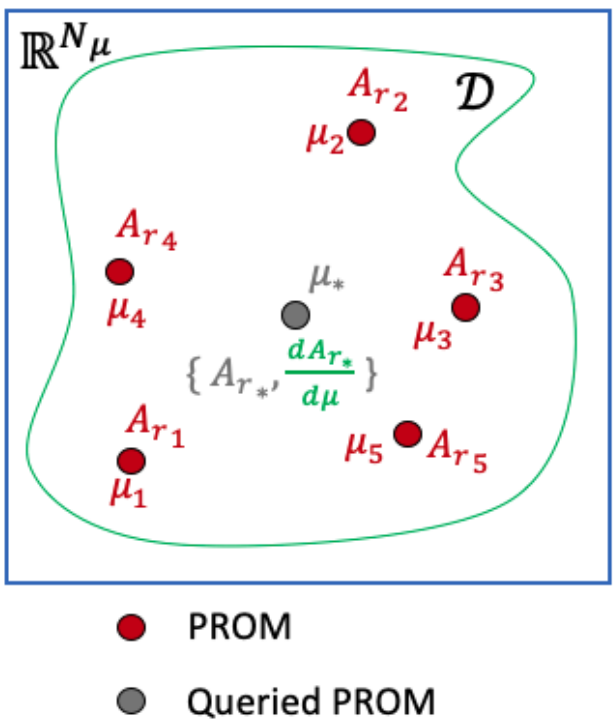


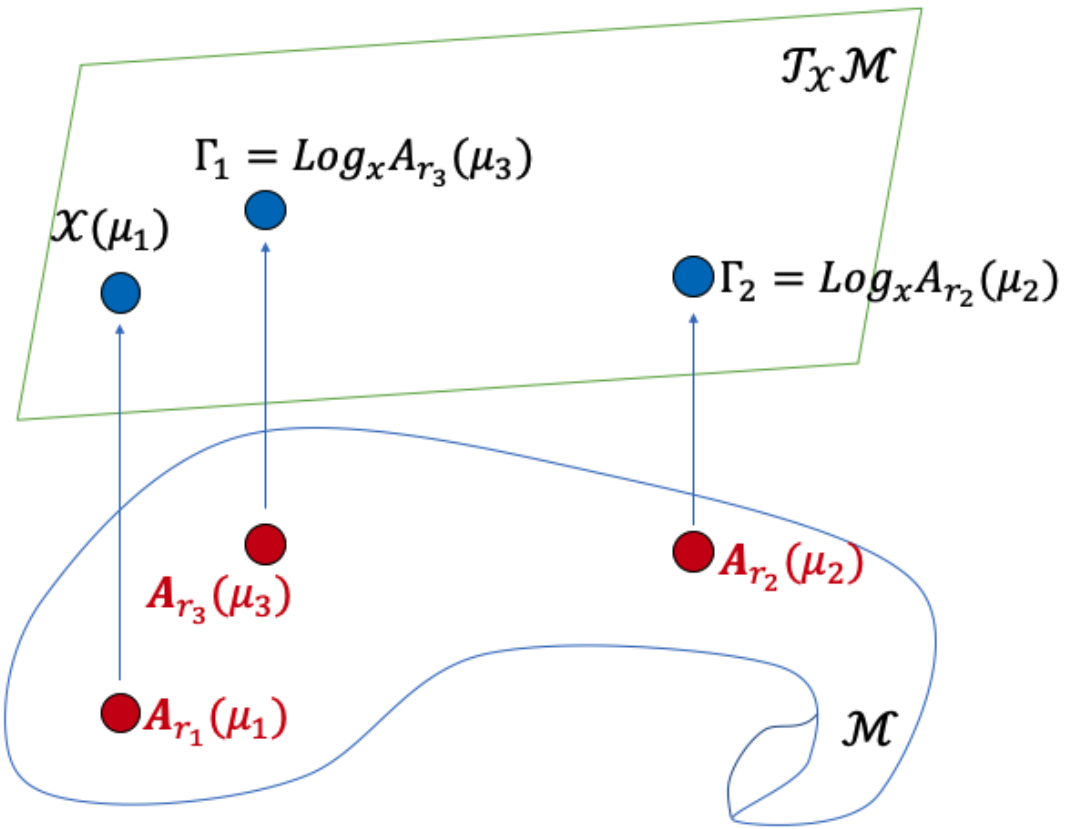


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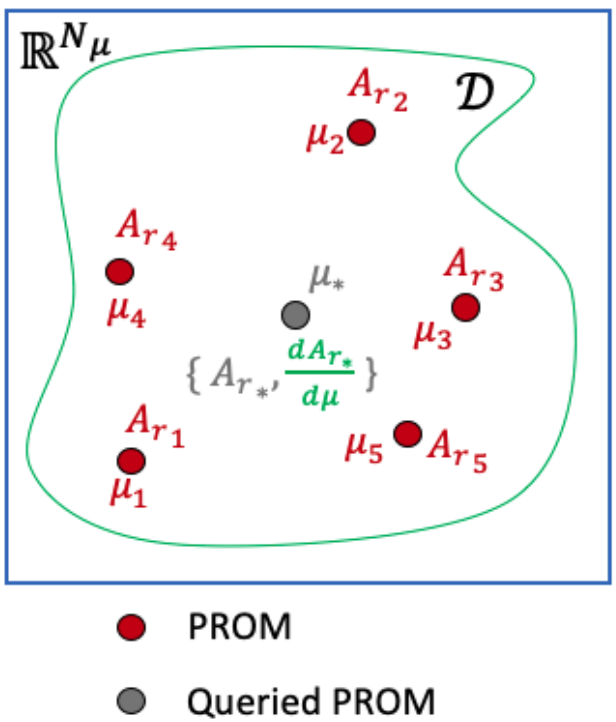


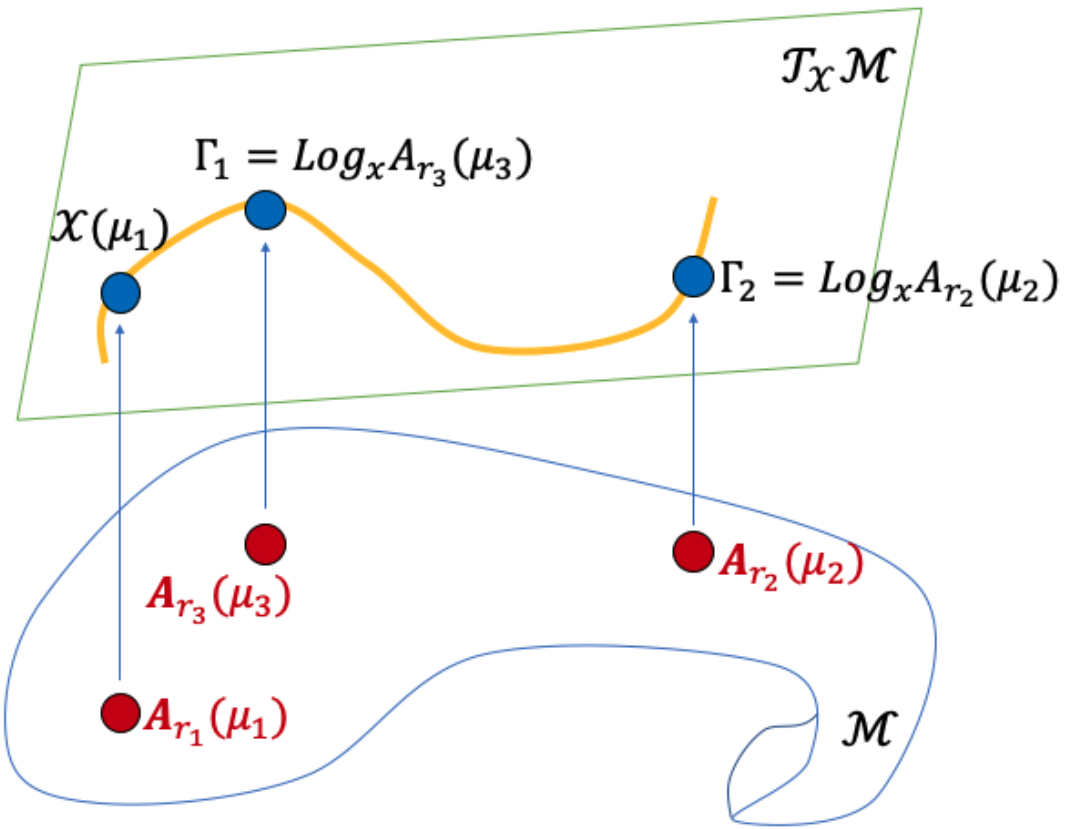
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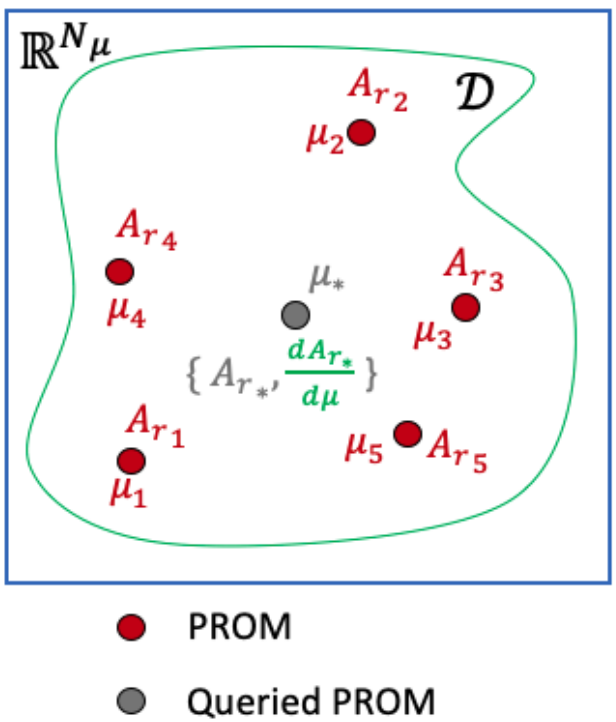


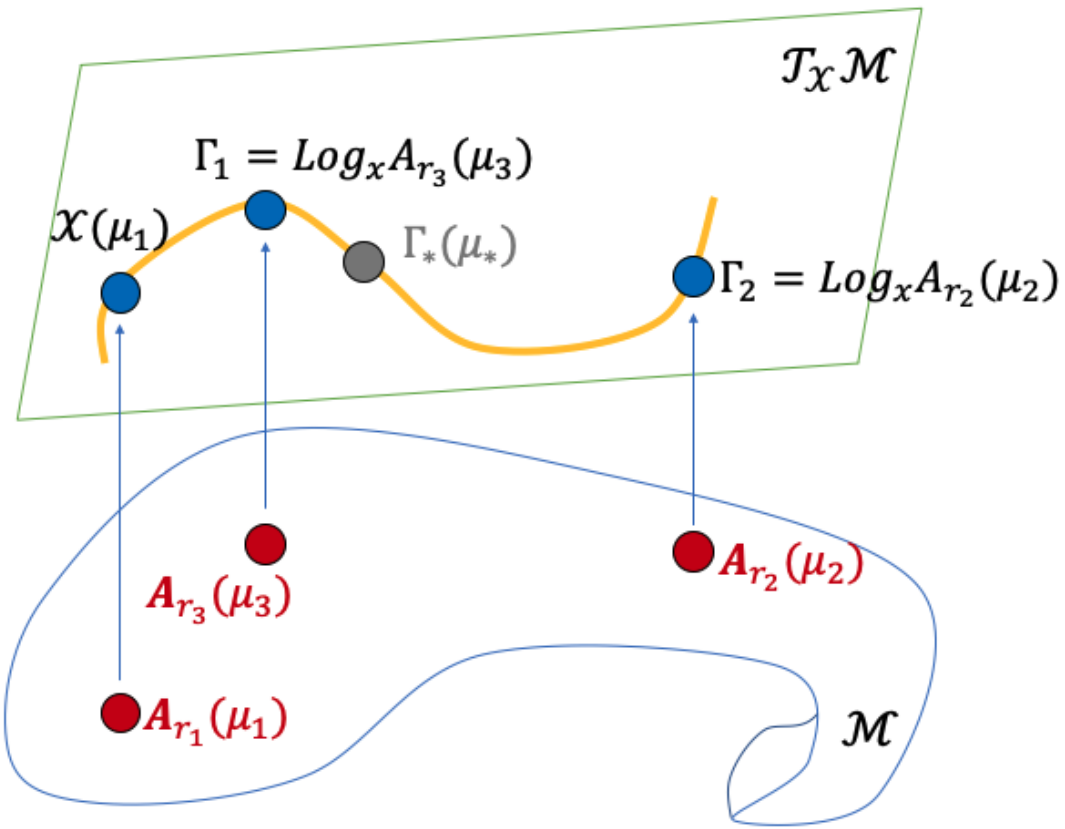
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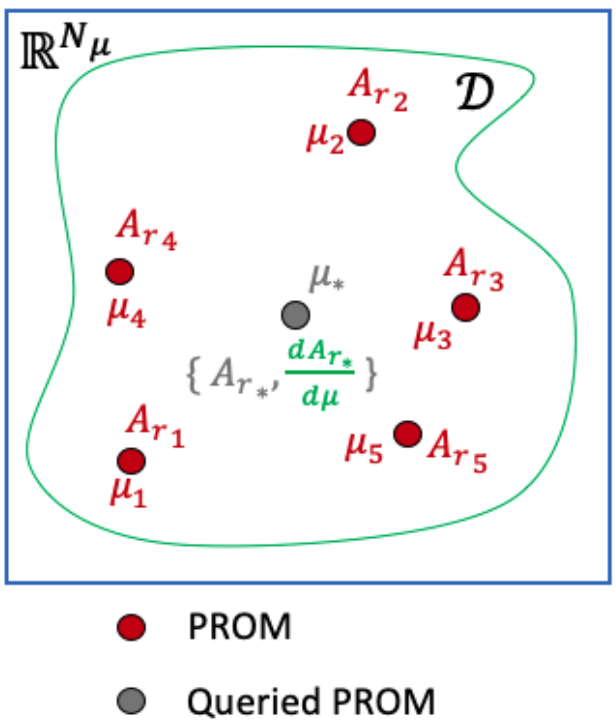


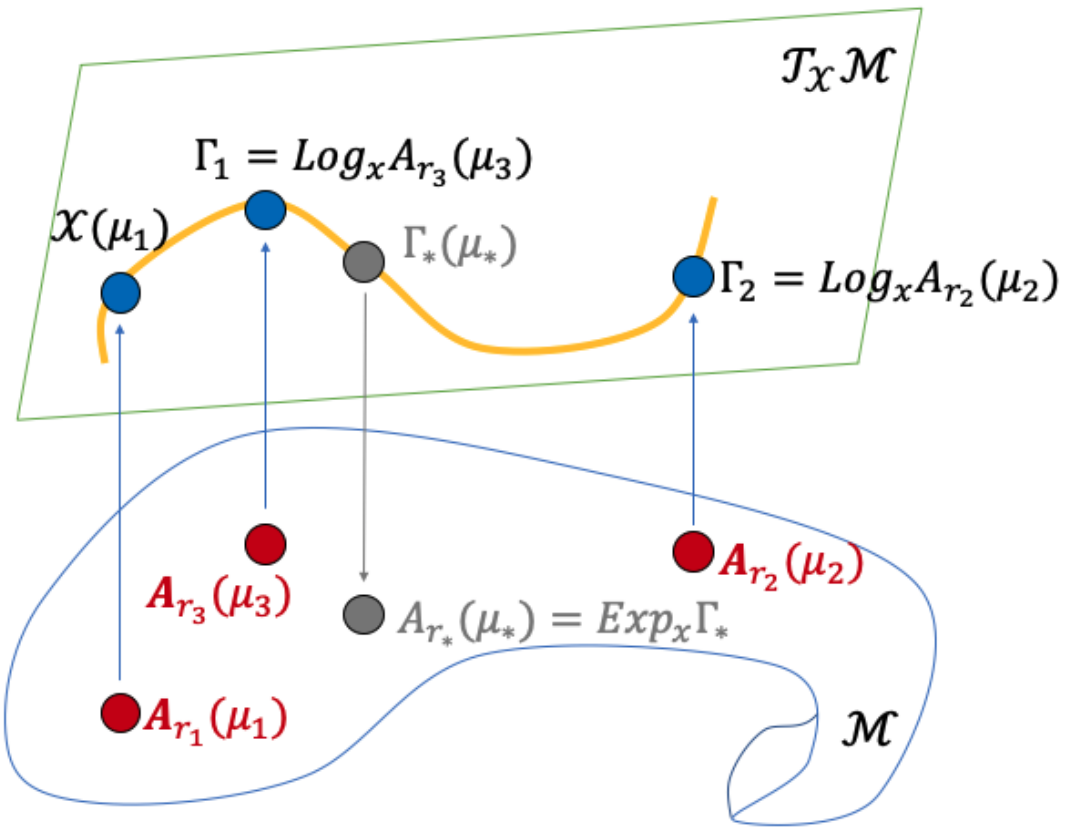
At a queried point $\boldsymbol{\mu}_\star \in \mathcal{D}$ reconstruct $\left\{ \mathbf{A}_r(\boldsymbol{\mu}_\star), \dfrac{d\mathbf{A}_r}{d\boldsymbol{\mu}}(\boldsymbol{\mu}_\star) \right\}$ using **interpolation** on matrix manifolds



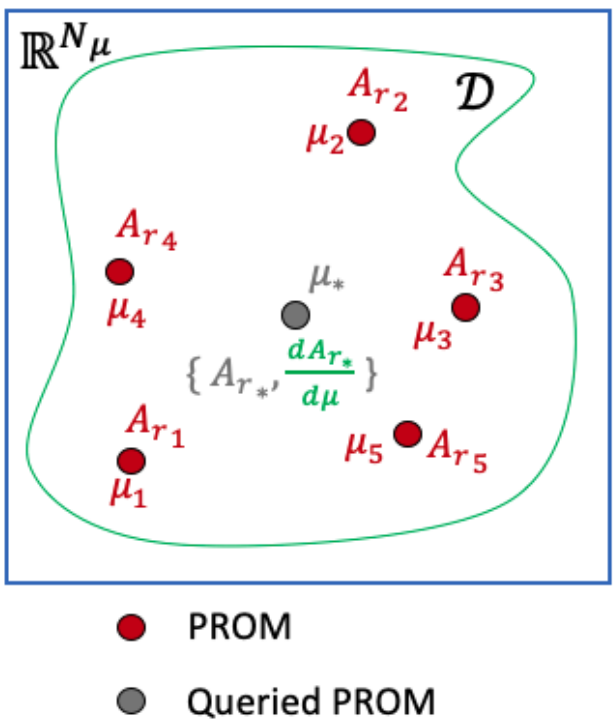


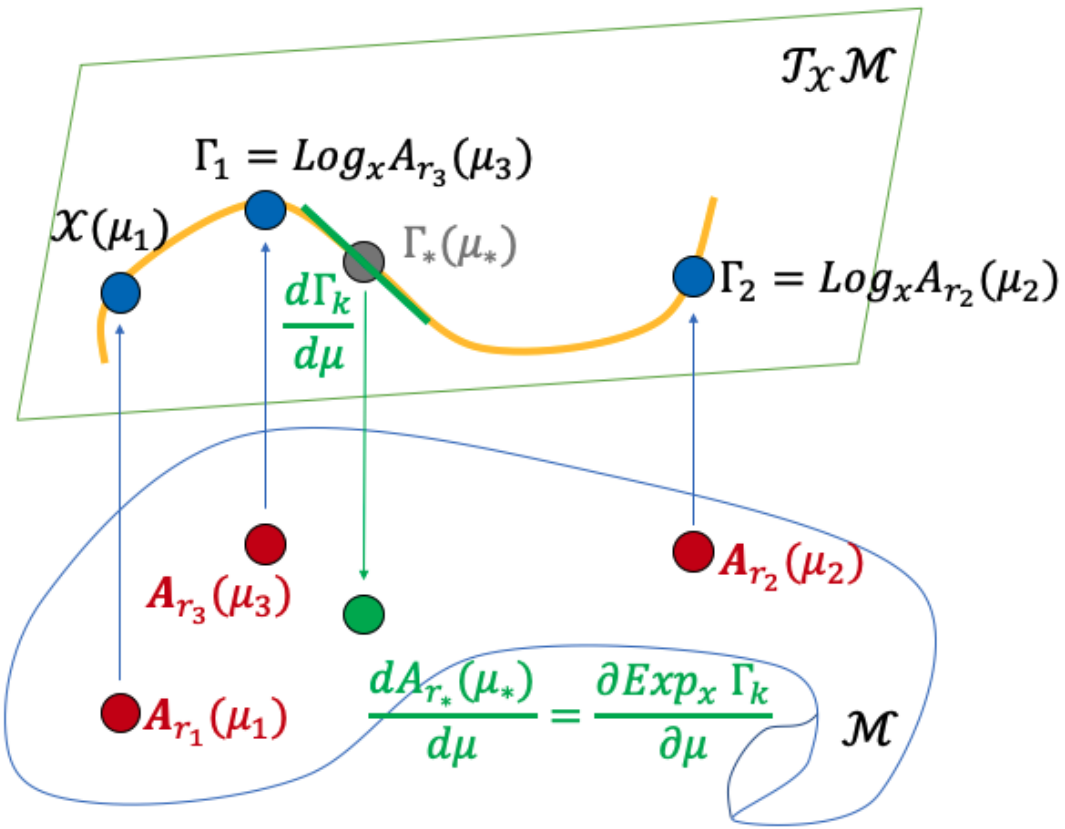
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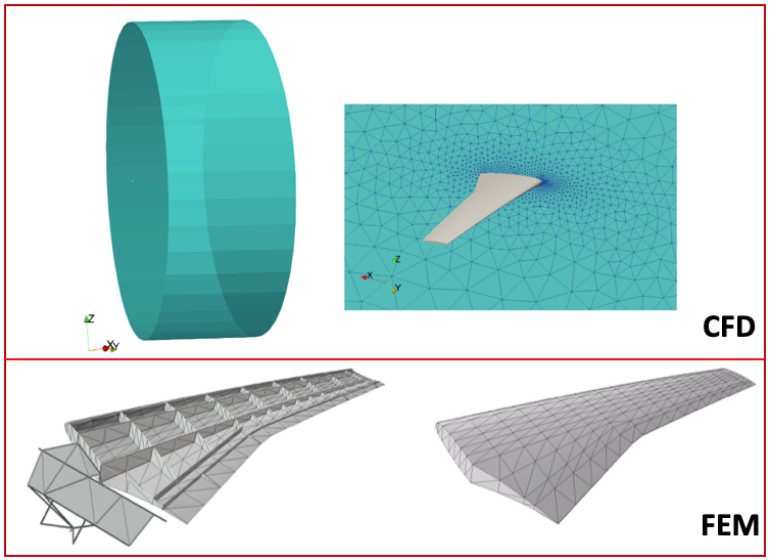




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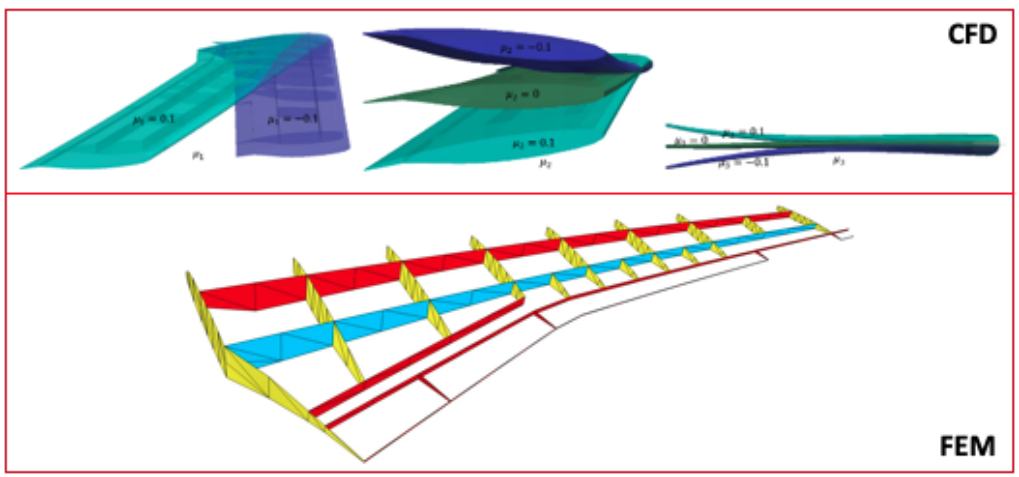






- NASA's Aeroelastic Research Wing number 2 (**ARW-2**)
- **Flow**: $M_\infty = 0.8, \alpha = 0^\circ$
- Inviscid (**CFD**) grid with 63,484 grid points
- Finite element structural model (**FEM**) with beam and shell elements and 2,556 DOF

- Parametric model[1], $\boldsymbol{\mu} \in \mathbb{R}^6$



- **Shape parameters**: back sweep angle μ_s^1, twist angle μ_s^2, and dihedral angle μ_s^3
- **Structural parameters**: three thickness increments for the outer spars (μ_m^1), the central spar (μ_m^2), and the ribs (μ_m^3)

[1] Youngsoo Choi , Gabriele Boncoraglio, Spenser Anderson, David Amsallem, and Charbel Farhat. "Gradient-based constrained optimization using a database of linear reduced-order models". In: Journal of Computational Physics 423 (2020), p. 109787.

Constraint: avoiding flutter







Constraint: avoiding flutter

- Parametric linear CFD-CSD-based aeroelastic model for flutter

$$\mathbf{R}(\mathbf{w}(\boldsymbol{\mu});\boldsymbol{\mu}) = \dot{\mathbf{w}}(\boldsymbol{\mu}) + \boldsymbol{\mathcal{N}}(\boldsymbol{\mu})\,\mathbf{w}(\boldsymbol{\mu}) = \mathbf{0}$$

- Flutter constraint: $\zeta_i(\boldsymbol{\mu}) \geqslant \zeta_{lb}$ for $i = 1, \cdots, n$;
  ζ_i are the damping ratios of the aeroelastic modes

- Database of linear local PROMs $\mathcal{DB} = \{\boldsymbol{\mathcal{N}}_r(\boldsymbol{\mu}_j)\}_{j=1}^{N_{\mathcal{DB}}}$

[1] Youngsoo Choi , Gabriele Boncoraglio, Spenser Anderson, David Amsallem, and Charbel Farhat. "Gradient-based constrained optimization using a database of linear reduced-order models". In: Journal of Computational Physics 423 (2020), p. 109787.

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Performance results for the evaluation of the flutter constraint and its **sensitivities**[1] for a single queried parameter vector

Computational model	# of CPUs	Wall-clock time (hours)	CPU time (hours)
HDM	32	0.492	15.744
Database of PROMs	1	0.017	0.017
Speed-up factor		28.9	926.1

[1] Youngsoo Choi , Gabriele Boncoraglio, Spenser Anderson, David Amsallem, and Charbel Farhat. "Gradient-based constrained optimization using a database of linear reduced-order models". In: Journal of Computational Physics 423 (2020), p. 109787.

Parametric nonlinear PDE

$$\mathbf{R}(\mathbf{w}(\boldsymbol{\mu});\boldsymbol{\mu}) = \mathbf{0}$$

with $\mathbf{R} : \mathbb{R}^{N_\mathbf{w}} \times \mathbb{R}^{N_{\boldsymbol{\mu}}} \to \mathbb{R}^{N_\mathbf{w}}$ and $\mathbf{w} \in \mathbb{R}^{N_\mathbf{w}}$

- Galerkin ($\mathbf{W}_\mathbf{w} = \mathbf{V}_\mathbf{w}$) or Petrov-Galerkin ($\mathbf{W}_\mathbf{w} \neq \mathbf{V}_\mathbf{w}$) PROM

$$\mathbf{r}(\mathbf{w}_r(\boldsymbol{\mu});\boldsymbol{\mu}) = \mathbf{W}_\mathbf{w}^T \mathbf{R}(\mathbf{w}_\text{ref} + \mathbf{V}_\mathbf{w}\mathbf{w}_r(\boldsymbol{\mu});\boldsymbol{\mu}) = \mathbf{0} \qquad (\star)$$

- A PROM possesses the minimum-residual property if Eq. ($\star$) is equivalent to

$$\min_{\mathbf{w}_r \in \mathbb{R}^{N_{\mathbf{w}_r}}} \| \mathbf{R}(\mathbf{w}_\text{ref} + \mathbf{V}_\mathbf{w}\mathbf{w}_r(\boldsymbol{\mu});\boldsymbol{\mu}) \|_{\boldsymbol{\Theta}} \qquad \boldsymbol{\Theta} \succ 0$$

  - the Jacobian of $\mathbf{R}$ is SPD, i.e., $\dfrac{\partial \mathbf{R}}{\partial \mathbf{w}} \succ 0$
  - choosing $\mathbf{W}_\mathbf{w} = \boldsymbol{\Theta} \dfrac{\partial \mathbf{R}}{\partial \mathbf{w}} \mathbf{V}_\mathbf{w}$

Despite the **reduced dimensionality**, $\mathcal{O}(N_{\mathbf{w}})$ operations are required to evaluate

$$\mathbf{W}_{\mathbf{w}}^T \mathbf{R}(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}} \mathbf{w}_r; \boldsymbol{\mu}) \qquad \mathbf{W}_{\mathbf{w}}^T \frac{\partial \mathbf{R}(\cdot)}{\partial \mathbf{w}} \mathbf{V}_{\mathbf{w}}$$

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Solution: *project-then-approximate* class of hyperreduction methods which directly approximate the projected quantities –
Energy-conserving sampling and weighting (ECSW) method

$$\mathbf{W}_{\mathbf{w}}^T \mathbf{R}(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}} \mathbf{w}_r; \boldsymbol{\mu}) = \sum_{e \in \mathcal{E}} \mathbf{W}_{\mathbf{w}}^T \mathbf{L}_e^T \left(\mathbf{R}\right)_e \left(\mathbf{L}_{e^+} \left(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}} \mathbf{w}_r\right); \boldsymbol{\mu}\right)$$

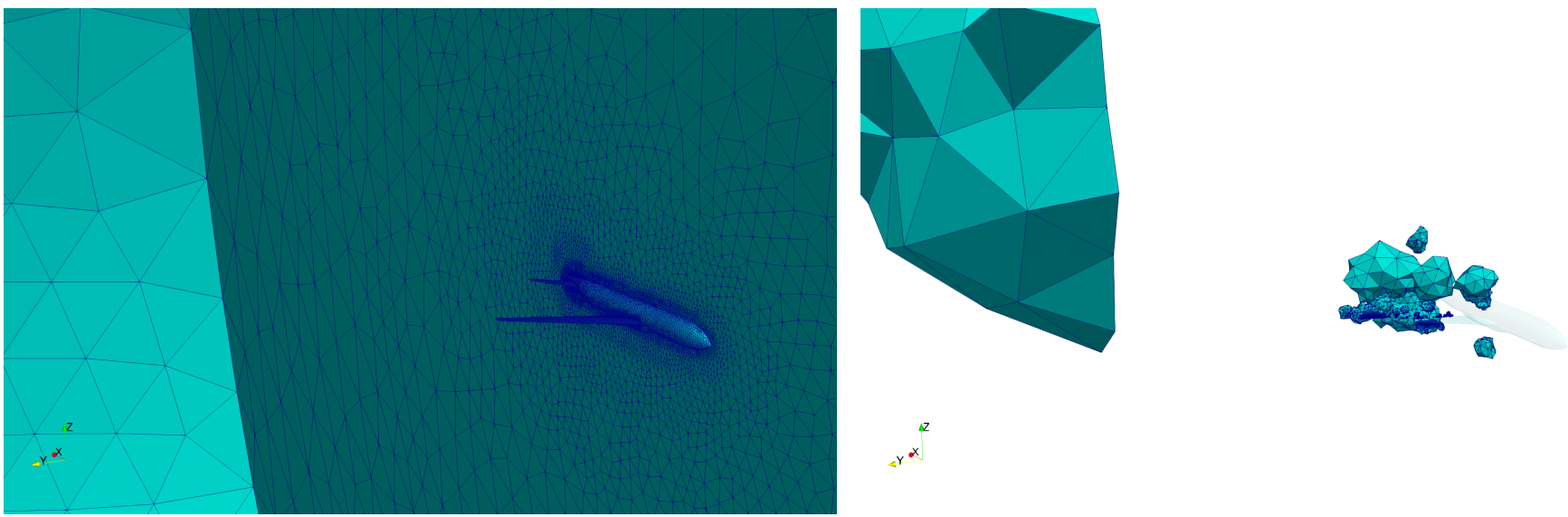
- $\mathcal{E} = \{e_1, \cdots, e_{N_\mathcal{E}}\}$: set of mesh entities, $|\mathcal{E}| = N_\mathcal{E}$
- $\mathbf{L}_e^T, \mathbf{L}_{e^+}$ are Boolean matrices

$$\mathbf{W}_{\mathbf{w}}^T \mathbf{R}(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}} \mathbf{w}_r; \boldsymbol{\mu}) \approx \sum_{e \in \tilde{\mathcal{E}}} \xi_e \mathbf{W}_{\mathbf{w}}^T \mathbf{L}_e^T \left(\mathbf{R}\right)_e \left(\mathbf{L}_{e^+} \left(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}} \mathbf{w}_r\right); \boldsymbol{\mu}\right)$$

- $\tilde{\mathcal{E}}$ is the sampled mesh, with $\tilde{\mathcal{E}} \subset \mathcal{E}$ and $|\tilde{\mathcal{E}}| = N_{\tilde{\mathcal{E}}} \ll |N_\mathcal{E}|$
- weights $\{\xi_{e_i}\}_{i=1}^{N_{\tilde{\mathcal{E}}}}$ (interpretation: generalized quadrature rule in a hyperspace)

Solution: *project-then-approximate* class of hyperreduction methods which directly approximate the projected reduced-order quantities: ECSW method

$$\mathbf{W}_{\mathbf{w}}^T \mathbf{R}(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}}\mathbf{w}_r; \boldsymbol{\mu}) \approx \sum_{e \in \tilde{\mathcal{E}}} \xi_e \mathbf{W}_{\mathbf{w}}^T \mathbf{L}_e^T \left(\mathbf{R}\right)_e \left(\mathbf{L}_{e^+} \left(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}}\mathbf{w}_r\right); \boldsymbol{\mu}\right)$$

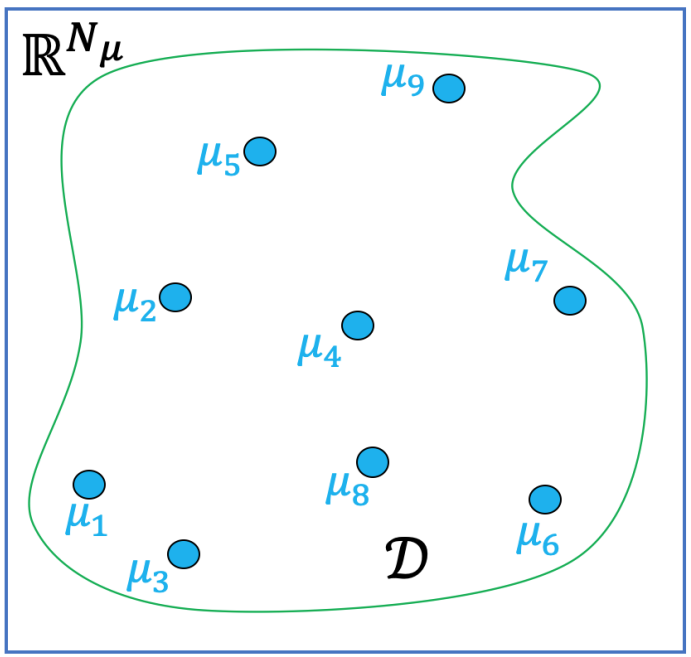


HPROM characterized by (1) ROB $\mathbf{V_w}$ and (2) sampled mesh

- Build the ROB $\mathbf{V_w}$

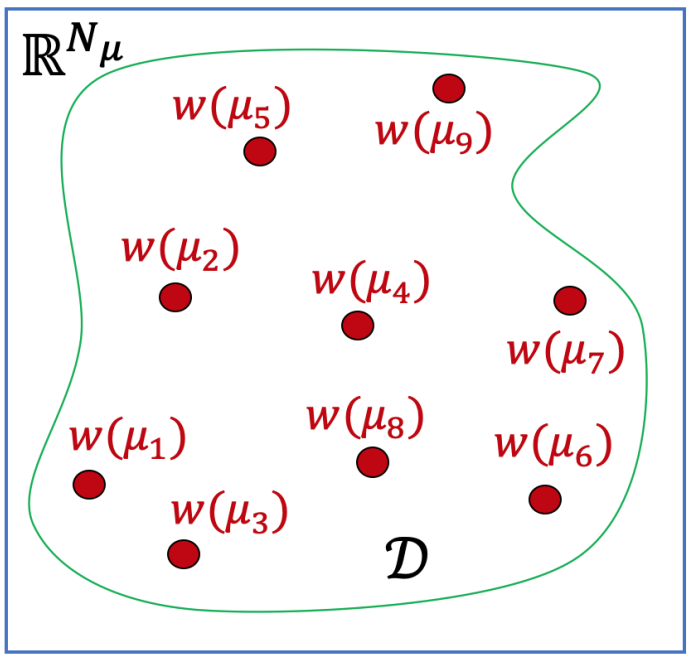
HPROM characterized by (1) ROB $\mathbf{V_w}$ and (2) sampled mesh

- Build the ROB $\mathbf{V_w}$
  - sample snapshots $\{\mathbf{w}(\boldsymbol{\mu}_i)\}_{i=1}^{N_{\mathcal{DB}}}$ using Greedy algorithm and form the snapshot matrix $\mathbf{S} = \left[\mathbf{w}(\boldsymbol{\mu}_1), \cdots, \mathbf{w}(\boldsymbol{\mu}_{N_{\mathcal{DB}}})\right] \in \mathbb{R}^{N_{\mathbf{w}} \times N_{\mathcal{DB}}}$



HPROM characterized by (1) ROB $\mathbf{V_w}$ and (2) sampled mesh

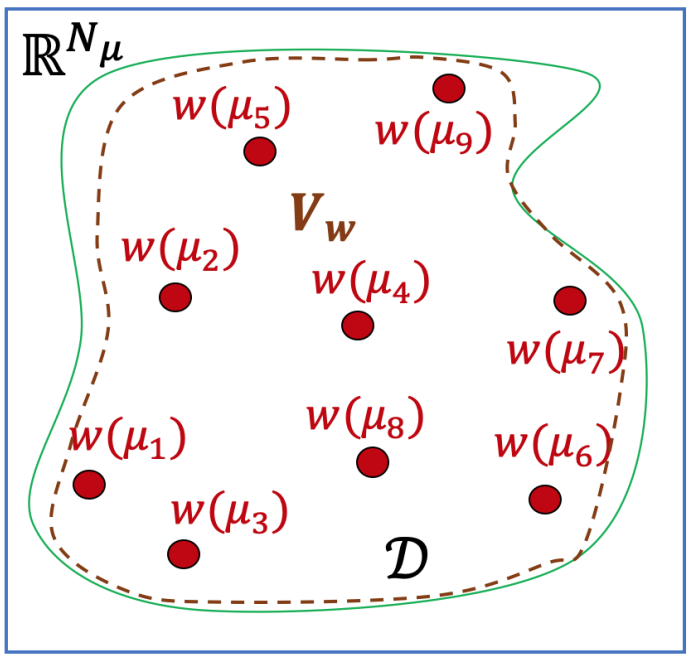
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  - compute $\mathbf{V_w}$ using POD

$$\mathbf{S} = \begin{bmatrix} \mathbf{V_w} & \mathbf{V_c} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_{\mathbf{w}}^T \\ \mathbf{U}_{\mathbf{c}}^T \end{bmatrix}$$

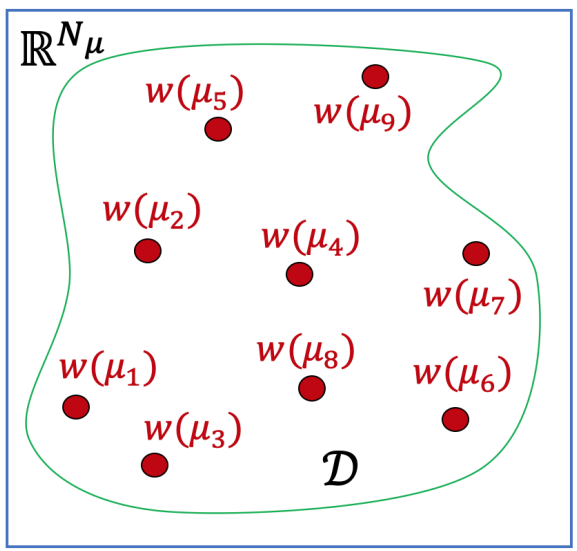


HPROM characterized by (1) ROB $\mathbf{V_w}$ and (2) sampled mesh

- Compute the sampled mesh quantities $\left\{\widetilde{\mathcal{E}}, \boldsymbol{\xi}_{\widetilde{\mathcal{E}}} = \{\xi_{e_i}\}_{i=1}^{N_{\widetilde{\mathcal{E}}}}\right\}$

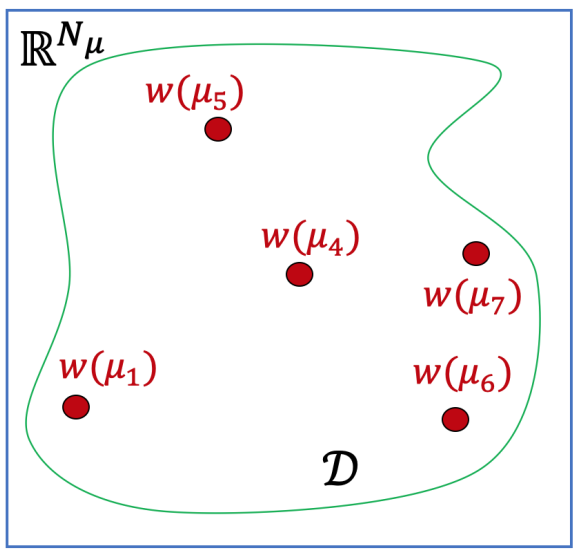
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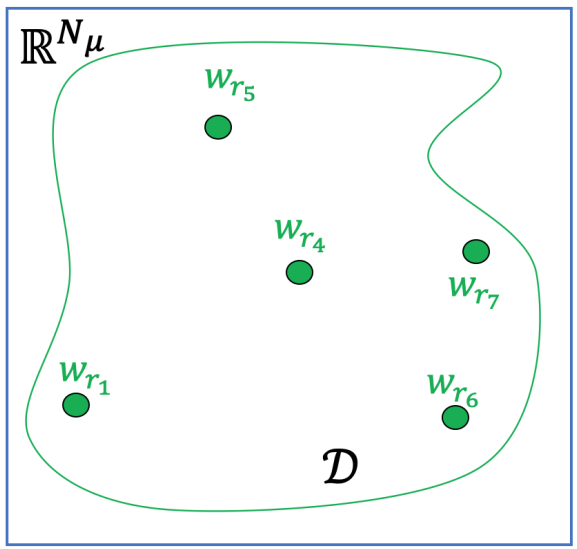
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HPROM characterized by (1) ROB $\mathbf{V}_{\mathbf{w}}$ and (2) sampled mesh

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  - compute generalized coordinates from M snapshots, $(M \leqslant N_{\mathcal{DB}})$

$$\{\mathbf{w}_r(\boldsymbol{\mu}_i)\}_{i=1}^{M} = \left\{\mathbf{V}_{\mathbf{w}}^T \left(\mathbf{w}(\boldsymbol{\mu}_i) - \mathbf{w}_{\text{ref}}\right)\right\}_{i=1}^{M}$$



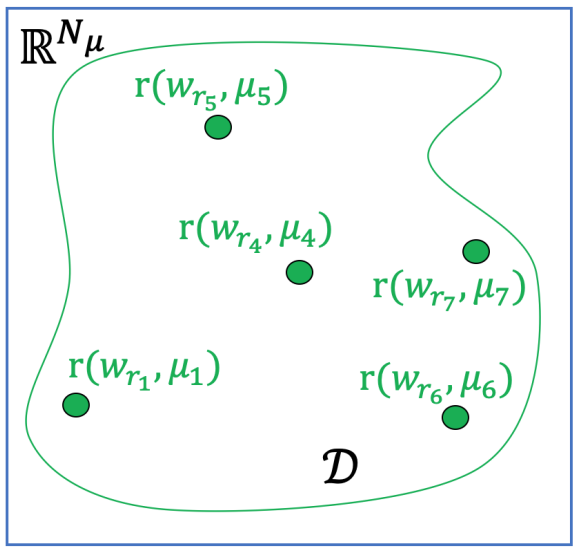
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  - compute projected reduced-order vectors as training data

$$\{\mathbf{r}(\mathbf{w}_r; \boldsymbol{\mu}_i)\}_{i=1}^{M} = \left\{\mathbf{W}_{\mathbf{w}}^T \mathbf{R}\left(\mathbf{w}_{\text{ref}} + \mathbf{V}_{\mathbf{w}}\mathbf{w}_r(\boldsymbol{\mu}_i); \boldsymbol{\mu}_i\right)\right\}_{i=1}^{M}$$



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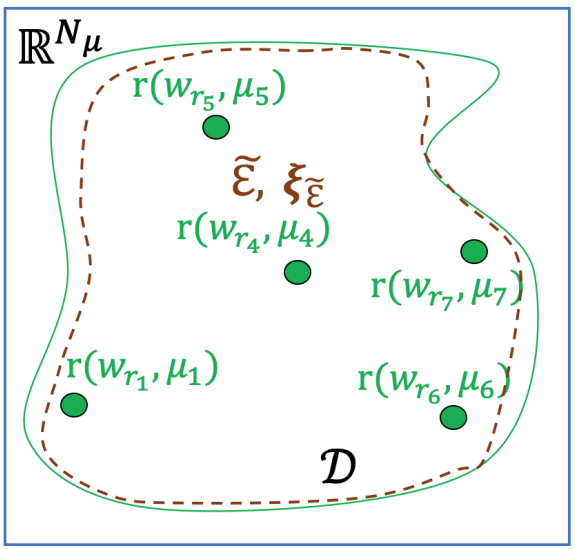
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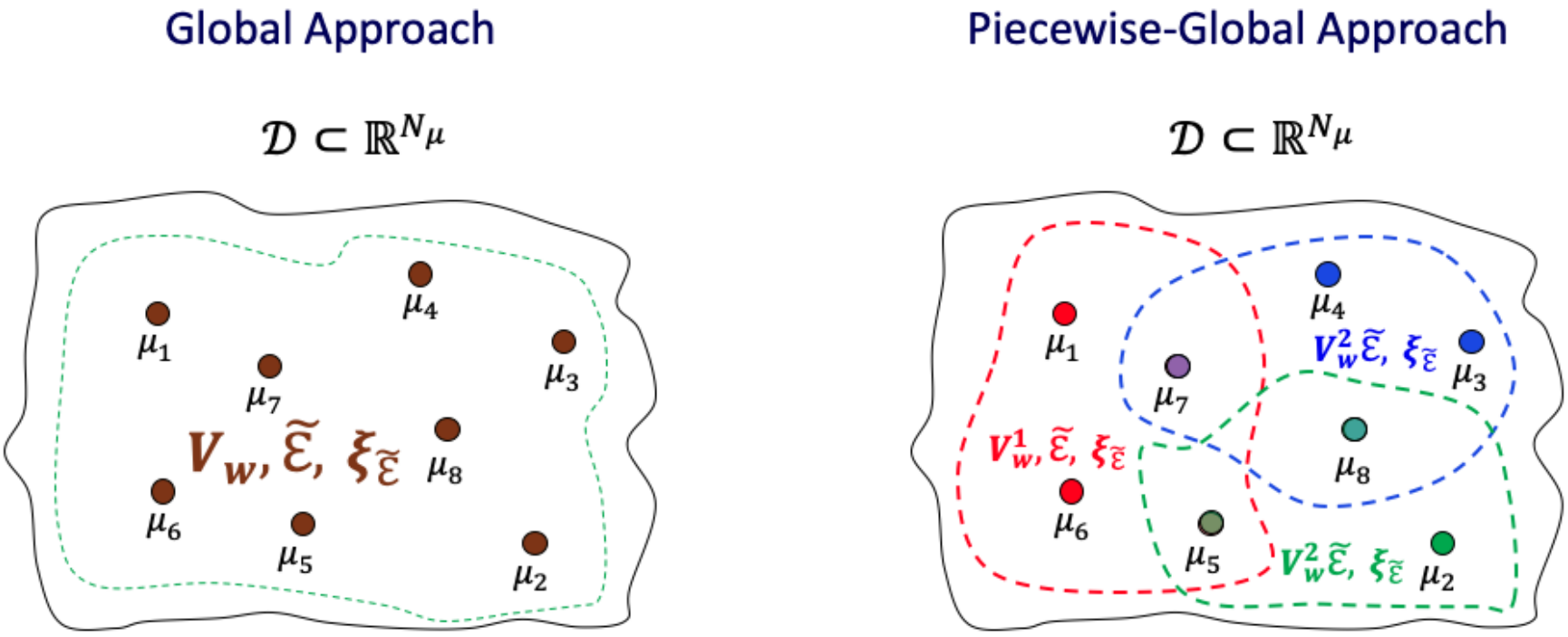
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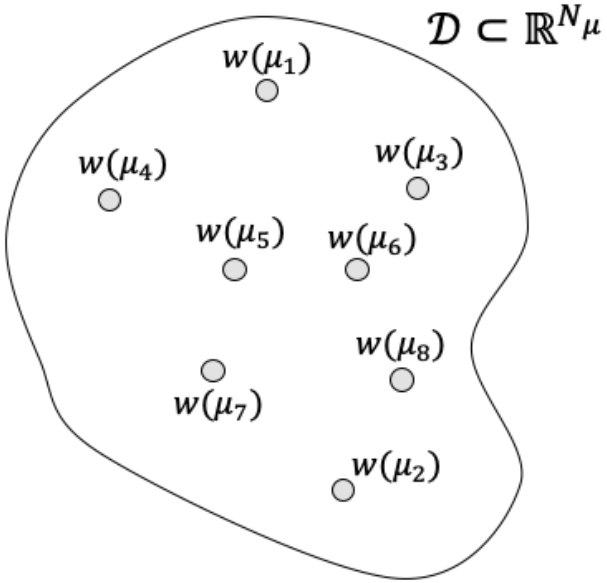
  - identify the optimal sampled mesh by solving a non-negative least-square problem derived from the approximation for $\forall i = 1, \cdots, M$

$$\mathbf{r}(\mathbf{w}_r;\boldsymbol{\mu}_i) \approx \sum_{e\,\in\,\widetilde{\mathcal{E}}} \xi_e \mathbf{W}_\mathbf{w}^T\mathbf{L}_e^T\left(\mathbf{R}\right)_e\left(\mathbf{L}_{e^+}\left(\mathbf{w}_{\text{ref}} + \mathbf{V}_\mathbf{w}\mathbf{w}_r(\boldsymbol{\mu}_i)\right);\boldsymbol{\mu}_i\right)$$

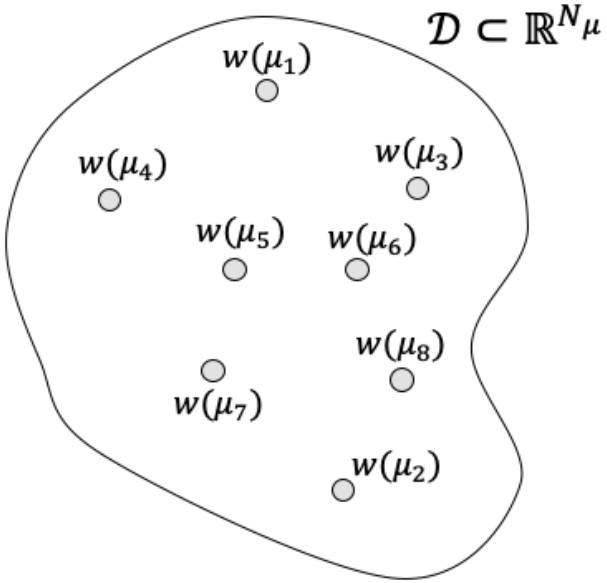




- The objective is to accelerate the optimization process using a database of piecewise global HPROMs
- The piecewise global HPROM needs to be accurate only within a region of the parameter space $\mathcal{D}$, and therefore can have a smaller dimension than otherwise

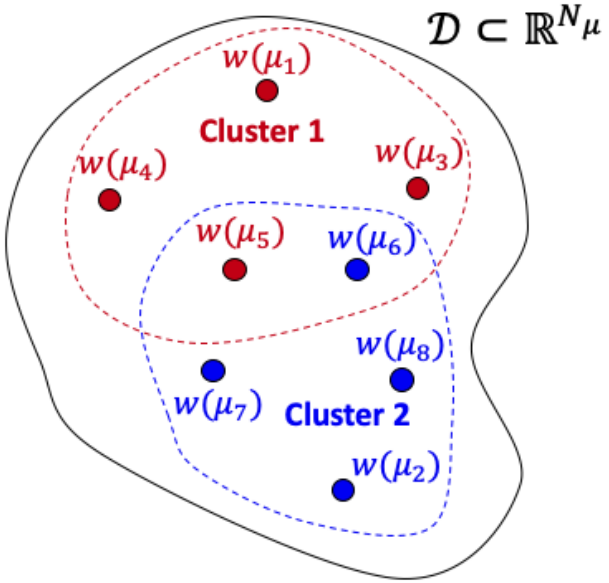


- What features can be used for clustering?



- What features can be used for clustering?
  - some examples
    - vector of optimization variables $\boldsymbol{\mu}$
    - QoIs such as objective functions and gradients
    - state variables $\mathbf{w}$
  - vector of features for clustering

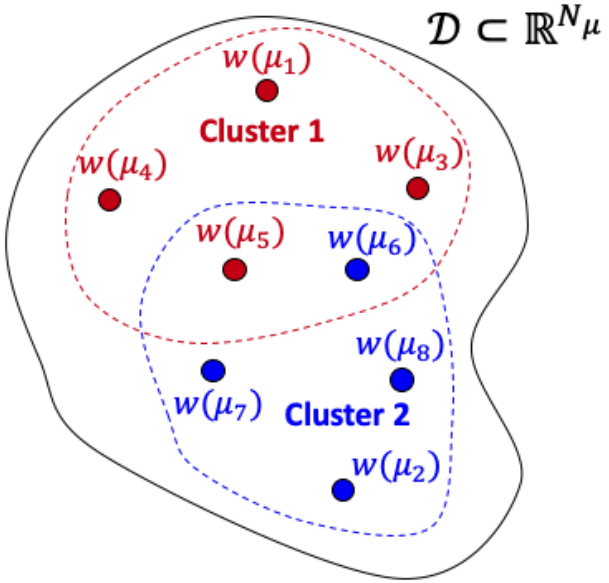
$$\mathbf{x}_i = \left[\mu_i^1, \cdots, \mu_i^{N_{\boldsymbol{\mu}}}, \mathrm{QoI}_1(\boldsymbol{\mu}_i), \cdots, \mathrm{QoI}_{N_{\mathrm{QoI}}}(\boldsymbol{\mu}_i)\right] \in \mathbb{R}^{(N_{\boldsymbol{\mu}}+N_{\mathrm{QoI}})}$$



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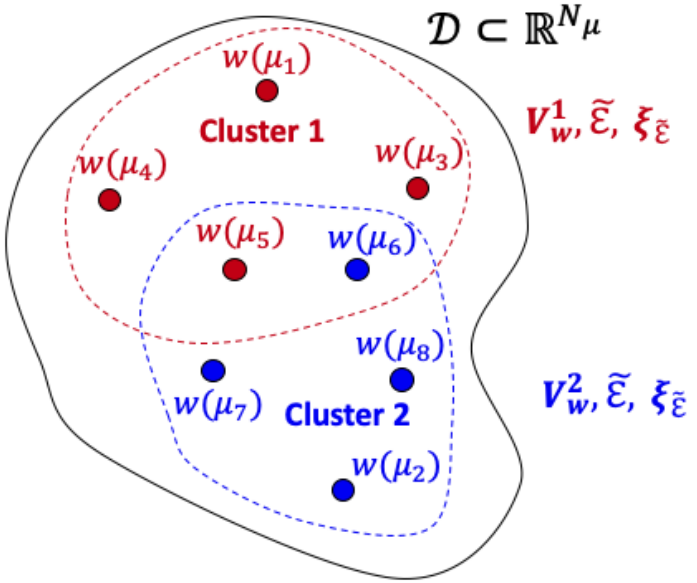
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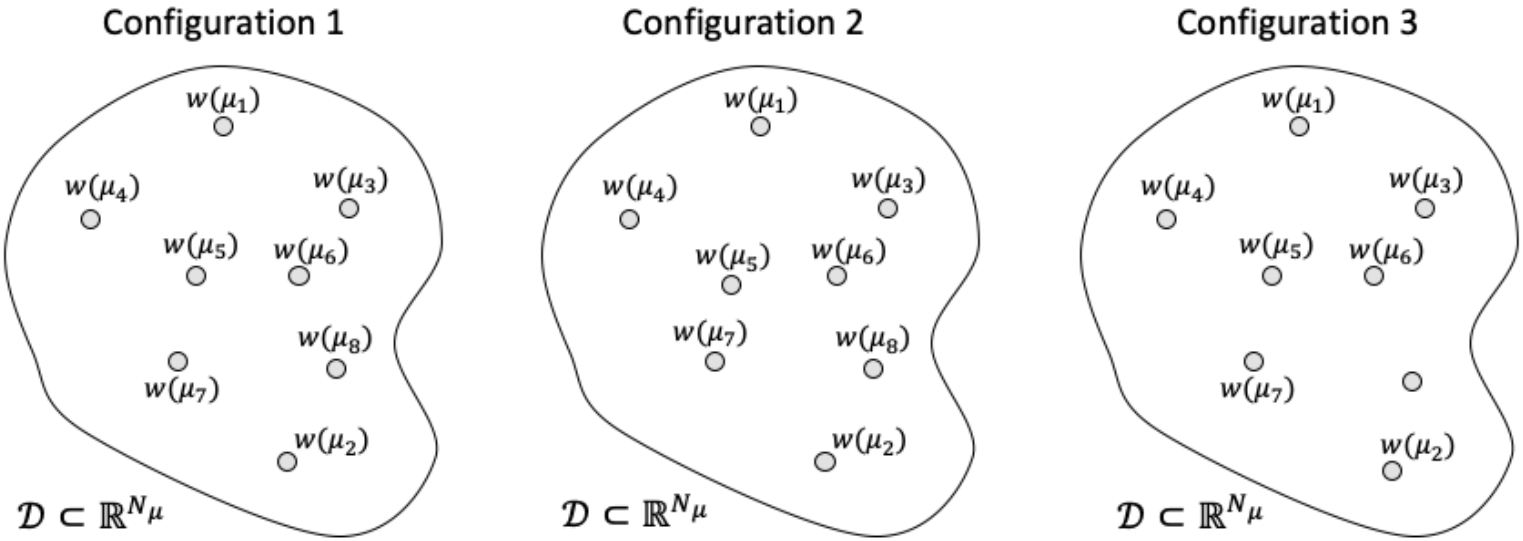
- Clustering?
  - soft clustering algorithms such as Fuzzy overlapping



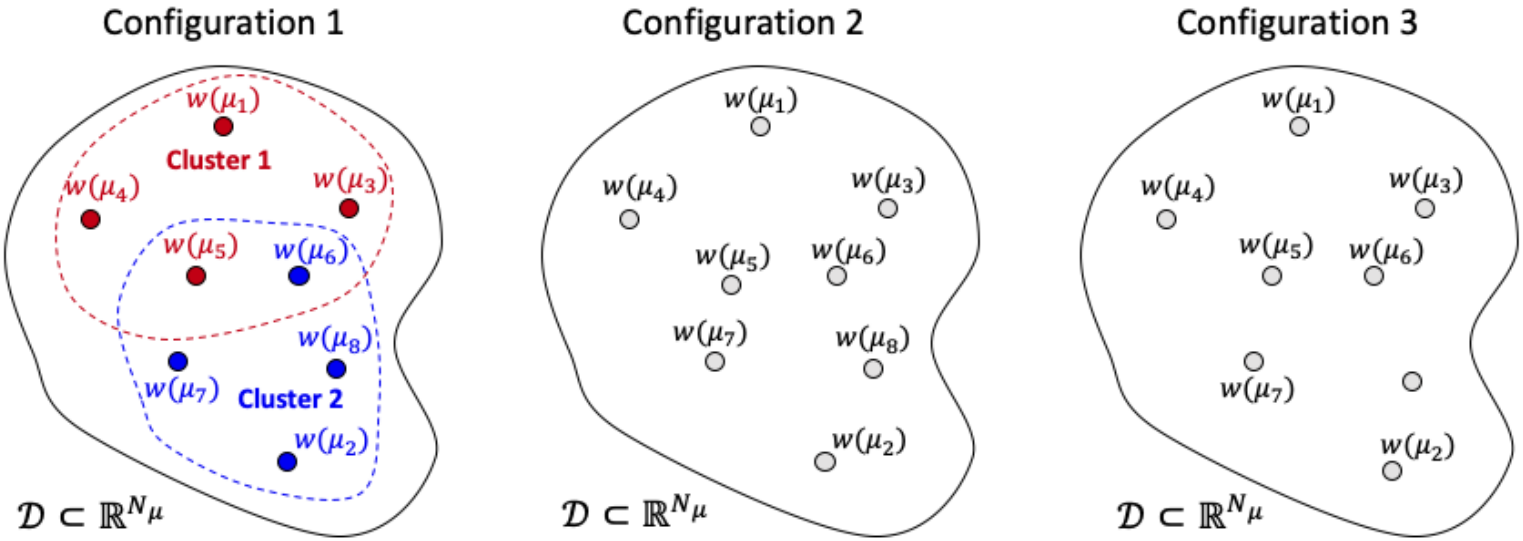
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  - vector of features for clustering

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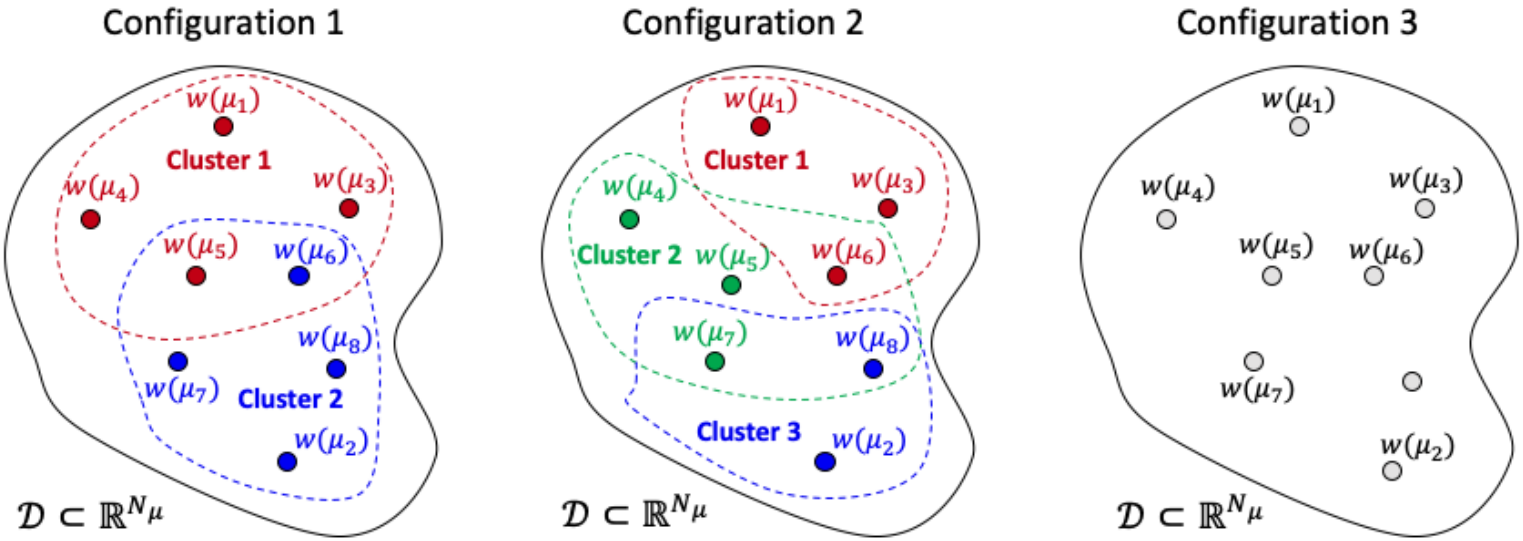
- Clustering?
  - soft clustering algorithms such as Fuzzy overlapping
- Piecewise-global (P-G) ROB $\mathbf{V}_i$ and HPROM is built for each cluster



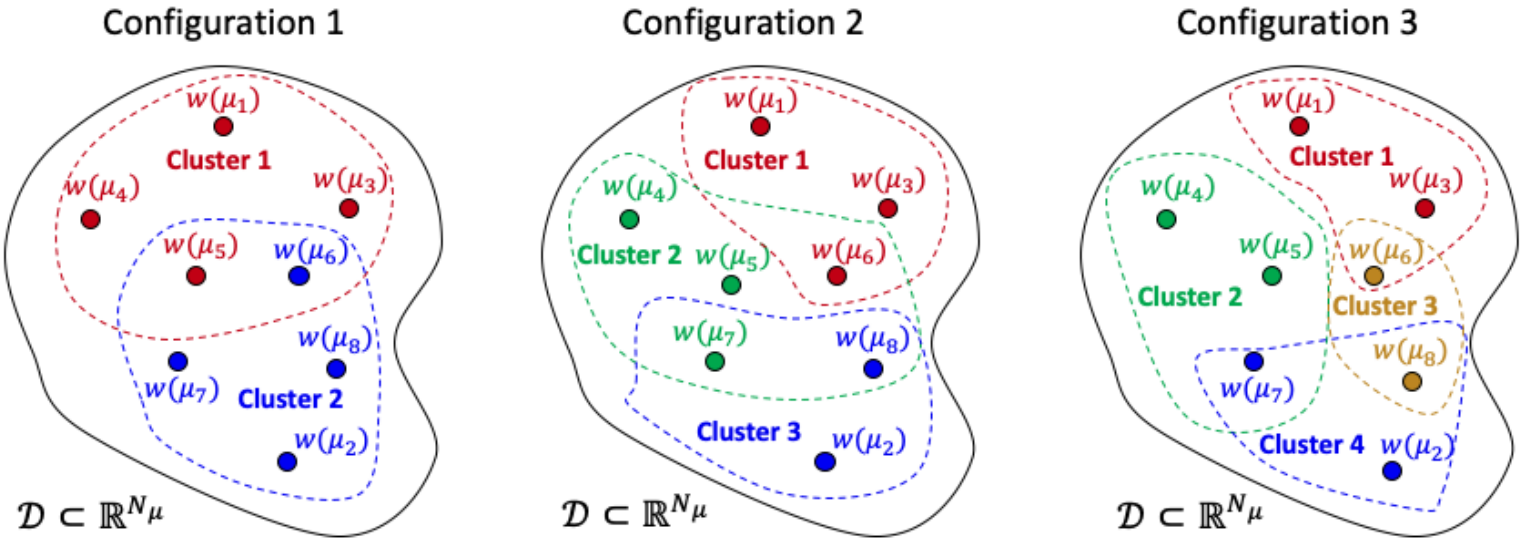
[2] Robert Tibshirani, Guenther Walther, and Trevor Hastie. "Estimating the number of clusters in a data set via the gap statistic". In: Journal of the Royal Statistical Society: Series B (Statistical Methodology) 63.2 (2001), pp. 411–423.



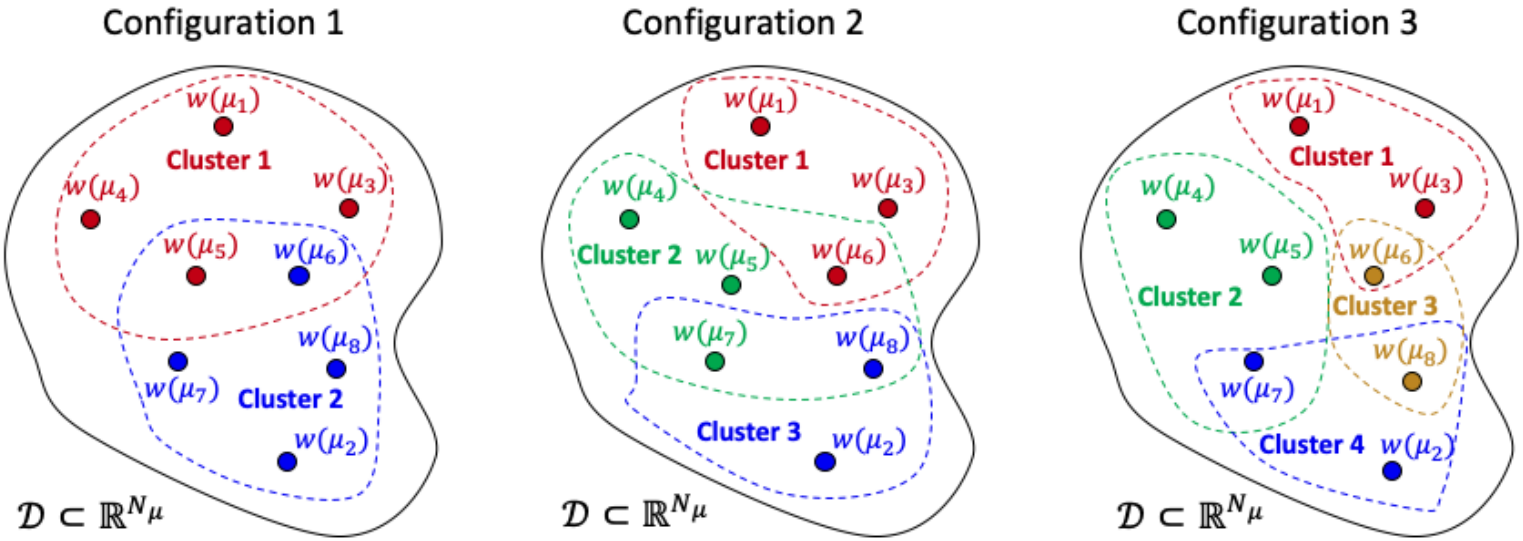
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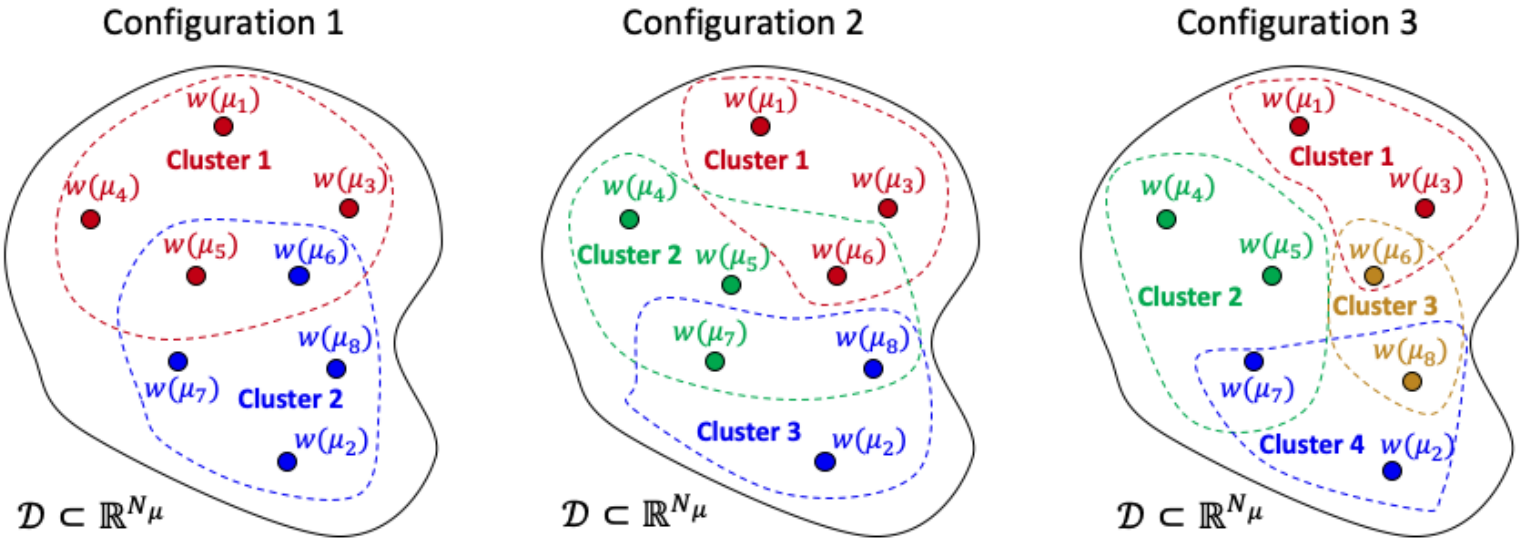


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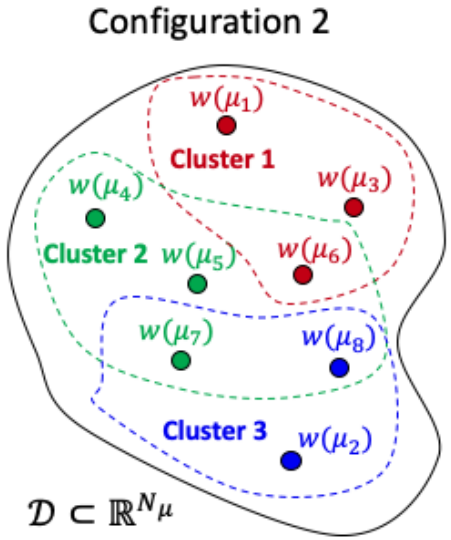
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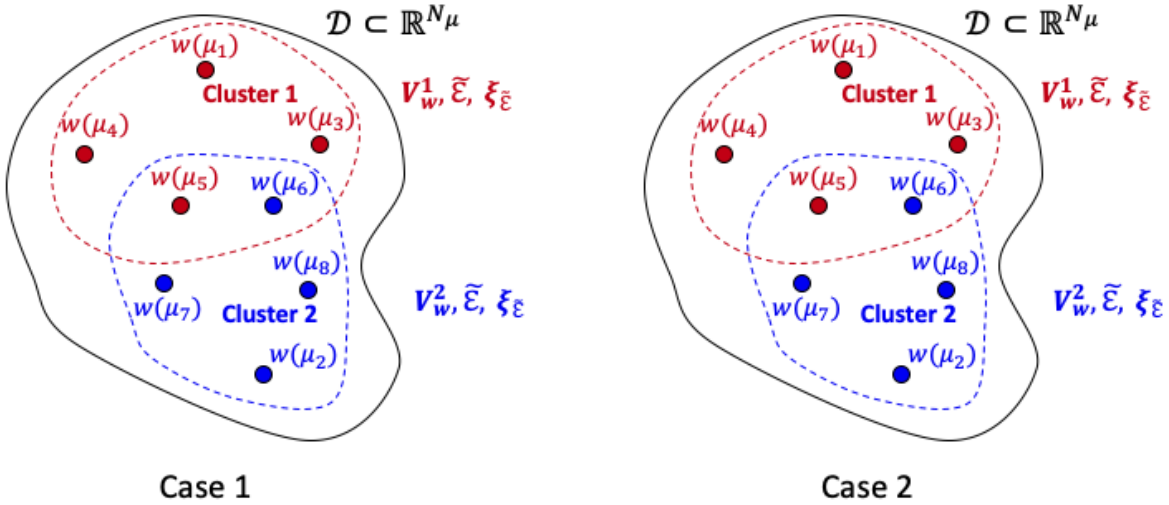
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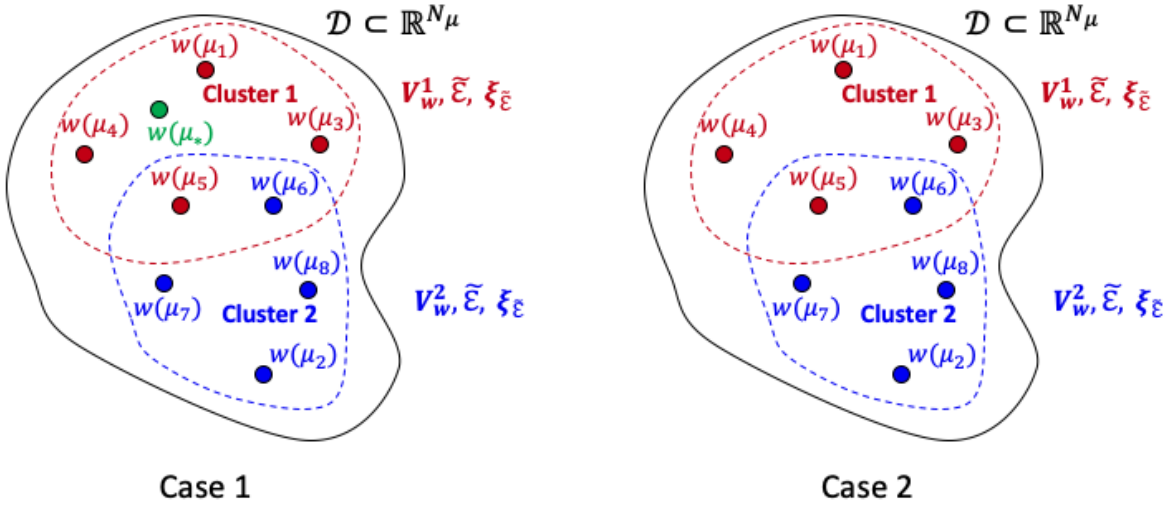
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Optimal piecewise-global model



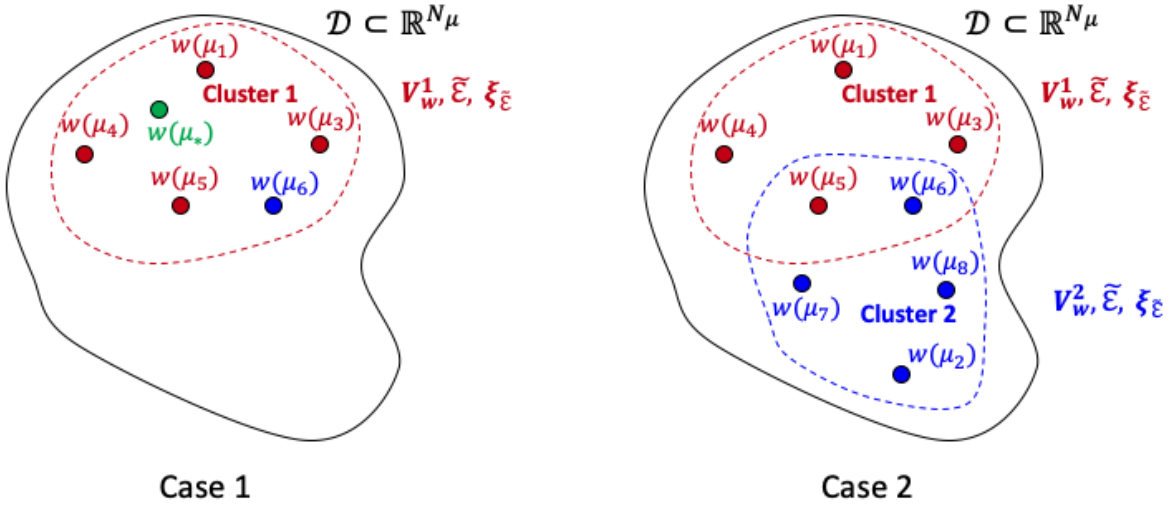
- Which piecewise-global model to select for $\boldsymbol{\mu}_*$?

Optimal piecewise-global model



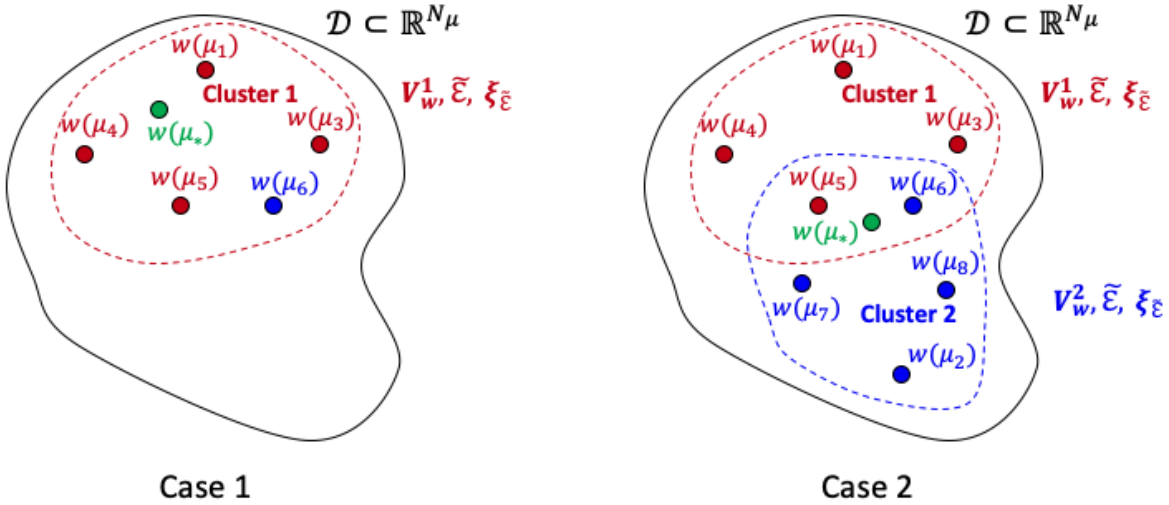
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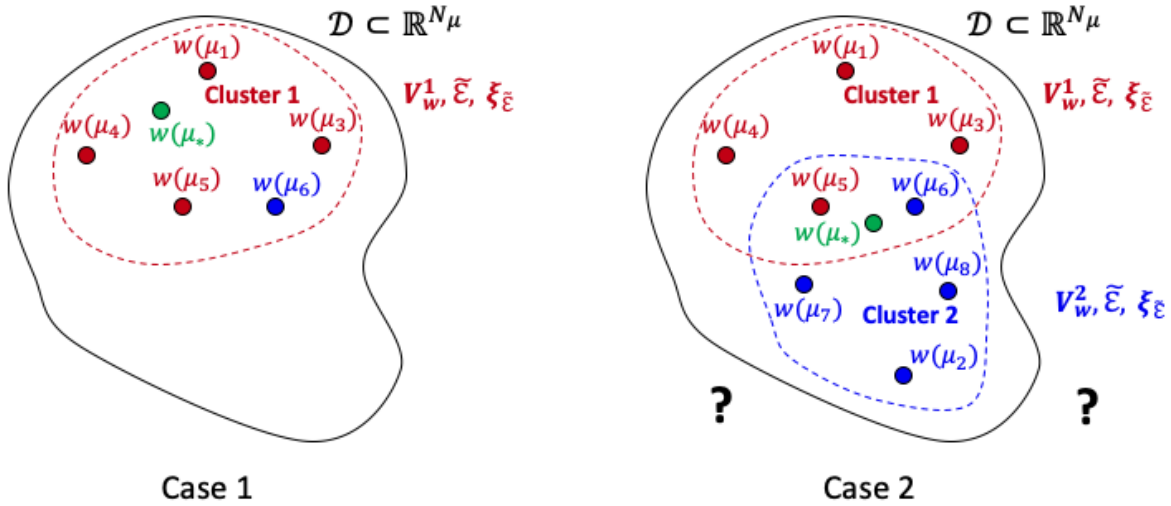
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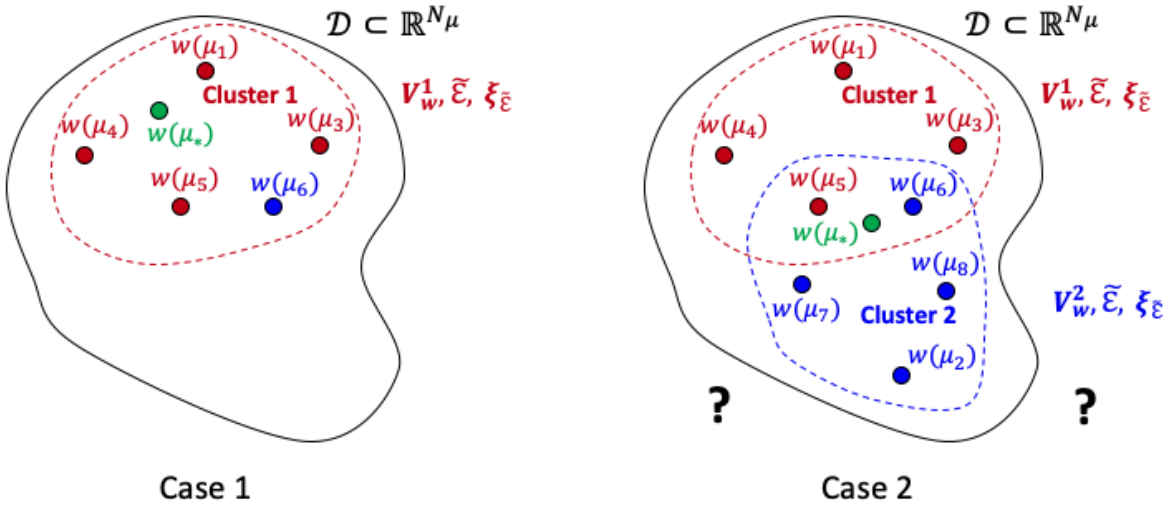
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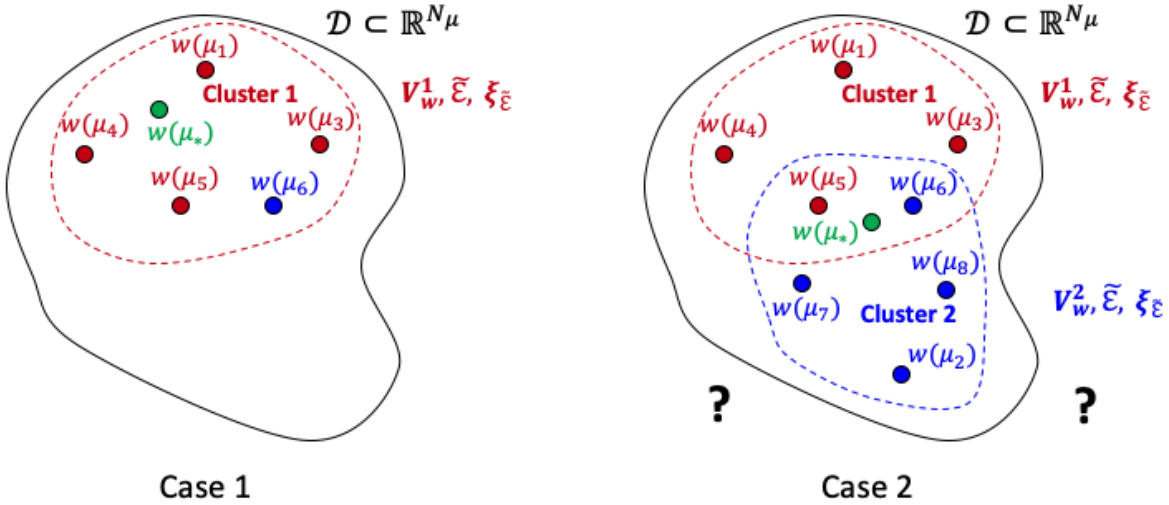
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Optimal piecewise-global model

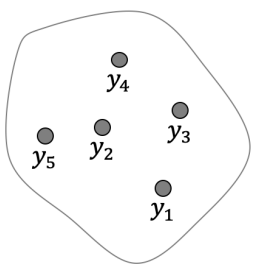


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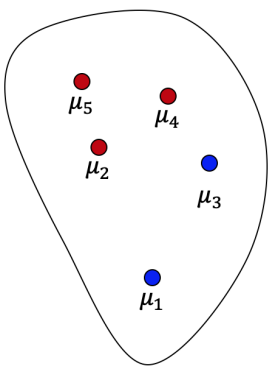
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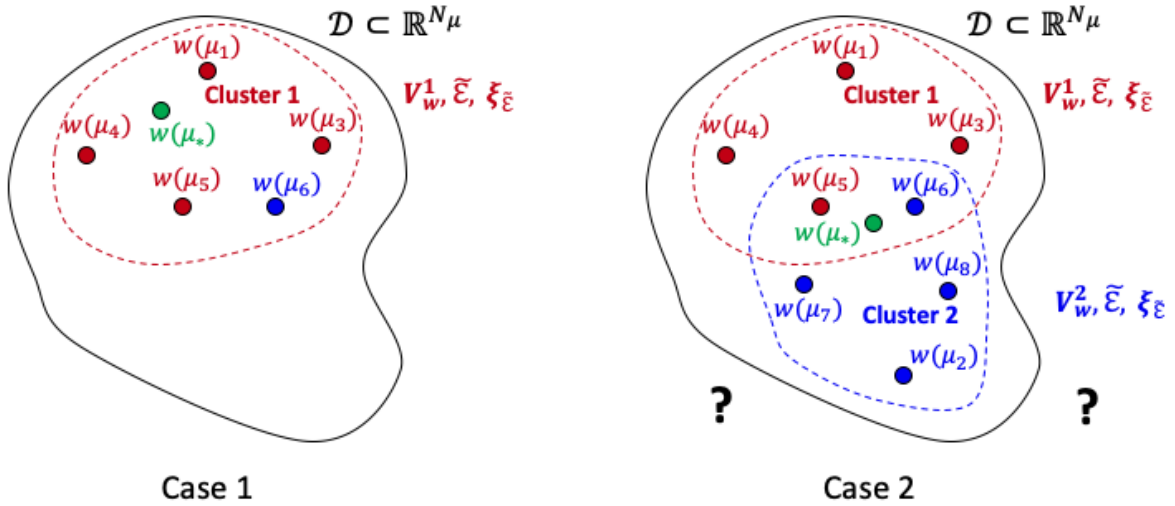


Label Space
$\mathcal{Y} \subset \mathbb{R}^{N_{cl}}$

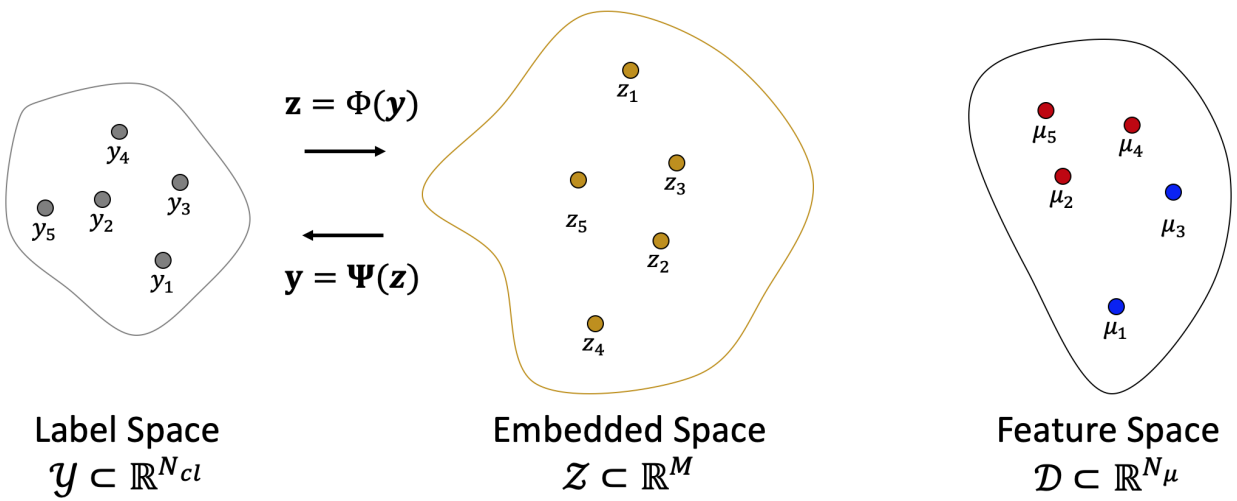


Feature Space
$\mathcal{D} \subset \mathbb{R}^{N_\mu}$

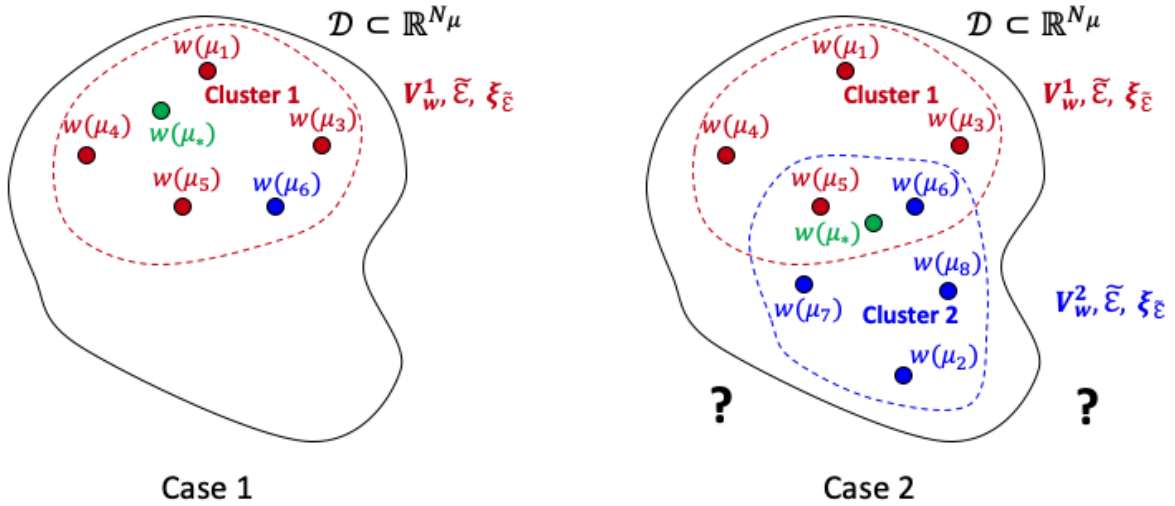
Optimal piecewise-global model



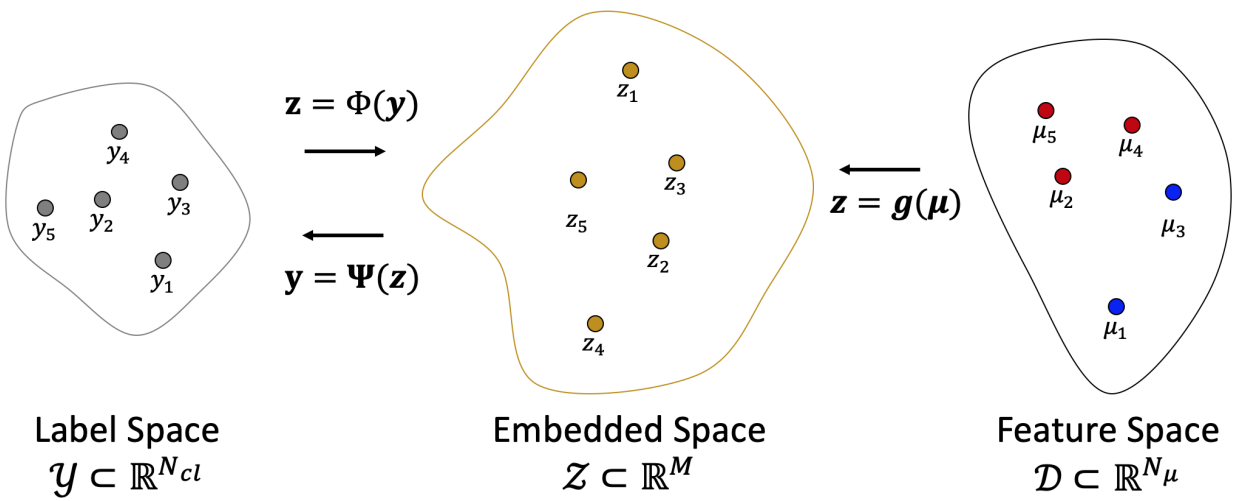
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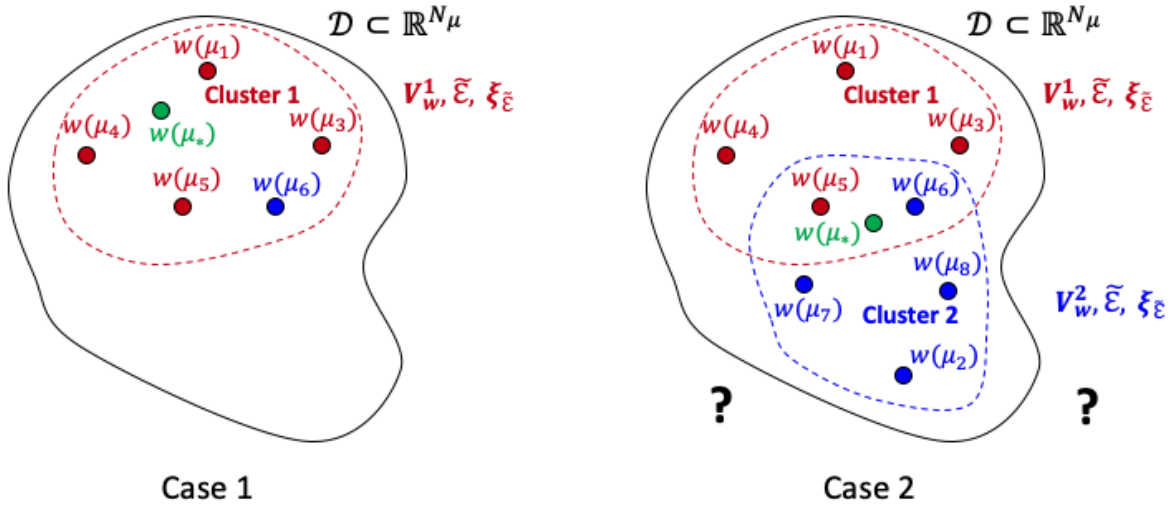
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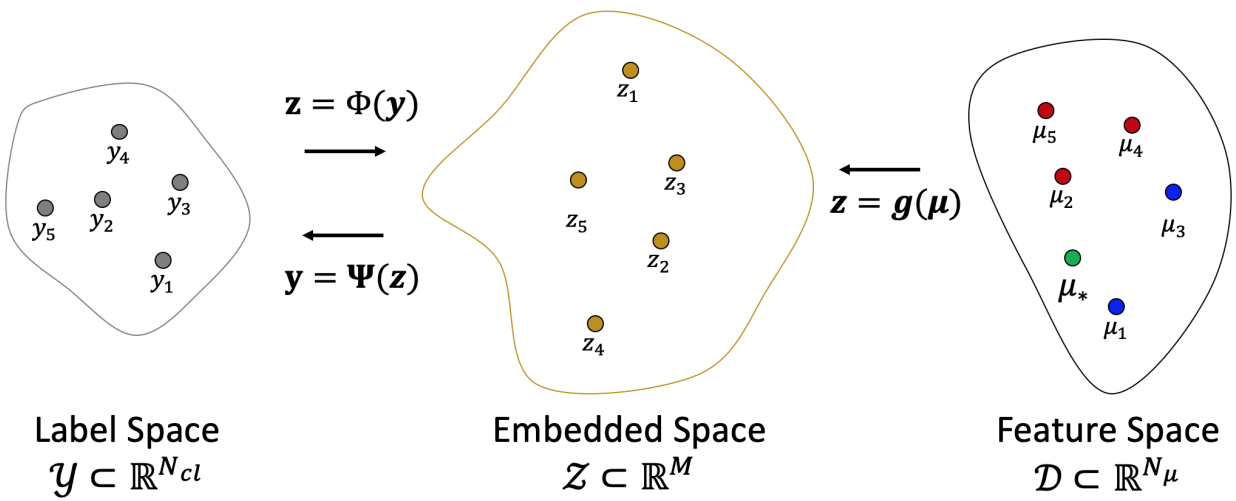
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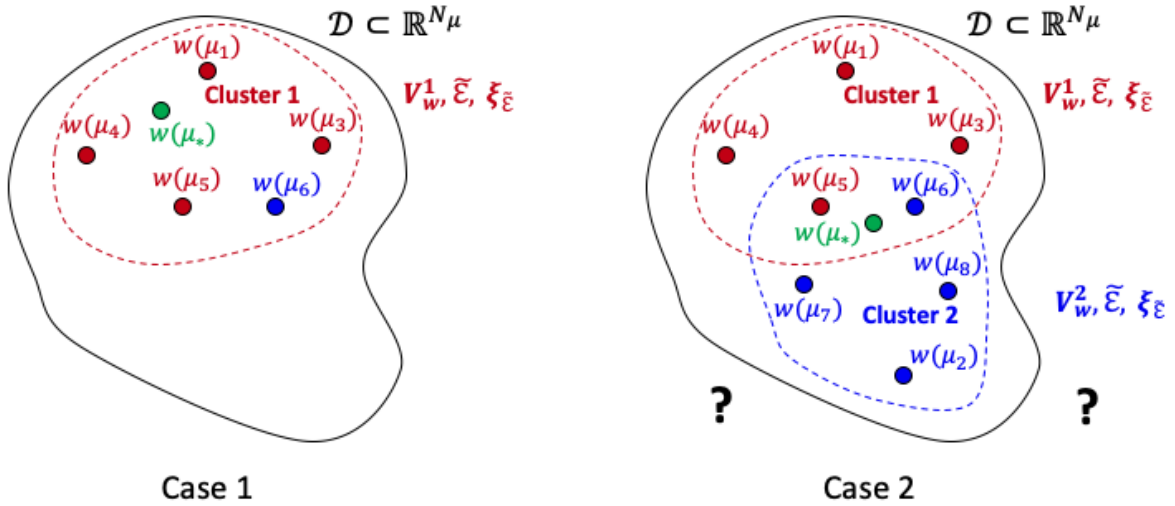
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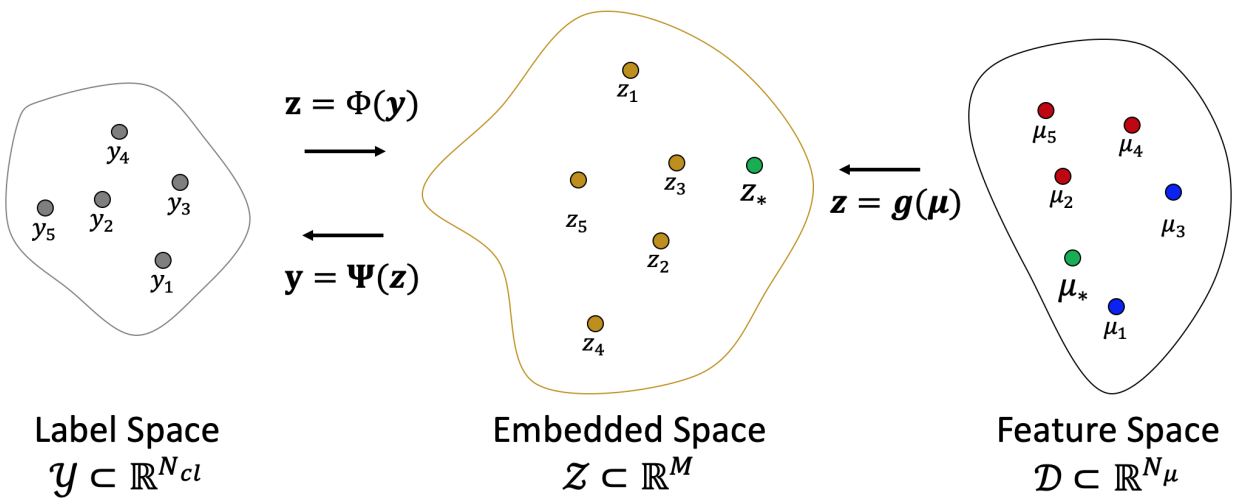
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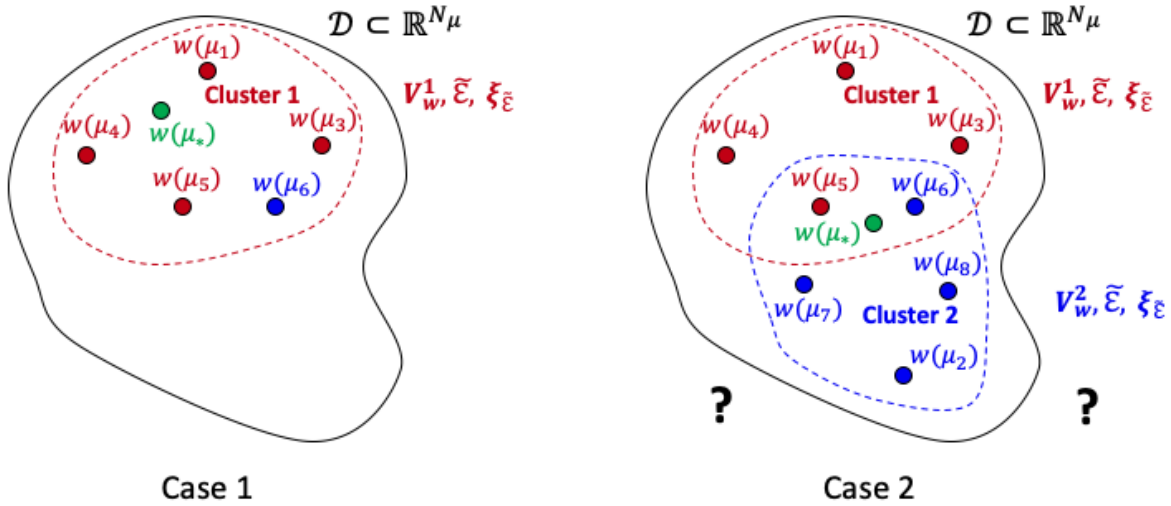


Optimal piecewise-global model

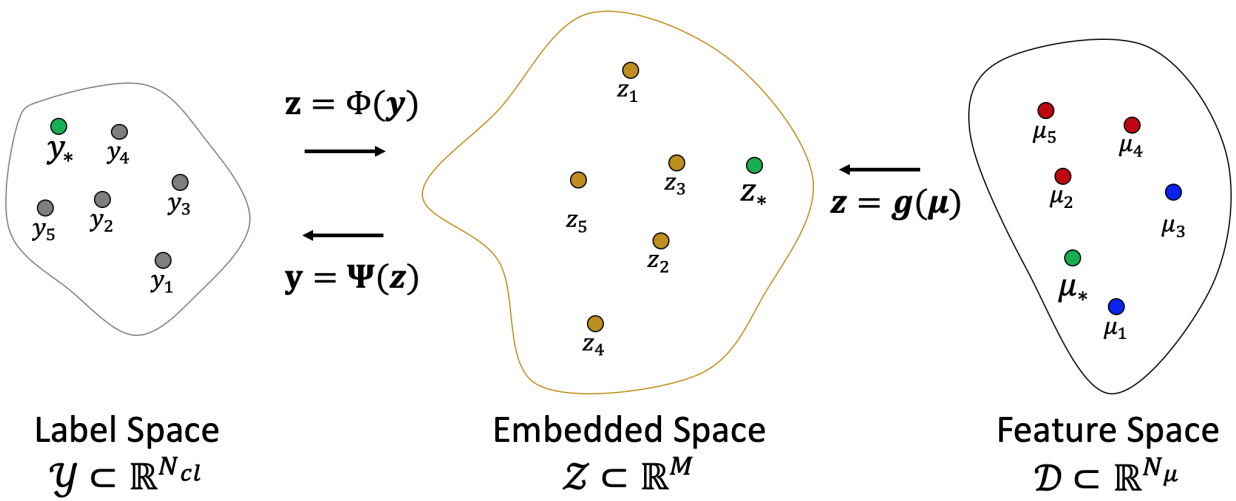


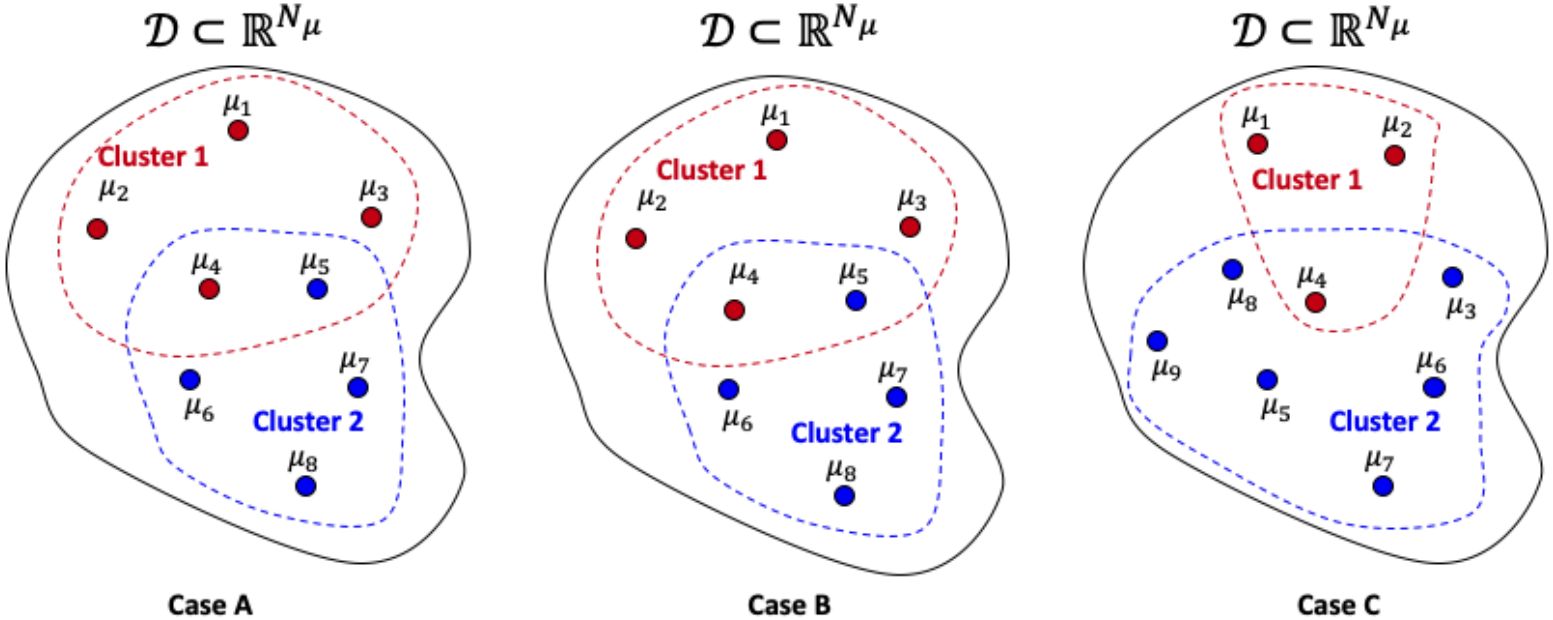
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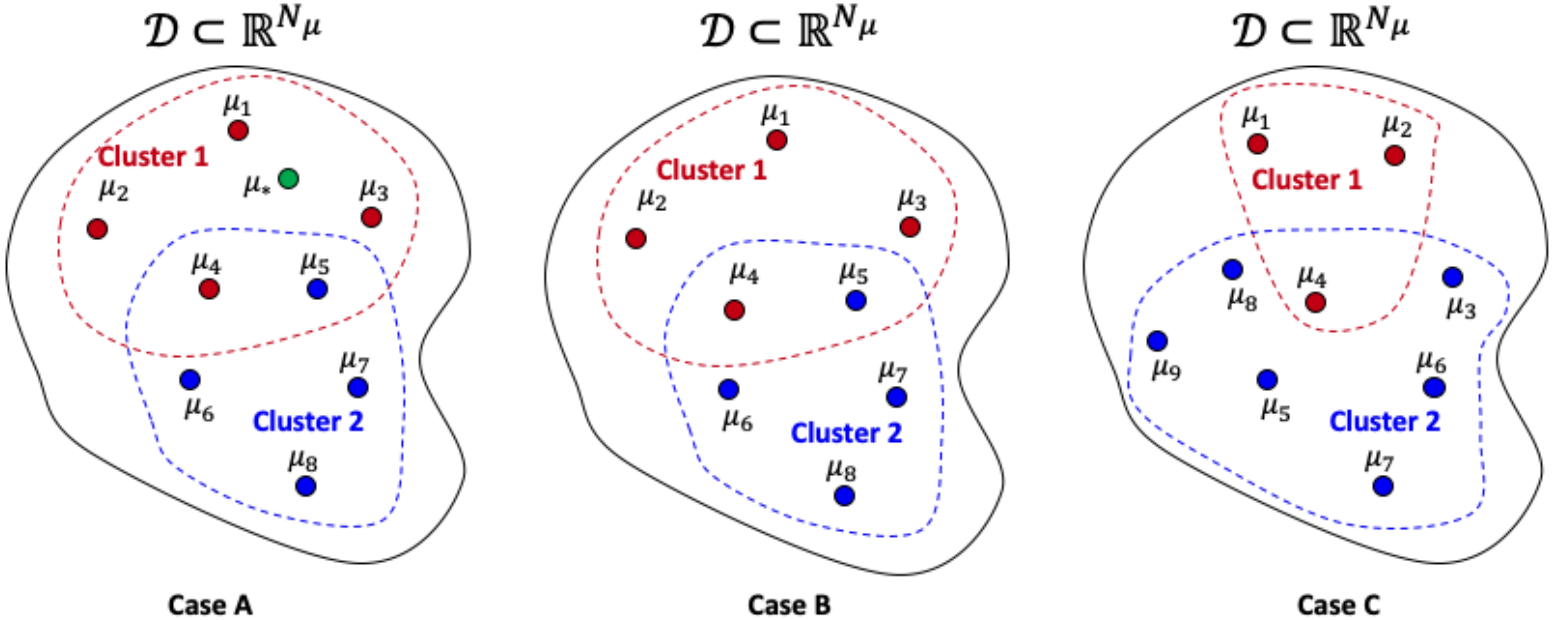
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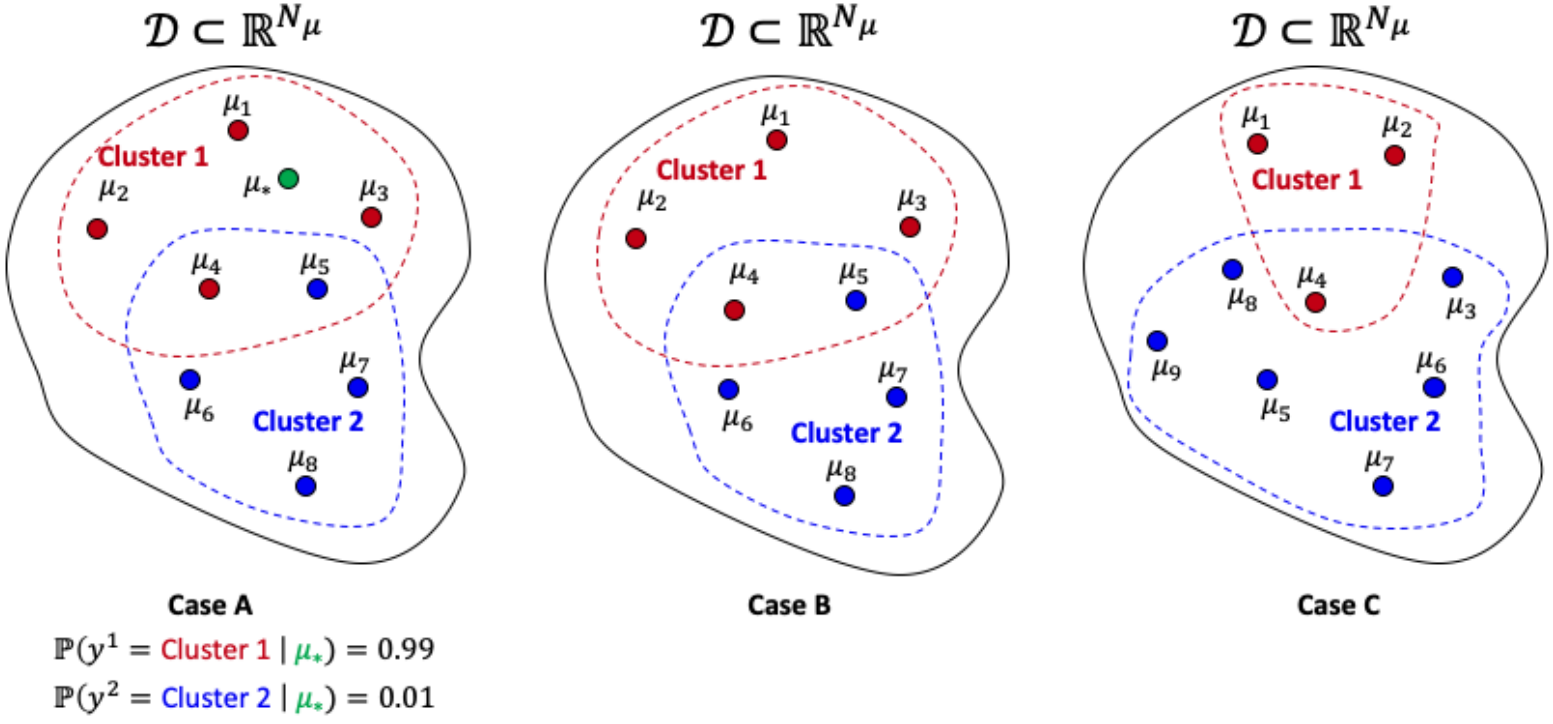
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[3] Kuan-Hao Huang and Hsuan-Tien Lin. "Cost-sensitive label embedding for multi-label classification". In: Machine Learning 106.9 (2017), pp. 1725–1746.



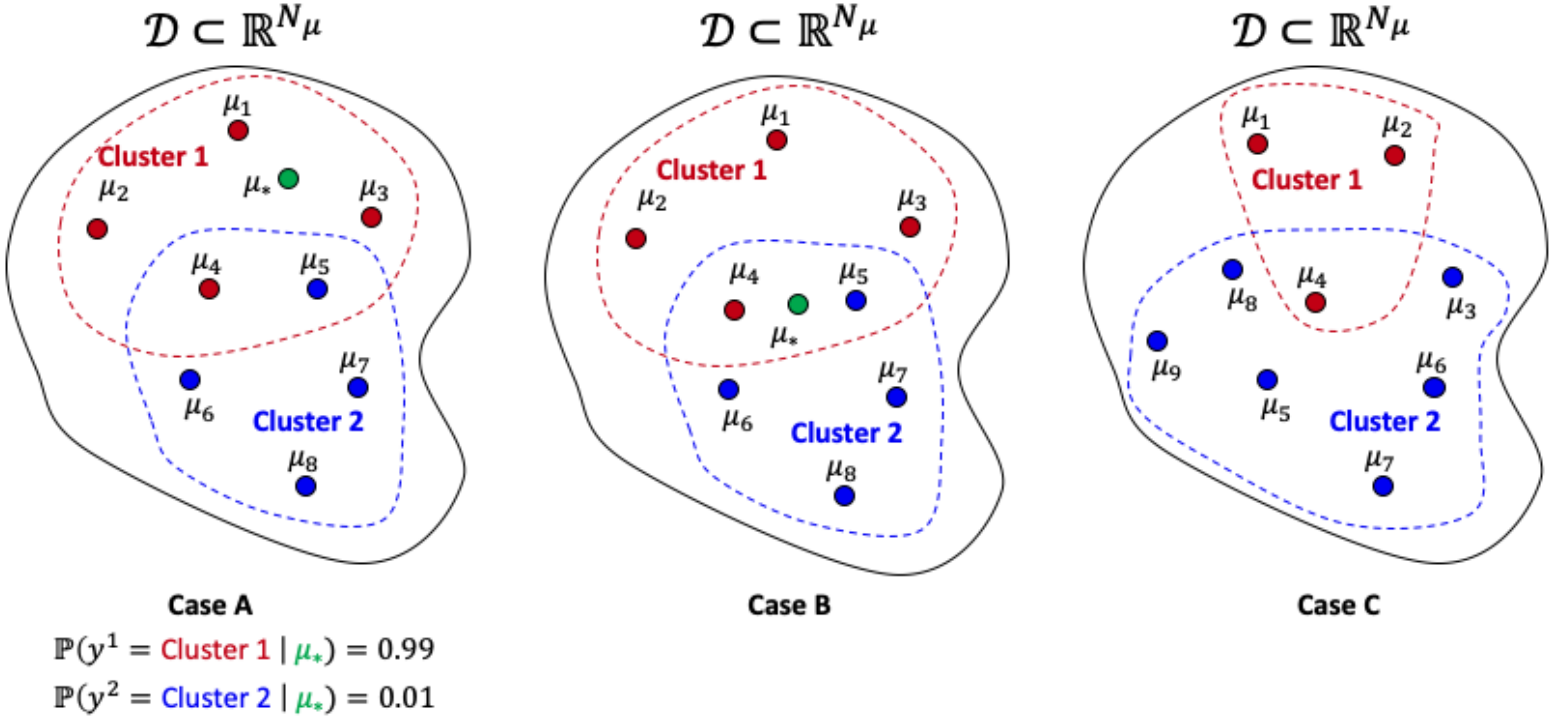
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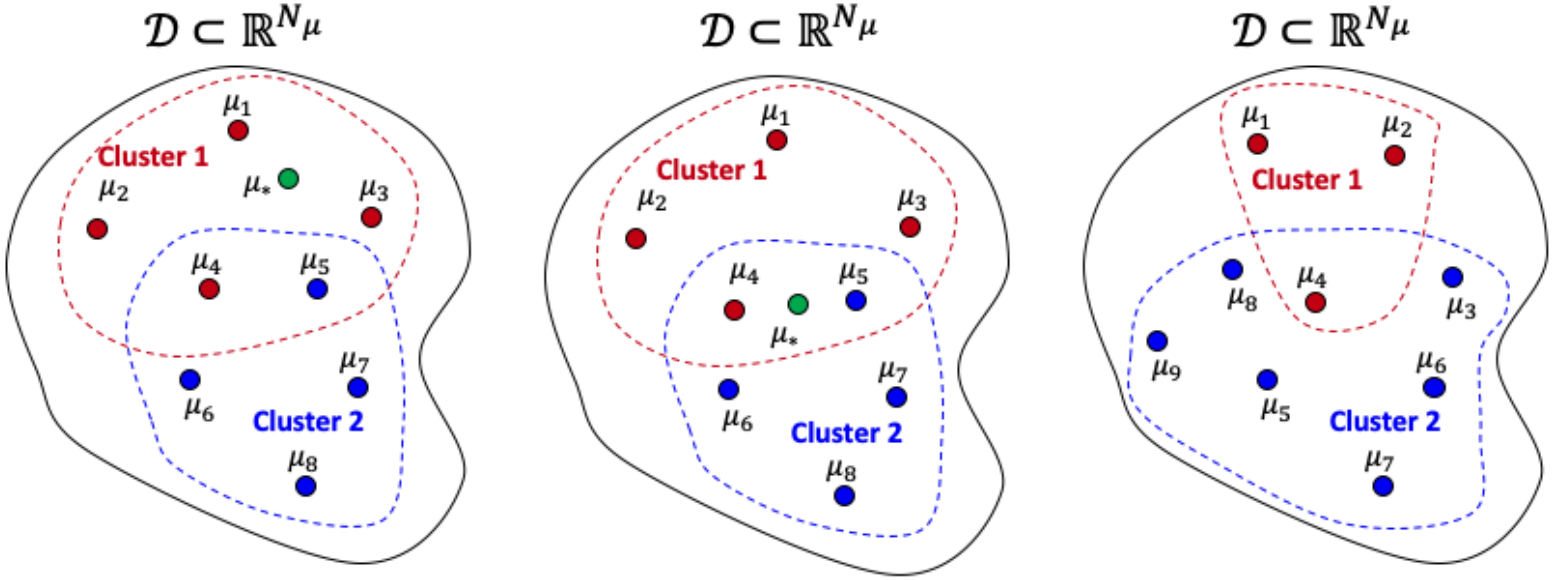
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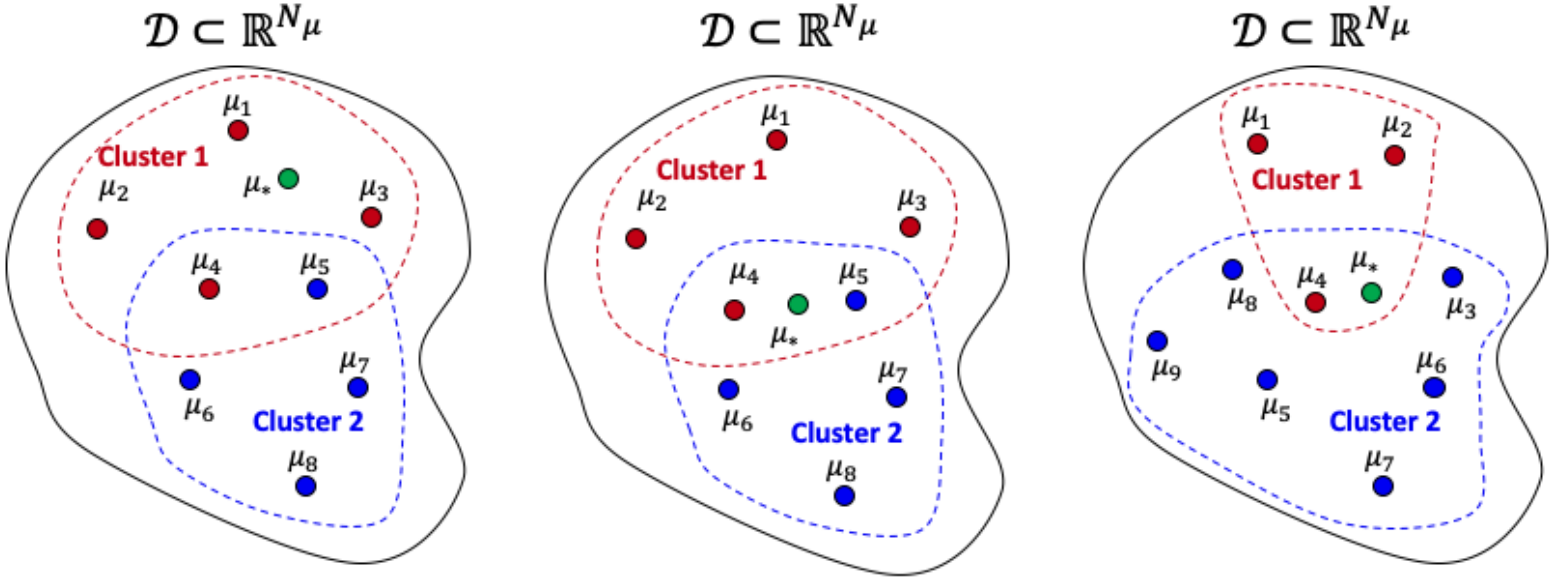
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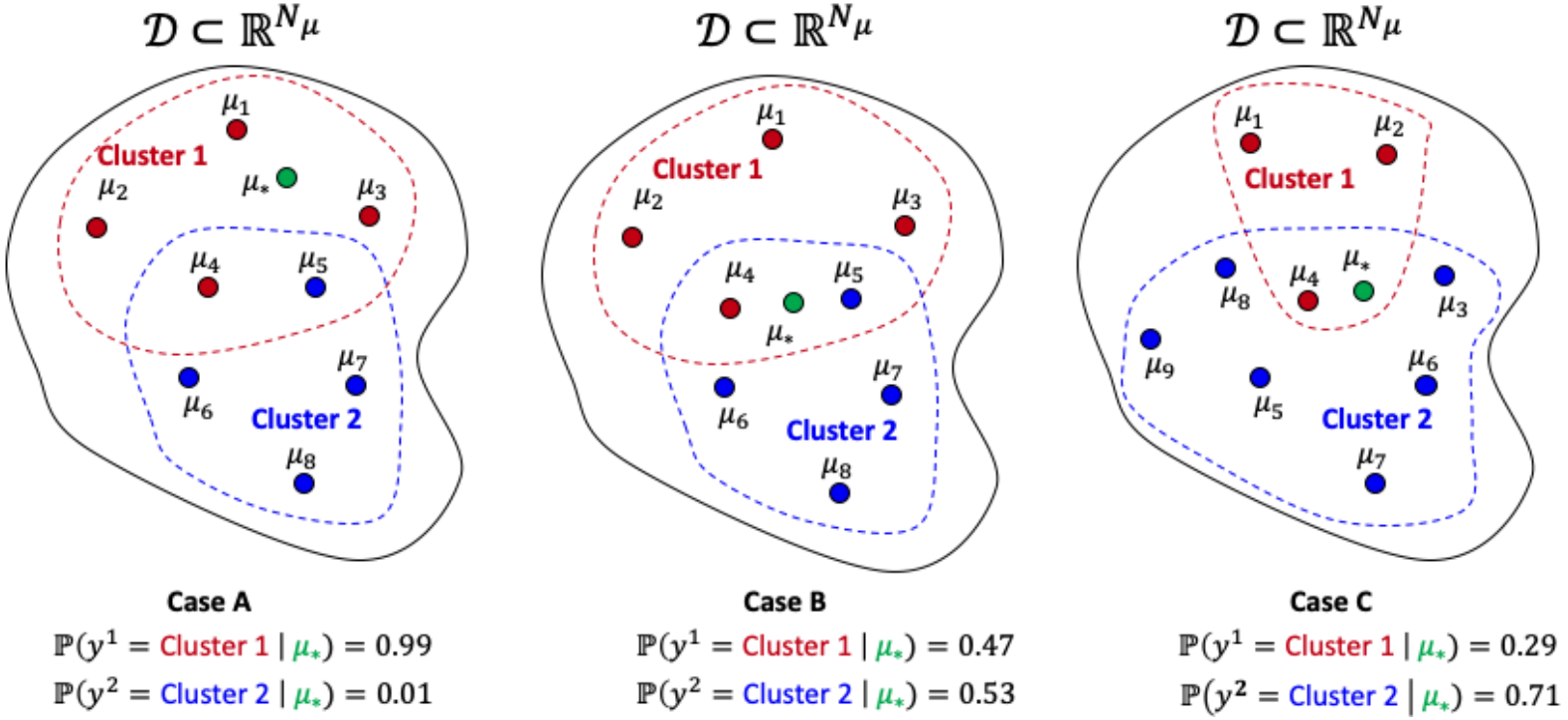
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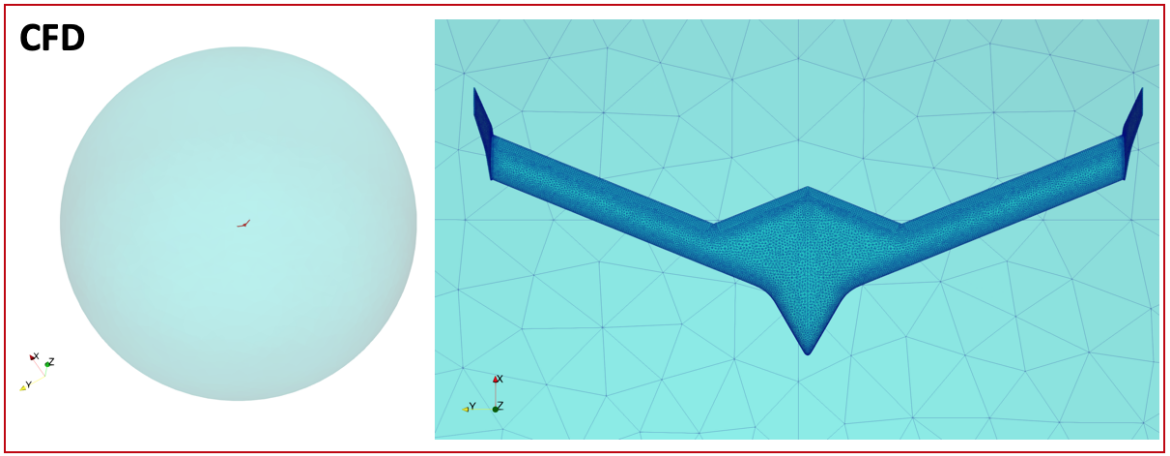
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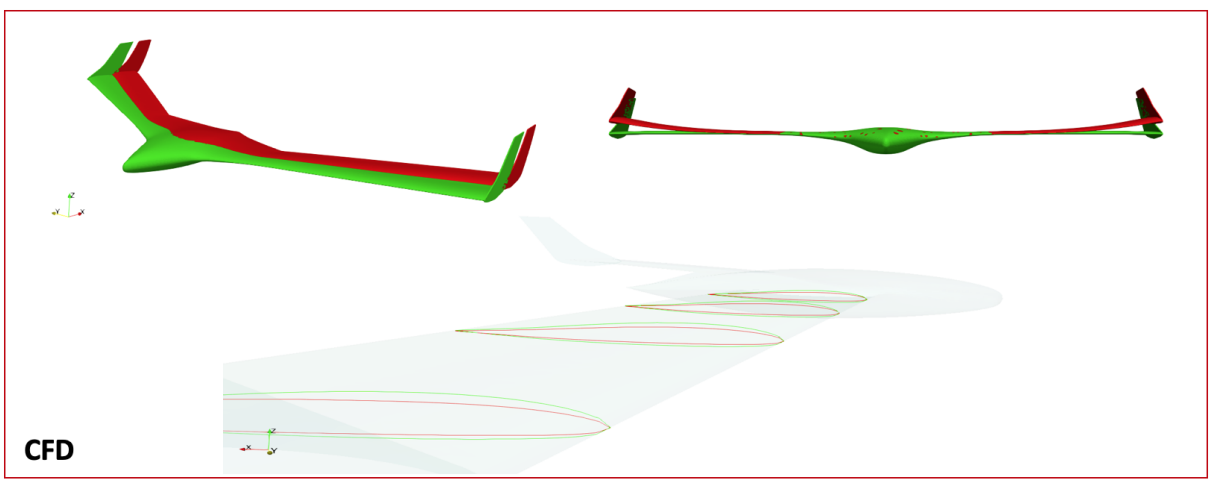
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- mAEWing2 flying aircraft
- **Flow**: $M_\infty = 0.85, \alpha = 2.32^\circ$
- Inviscid (**CFD**) grid with 199,786 grid points

- Parametric CFD model with 33 design parameters ($\boldsymbol{\mu} \in \mathbb{R}^{33}$), "reduced" to 10 generalized parameters ($\boldsymbol{\mu}_r \in \mathbb{R}^{10}$) using the method of active subspaces (see later)[4]

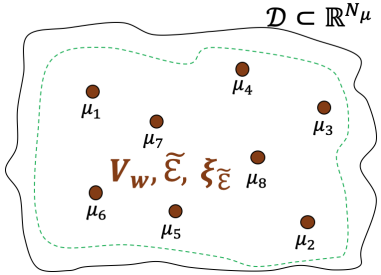


- **Design parameters** associated with the back sweep angle, the dihedral angle, and the airfoil shape

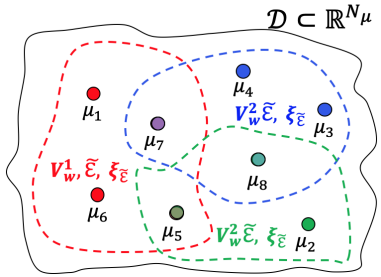
[4] Gabriele Boncoraglio and Charbel Farhat. "Optimization in High-Dimensional Parameter Spaces Using Piecewise-Global Nonlinear Hyperreduced Models and Active Subspaces". In: Submitted. 2021.

Parametric global vs piecewise-global HPROM

- 1,193 sampled snapshots, i.e., $\{\mathbf{w}(\boldsymbol{\mu}_i)\}_{i=1}^{1,193}$
- POD with energy criterion = 99.99999% and ECSW tol. $= 10^{-3}$



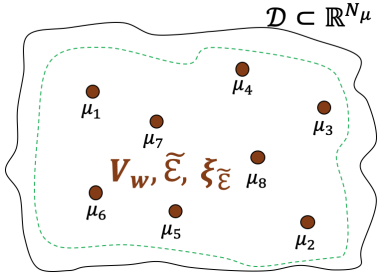
- 1 Global HPROM
  - global ROB $\mathbf{V_w}$ has dimension 1,179
  - sampled mesh has 57,457 nodes ($|\widetilde{\mathcal{E}}| = 57,457$; 28.8% of the original mesh)

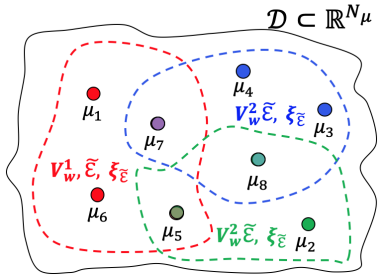


- Database of 17 piecewise-global HPROMs
  - each piecewise-global ROB $\mathbf{V}_\mathbf{w}^i$ has on average dimension 130
  - each sampled mesh has on average 11,071 nodes ($|\widetilde{\mathcal{E}}| = 11,071$; 5.5% of the original mesh).

Parametric global vs piecewise-global HPROM

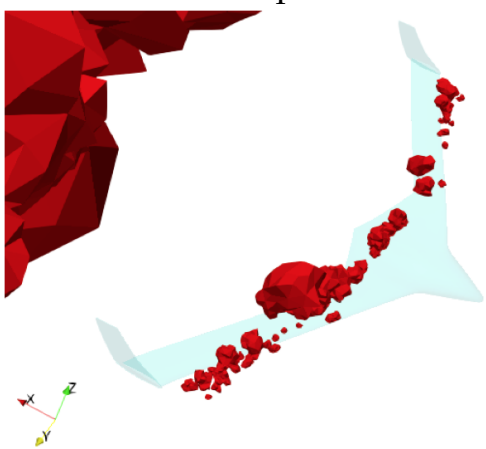
- 1,193 sampled snapshots, i.e., $\{\mathbf{w}(\boldsymbol{\mu}_i)\}_{i=1}^{1,193}$
- POD with energy criterion = 99.99999% and ECSW tol. $= 10^{-3}$

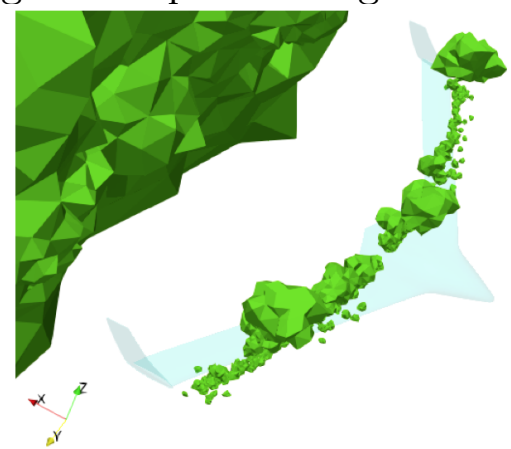


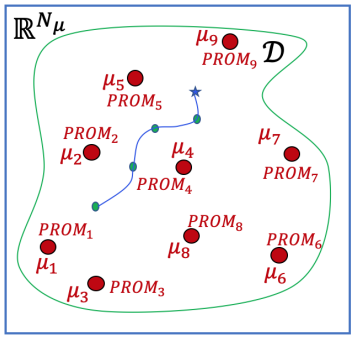


- 1 Global HPROM
  - global ROB $\mathbf{V_w}$ has dimension 1,179
  - sampled mesh has 57,457 nodes ($|\widetilde{\mathcal{E}}| = 57,457$; 28.8% of the original mesh)
- Database of 17 piecewise-global HPROMs
  - each piecewise-global ROB $\mathbf{V}_\mathbf{w}^i$ has on average dimension 130
  - each sampled mesh has on average 11,071 nodes ($|\widetilde{\mathcal{E}}| = 11,071$; 5.5% of the original mesh).

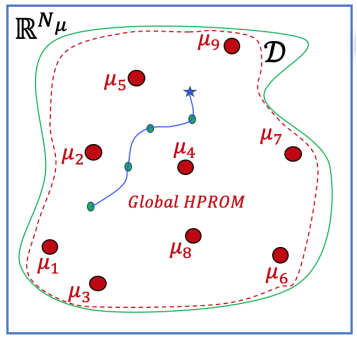
- (*left*) part of the sampled mesh belonging to the piecewise-global HPROM$_1$; and (*right*) part of the sampled mesh belonging to the piecewise-global HPROM$_2$





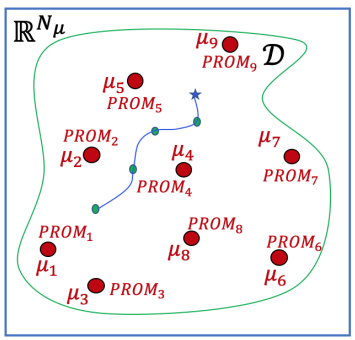


Database $\mathcal{DB}$ of local linear PROMs

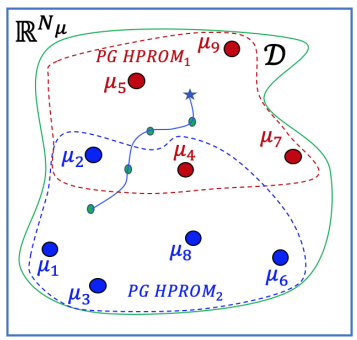


Global nonlinear HPROM

1. Exploit nonlinear, piecewise-global HPROMs in $\mathcal{D}$

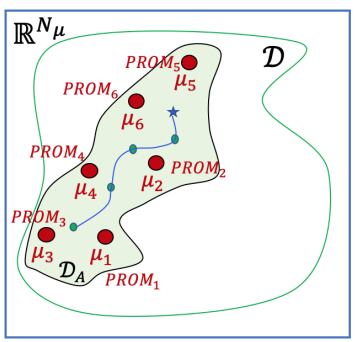


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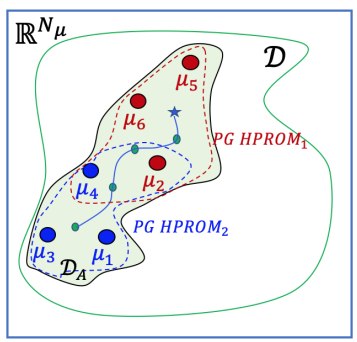


Piecewise-Global nonlinear HPROMs

2. Train/exploit linear, local PROMs and nonlinear, piecewise-global HPROMs, and solve optimization problem in $\mathcal{D}_A \subset \mathcal{D}$



Database $\mathcal{DB}$ of local linear PROMs



Piecewise-Global nonlinear HPROMs

- PDE-constrained optimization problem

$$\begin{aligned} \min_{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{N_{\boldsymbol{\mu}}}} \quad & f(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{c}(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}) \geqslant 0 \end{aligned} \tag{$\star$}$$

- Solution of problem $(\star)$ is contained in the AS, i.e., $\mathcal{D}_{AS} \subset \mathcal{D}$
- Each design parameter vector $\boldsymbol{\mu} \in \mathcal{D}_{AS} \subset \mathcal{D}$

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{\text{ref}} + \mathbf{V}_{\boldsymbol{\mu}} \boldsymbol{\mu}_r$$

  - $\mathbf{V}_{\boldsymbol{\mu}} \in \mathbb{R}^{N_{\boldsymbol{\mu}} \times N_{\boldsymbol{\mu}_r}}$ is a ROB ($N_{\boldsymbol{\mu}} \gg N_{\boldsymbol{\mu}_r}$)
  - $\boldsymbol{\mu}_r \in \mathbb{R}^{N_{\boldsymbol{\mu}_r}}$ are the generalized coordinates of $\boldsymbol{\mu}$

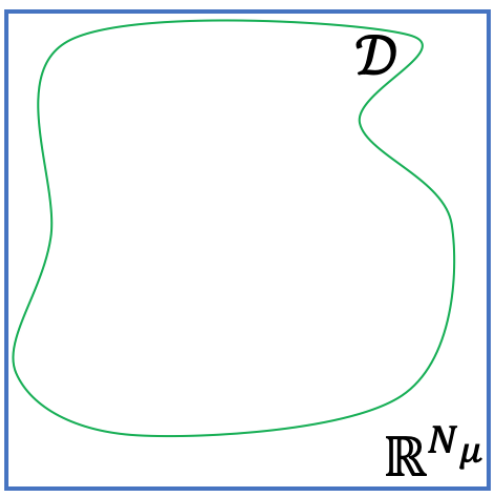
- PDE-constrained optimization problem

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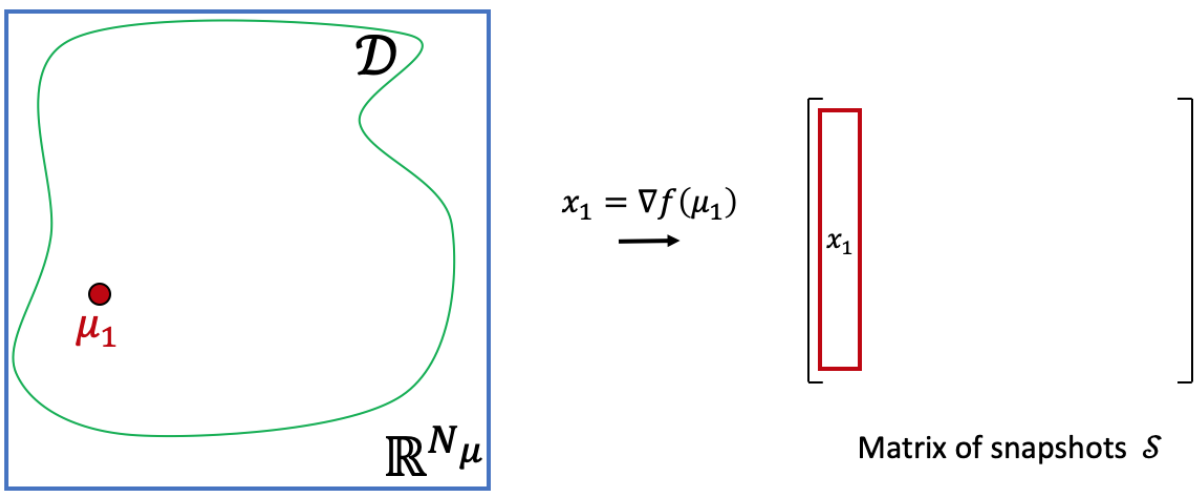
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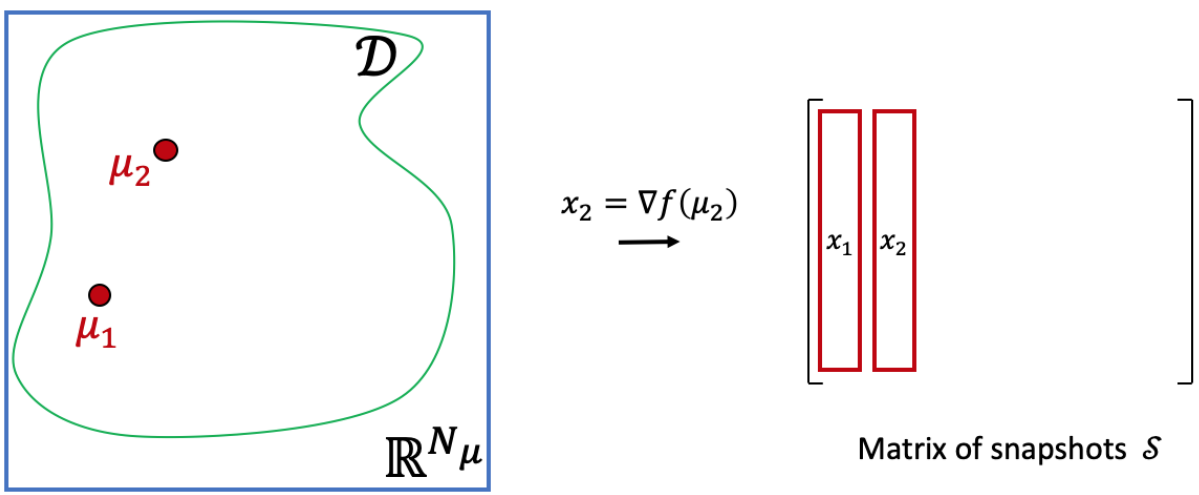
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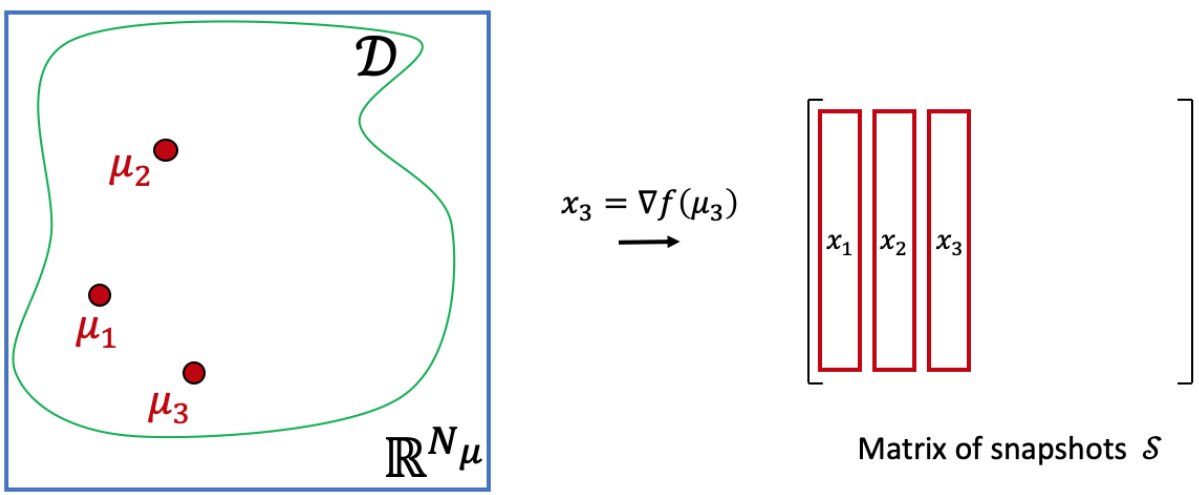
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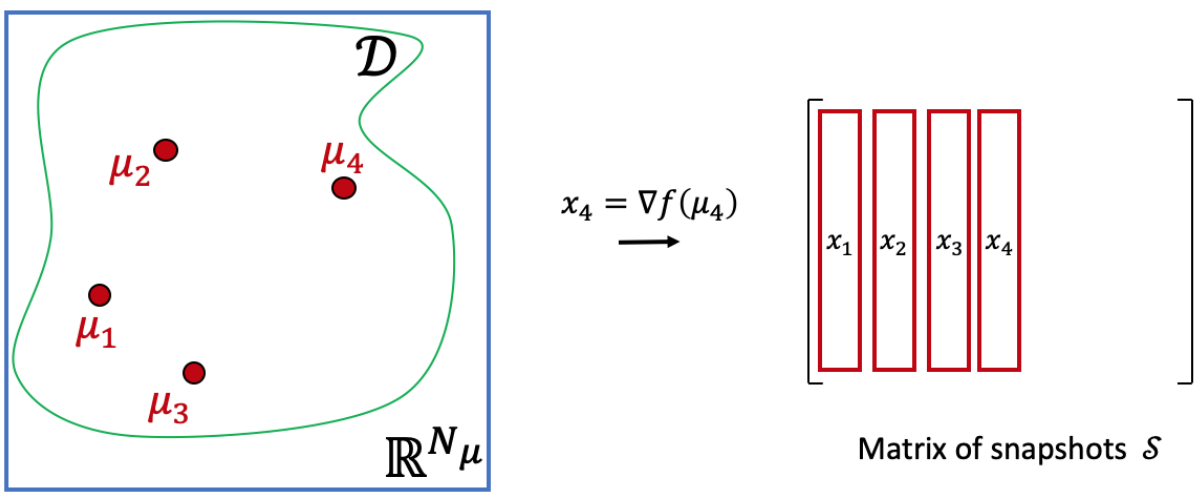
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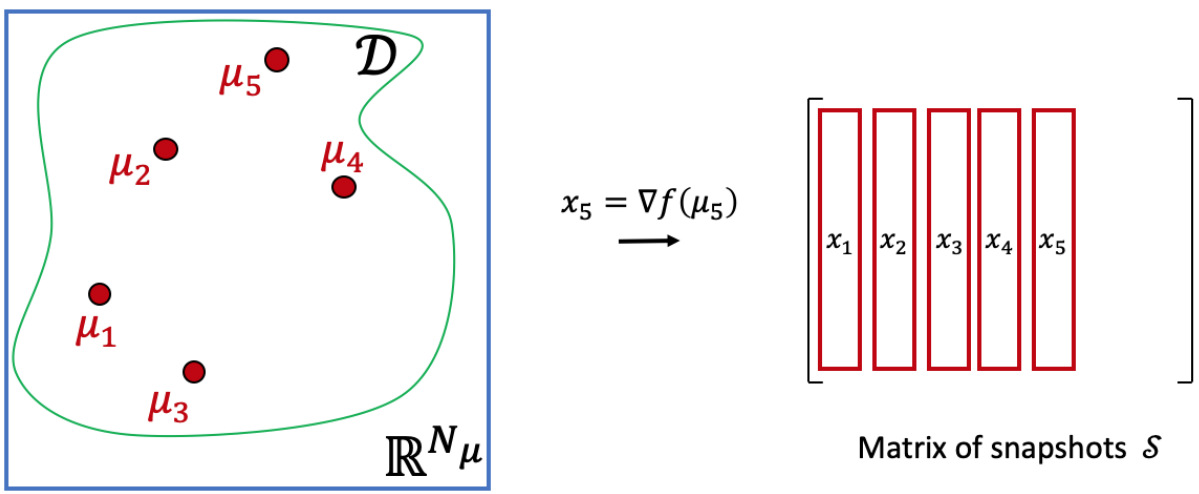
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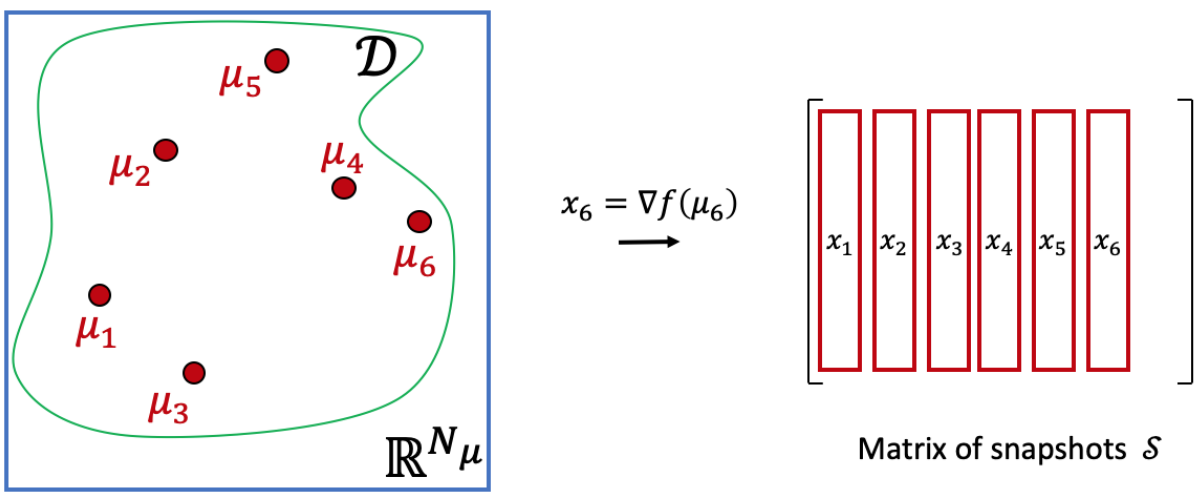
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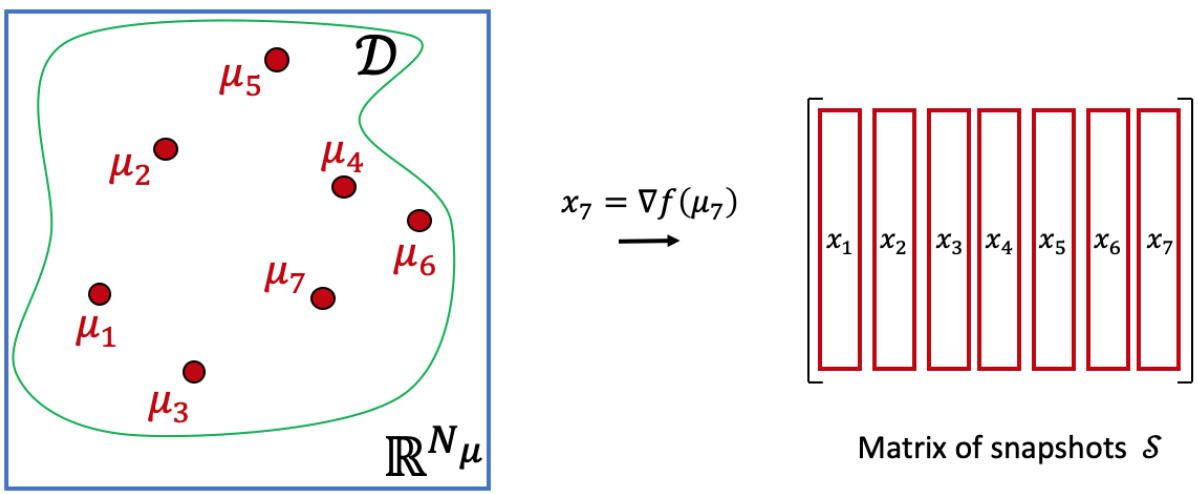
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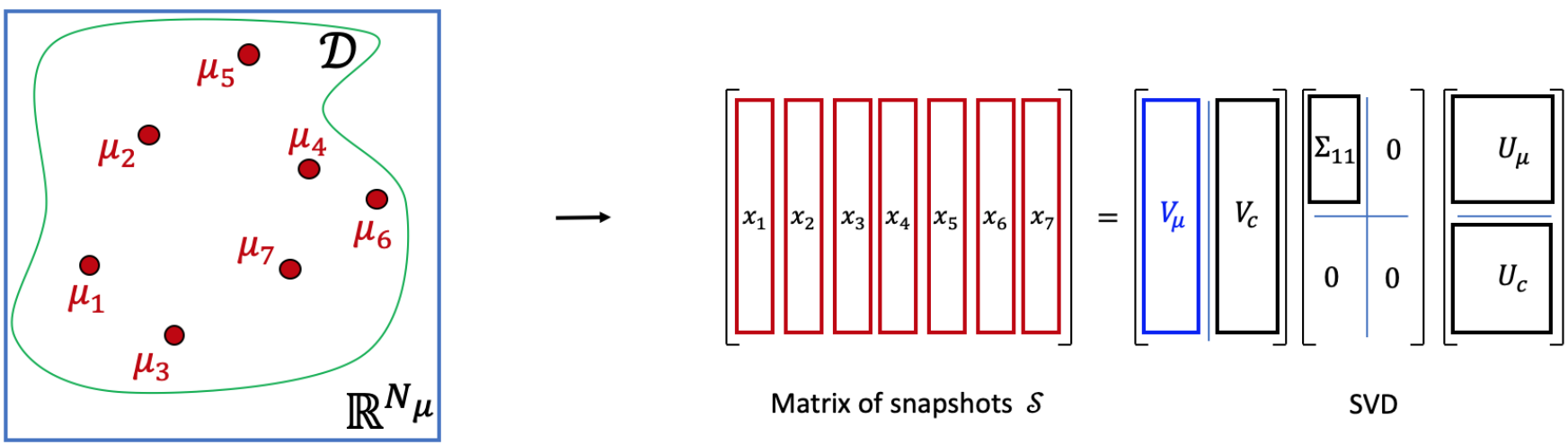
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The classical construction of the AS suffers from several drawbacks

- The guideline for estimating the number m of gradients to sample may still call for sampling a very large number of gradients
  - Constantine[5] suggests

$$m = \alpha \; k \; \log(N_{\boldsymbol{\mu}})$$

    where $2 \leqslant \alpha \leqslant 10$ and k is the number of singular values that are to be approximated
- The construction does not account for the constraints $\mathbf{c}(\cdot) \geqslant \mathbf{0}$
- Sampling a priori the gradients of $f(\cdot)$ (e.g., random sampling) does not necessarily lead to an AS which contains an optimal solution[6]

[5] Paul G Constantine. Active subspaces: Emerging ideas for dimension reduction in parameter studies. SIAM, 2015.

[6] Gabriele Boncoraglio, Charbel Farhat, and Charbel Bou-Mosleh. "Model reduction framework with a new take on active subspaces for optimization problems with linearized fluid-structure interaction constraints". In: International Journal for Numerical Methods in Engineering (2020).

- Same AS assumption: $\boldsymbol{\mu} = \boldsymbol{\mu}_{\text{ref}} + \mathbf{V}_{\boldsymbol{\mu}} \boldsymbol{\mu}_r$
- Recall that the update of each iterate $\boldsymbol{\mu}_k$ can be written as

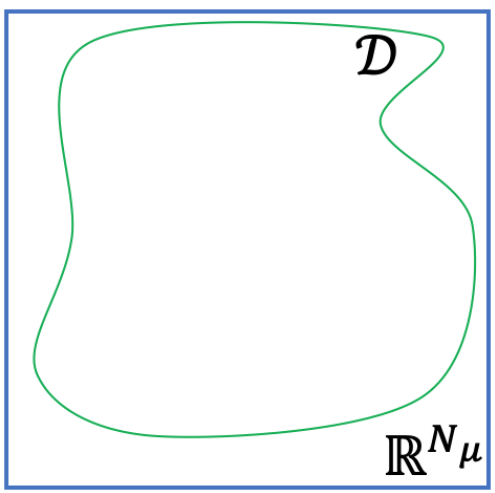
$$\boldsymbol{\mu}_{k+1} = \boldsymbol{\mu}_k + \Delta\boldsymbol{\mu}_k$$

  where $\Delta\boldsymbol{\mu}_k \in \mathbb{R}^{N_\mu}$ is determined by the optimization procedure
  - unconstrained optimization problem, a gradient-based procedure: $\Delta\boldsymbol{\mu}_k = -\eta_k \mathbf{C}_k \nabla f(\boldsymbol{\mu}_k)$
  - constrained optimization problem: $\Delta\boldsymbol{\mu}_k$ can be computed using the Karush-Kuhn-Tucker (KKT) conditions
- Alternative idea: directly sample $\Delta\boldsymbol{\mu}_k$ to construct the ROB $\mathbf{V}_{\boldsymbol{\mu}}$ by solving an auxiliary **cheaper** optimization problem

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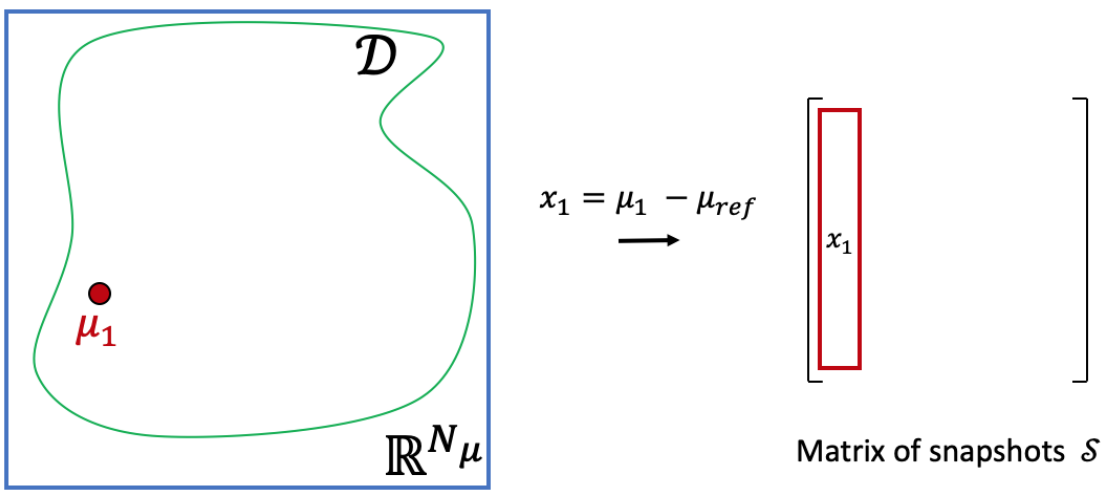
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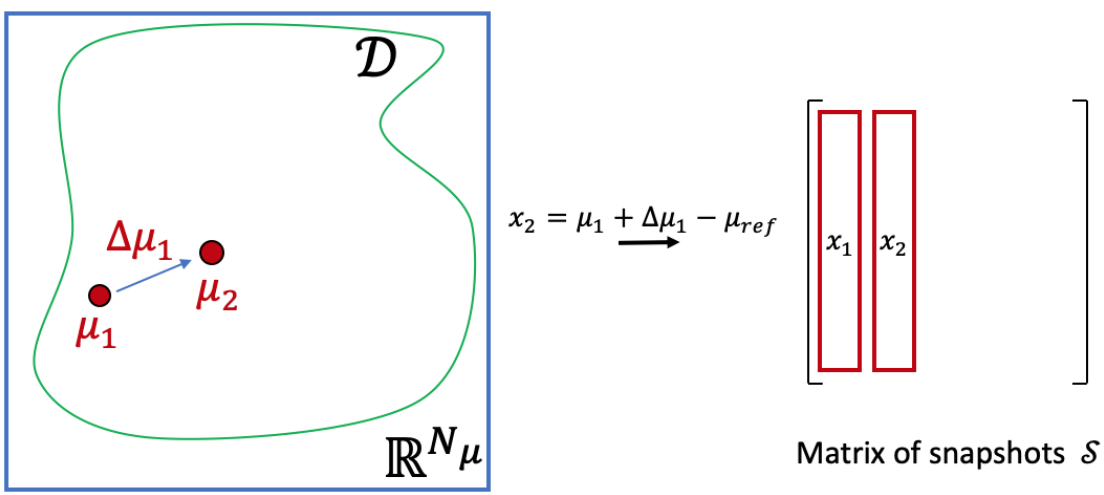
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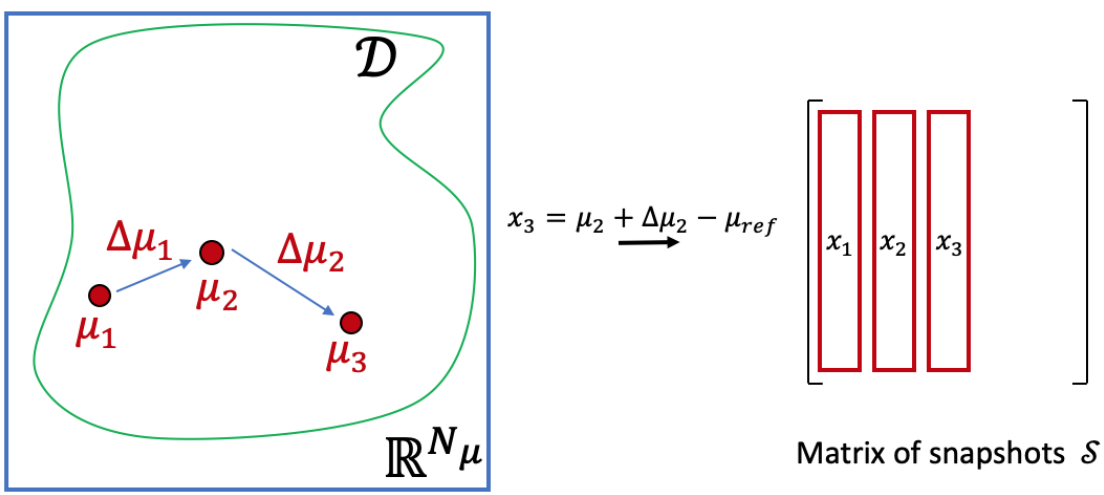
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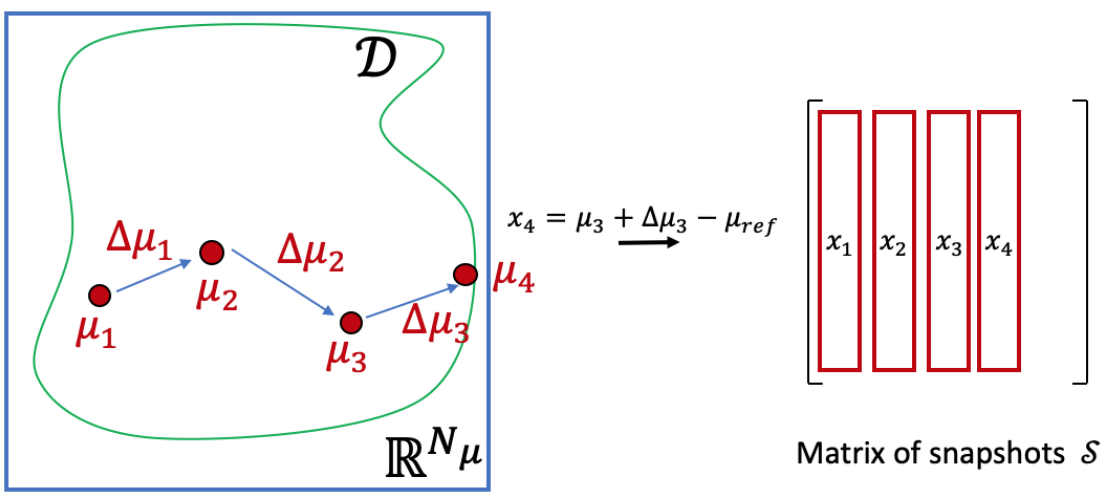
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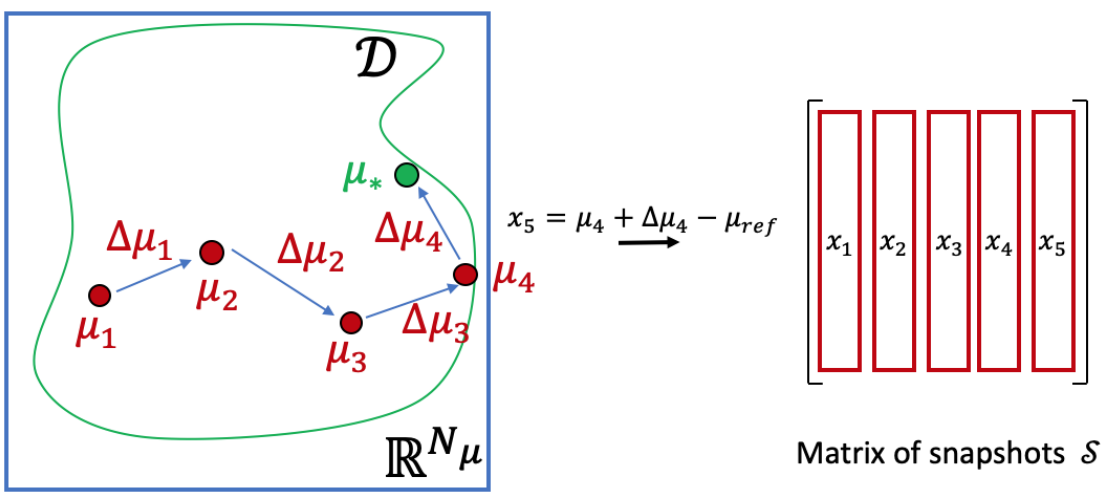
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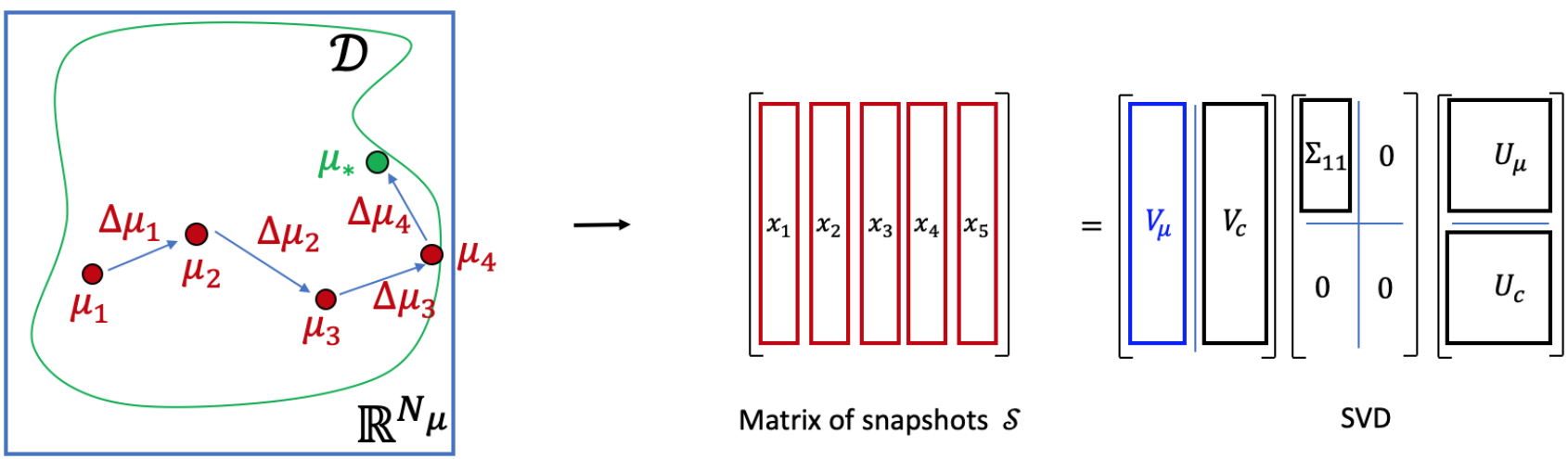
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- Alternative idea: directly sample $\Delta\boldsymbol{\mu}_k$ to construct the ROB $\mathbf{V}_{\mu}$ by solving an auxiliary **cheaper** optimization problem



- Same AS assumption: $\boldsymbol{\mu} = \boldsymbol{\mu}_{\text{ref}} + \mathbf{V}_{\boldsymbol{\mu}} \boldsymbol{\mu}_r$
- Recall that the update of each iterate $\boldsymbol{\mu}_k$ can be written as

$$\boldsymbol{\mu}_{k+1} = \boldsymbol{\mu}_k + \Delta\boldsymbol{\mu}_k$$

  where $\Delta\boldsymbol{\mu}_k \in \mathbb{R}^{N_\mu}$ is determined by the optimization procedure
  - unconstrained optimization problem, a gradient-based procedure: $\Delta\boldsymbol{\mu}_k = -\eta_k \mathbf{C}_k \nabla f(\boldsymbol{\mu}_k)$
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- Alternative idea: directly sample $\Delta\boldsymbol{\mu}_k$ to construct the ROB $\mathbf{V}_{\boldsymbol{\mu}}$ by solving an auxiliary **cheaper** optimization problem



- Auxiliary optimization problem: **related** but **cheaper** than original problem
  - single optimization problem: version without some of the expensive PDE-constraints

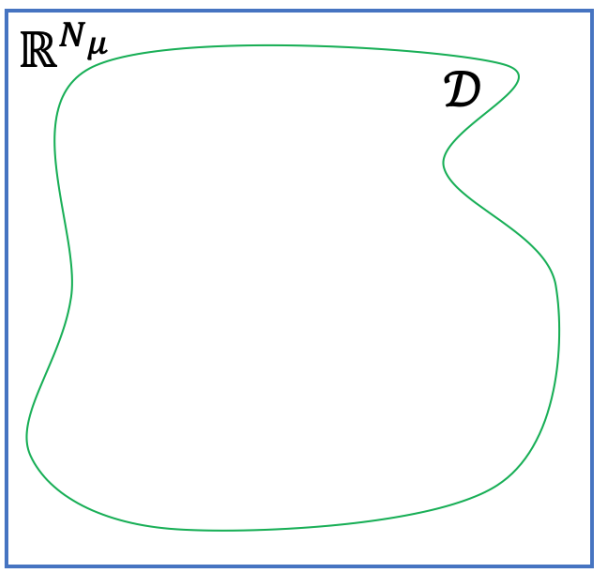
$$\begin{aligned} \min_{\boldsymbol{\mu}\ ,\mathbf{w}_L,\mathbf{w}_{NL}} \quad & f(\mathbf{w}_L,\mathbf{w}_{NL},\boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{c}(\mathbf{w}_L,\mathbf{w}_{NL},\boldsymbol{\mu}) \geqslant 0 \\ & \mathbf{R}_L(\mathbf{w}_L,\boldsymbol{\mu}) = \mathbf{0} \\ & \mathbf{R}_{NL}(\mathbf{w}_{NL},\boldsymbol{\mu}) = \mathbf{0} \end{aligned} \quad \rightarrow \quad \begin{aligned} \min_{\boldsymbol{\mu}\ ,\mathbf{w}_{NL}} \quad & f(\mathbf{w}_{NL},\boldsymbol{\mu}) \\ \text{subject to} \quad & \mathbf{c}(\mathbf{w}_{NL},\boldsymbol{\mu}) \geqslant 0 \\ & \mathbf{R}_{NL}(\mathbf{w}_{NL},\boldsymbol{\mu}) = \mathbf{0} \end{aligned}$$

  - multi-start optimization strategy: solve only one optimization instance

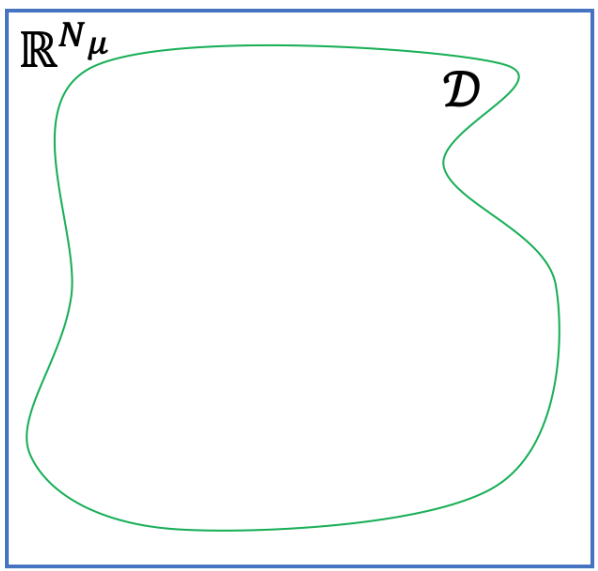
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  - multi-start optimization strategy: solve only one optimization instance



Single optimization instance

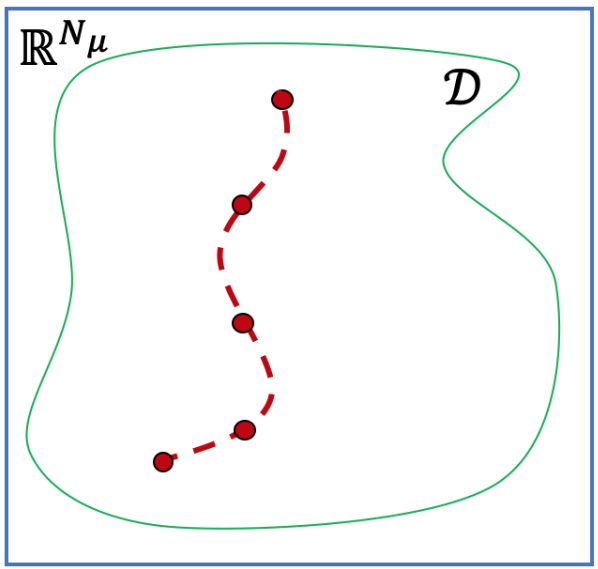


Multiple optimization instances

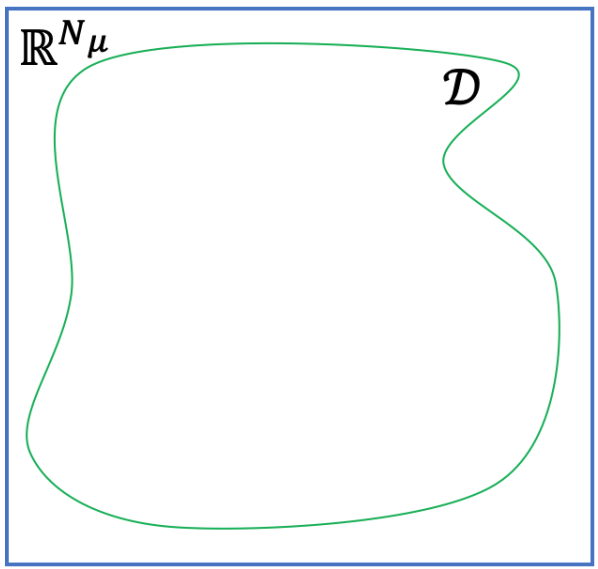
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Single optimization instance

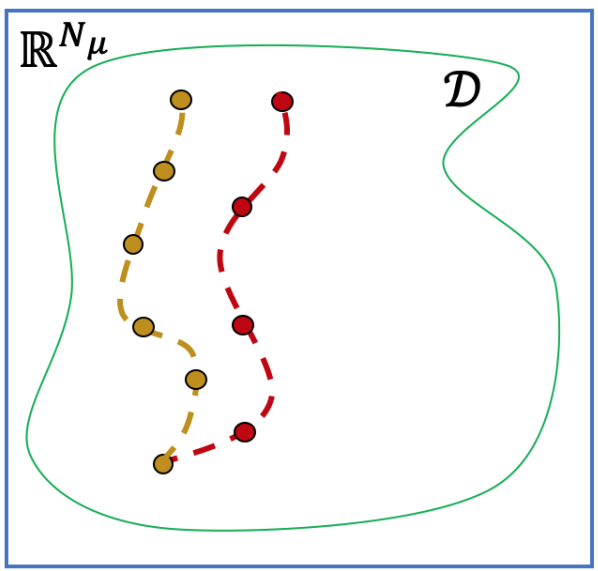


Multiple optimization instances

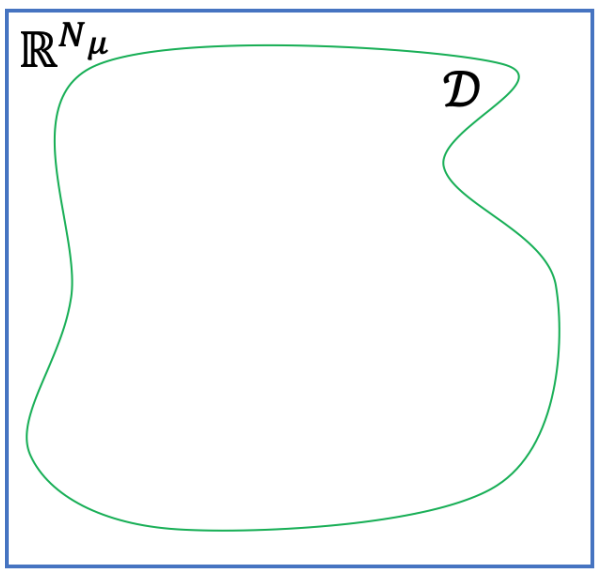
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  - multi-start optimization strategy: solve only one optimization instance



Single optimization instance

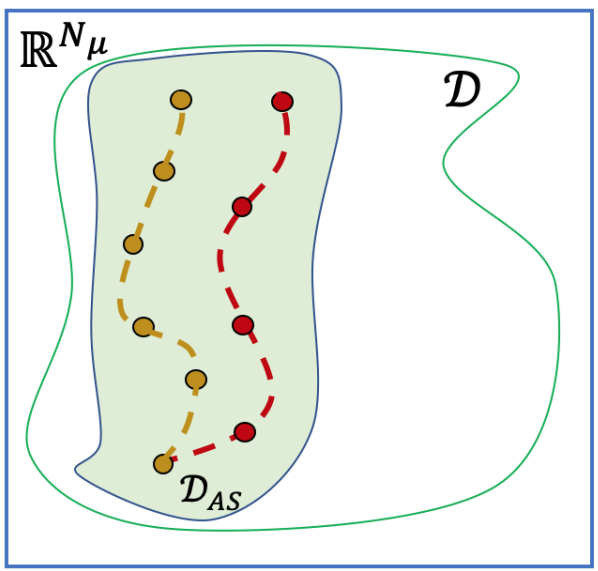


Multiple optimization instances

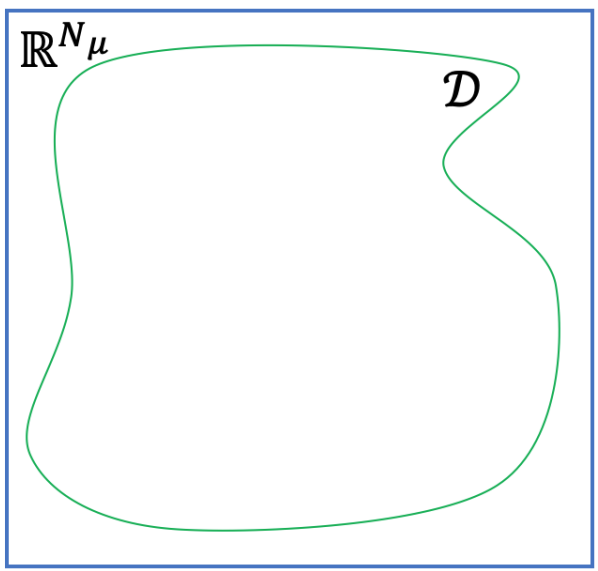
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Single optimization instance

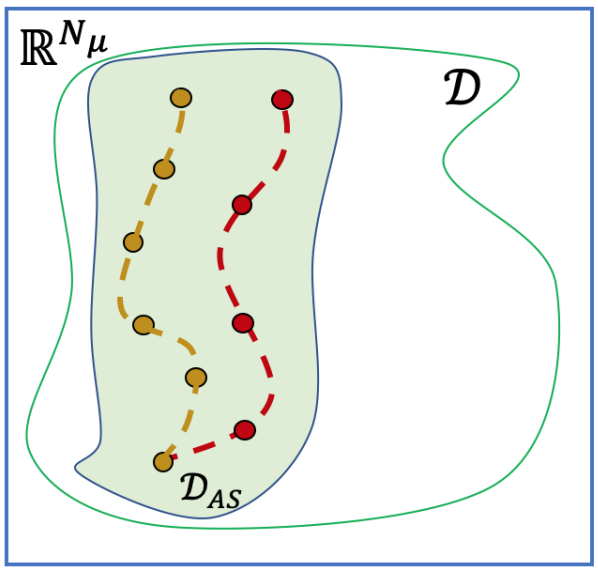


Multiple optimization instances

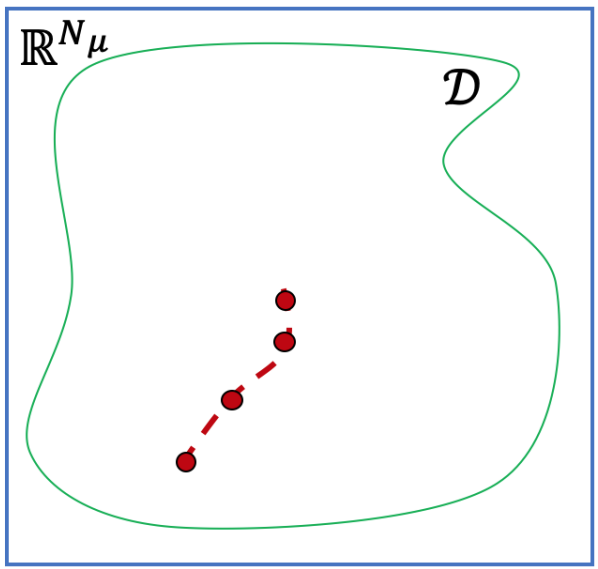
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Single optimization instance

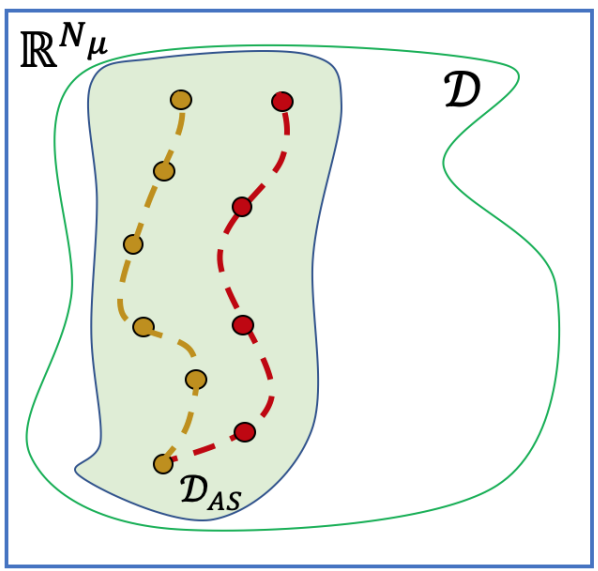


Multiple optimization instances

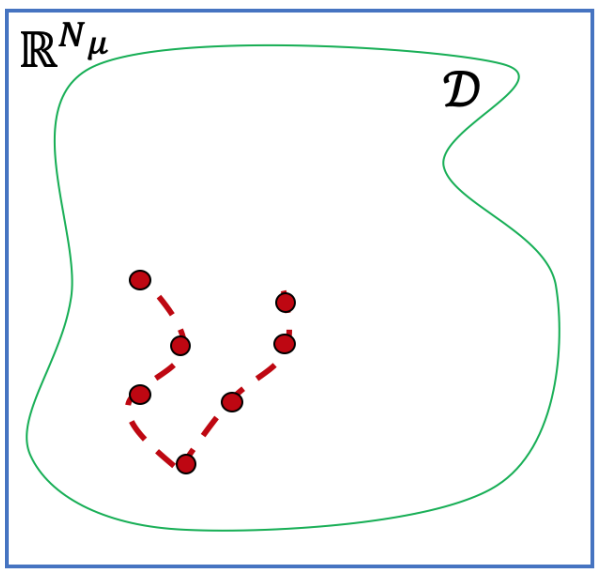
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  - multi-start optimization strategy: solve only one optimization instance



Single optimization instance

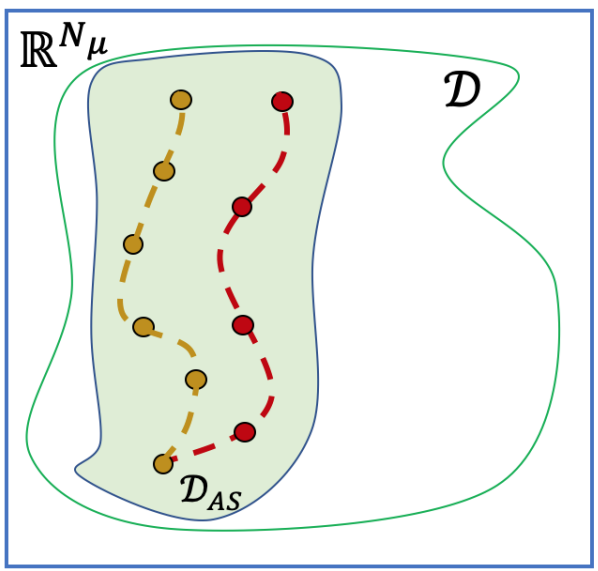


Multiple optimization instances

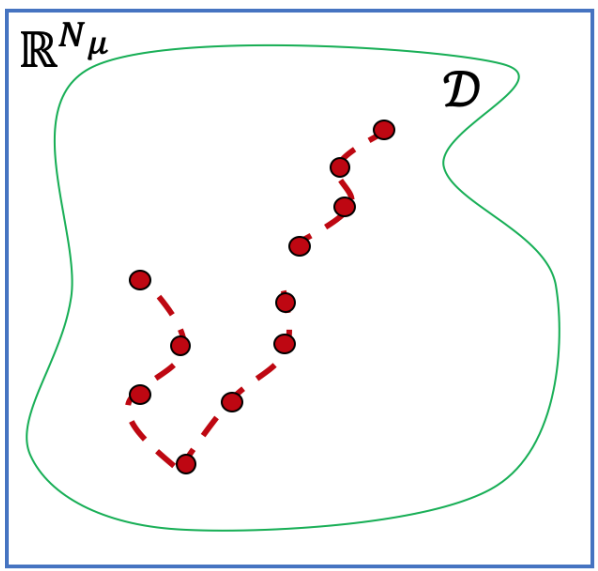
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Single optimization instance

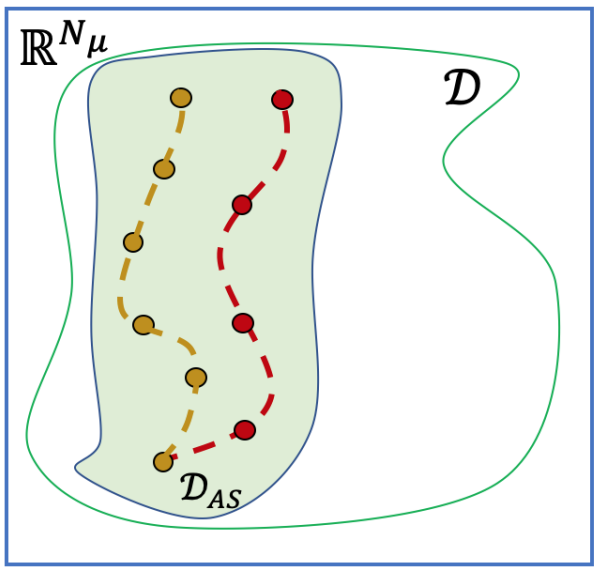


Multiple optimization instances

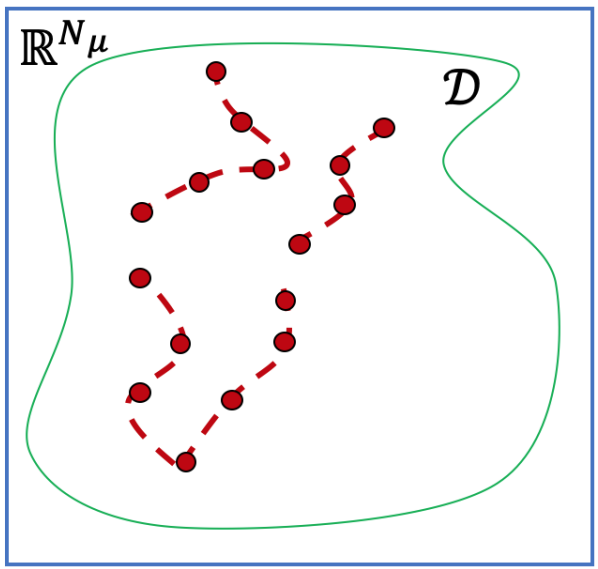
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  - multi-start optimization strategy: solve only one optimization instance



Single optimization instance

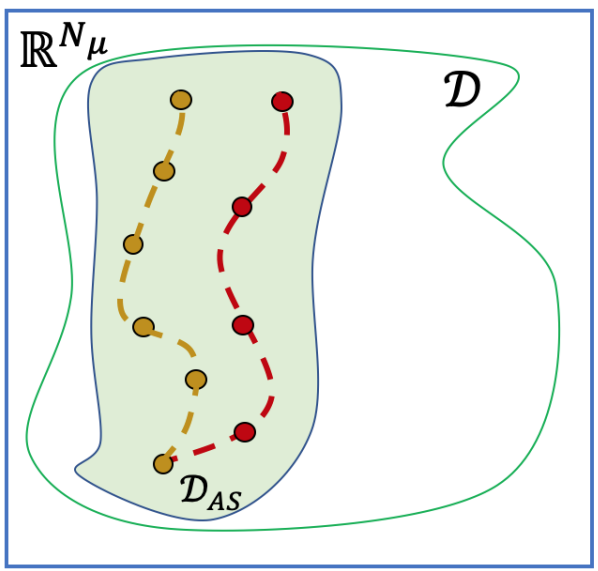


Multiple optimization instances

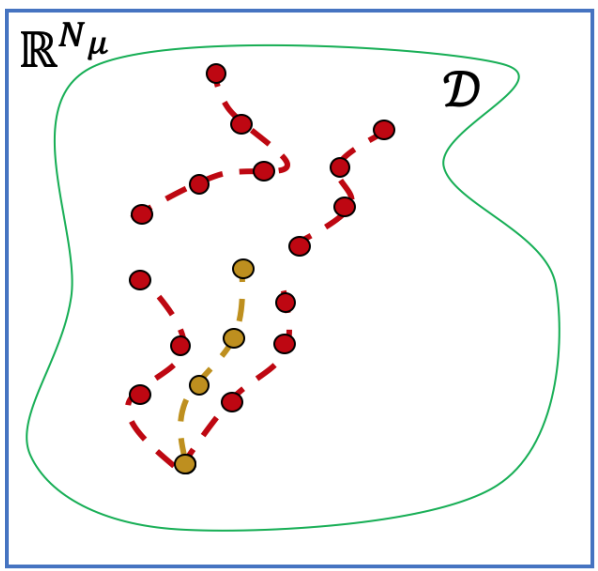
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  - multi-start optimization strategy: solve only one optimization instance



Single optimization instance

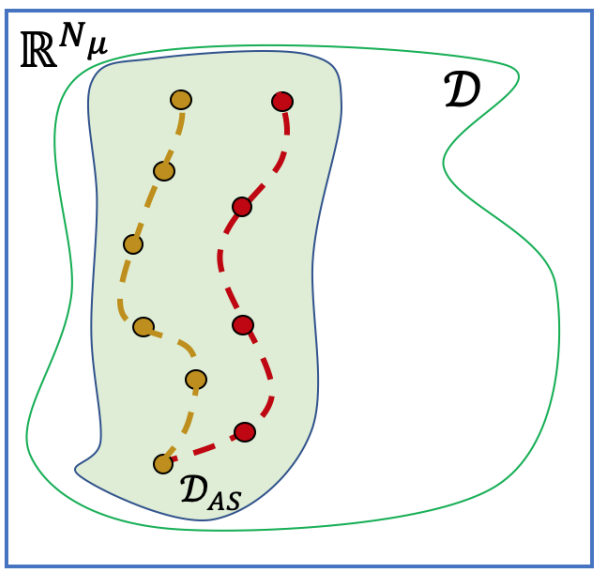


Multiple optimization instances

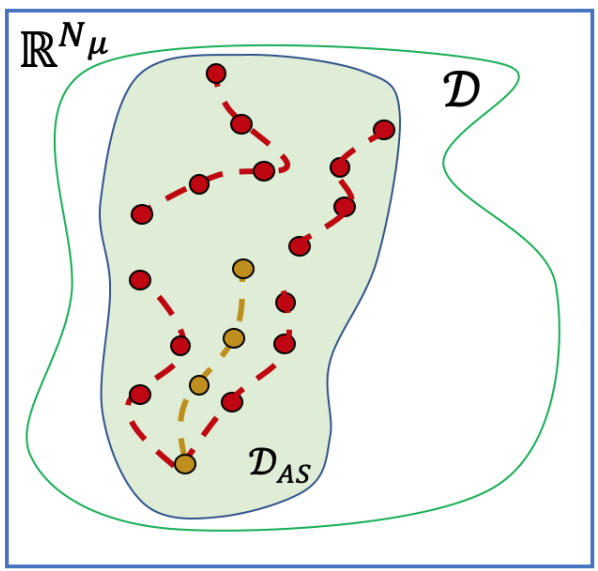
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  - multi-start optimization strategy: solve only one optimization instance



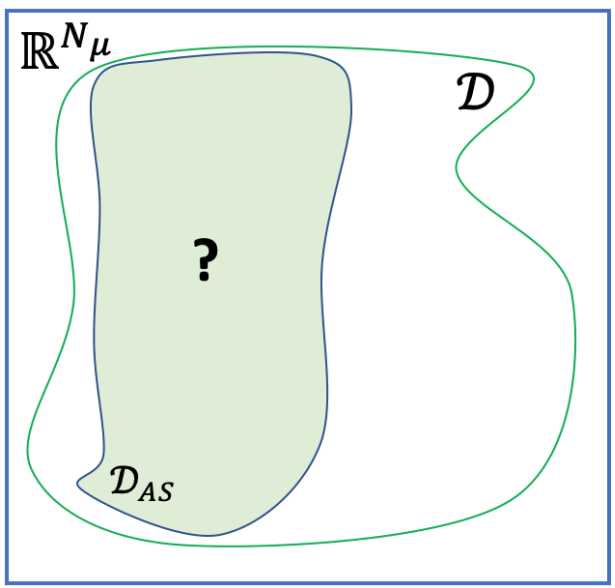
Single optimization instance



Multiple optimization instances

- Compute the ROB $\mathbf{V}_{\boldsymbol{\mu}} \in \mathbb{R}^{N_{\boldsymbol{\mu}} \times N_{\boldsymbol{\mu}_r}}$ representing the AS, where the AS dimension is $N_{\boldsymbol{\mu}_r}$
- Train PROMs in the **feasible** active subspace $\mathcal{D}_{AS}$
  1. find set of feasible candidate points
     - sample $\{\boldsymbol{\mu}_{r_i}\}_{i=1}^{N}$ in $\mathbb{R}^{N_{\boldsymbol{\mu}_r}}$ using a priori sampling
     - solve for each $\boldsymbol{\mu}_{r_i}$ the feasibility problem

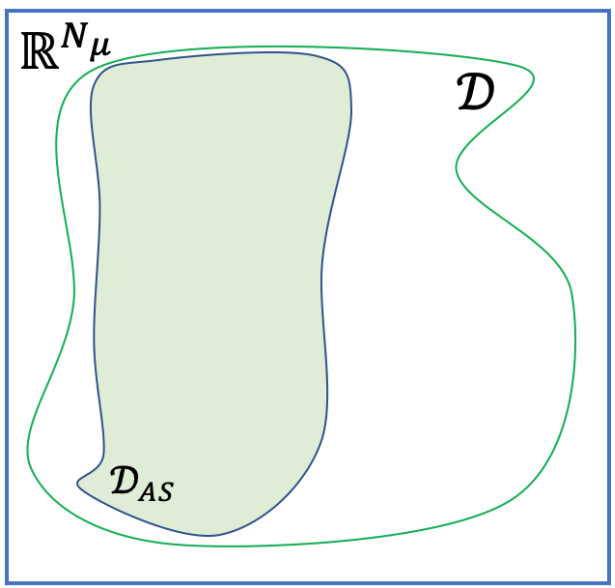
$$\boldsymbol{\mu}_i{}^{\star} = \begin{array}{ll} \min\limits_{\boldsymbol{\mu} \in \mathbb{R}^{N_\mu}} & \mathbf{0}^{\intercal}\boldsymbol{\mu} \\ \text{s.t.} & \mathbf{V}_{\mu}^{\intercal}\boldsymbol{\mu} = (\mathbf{V}_{\mu}^{\intercal}\boldsymbol{\mu}_{\text{ref}} + \boldsymbol{\mu}_{r_i}) \\ & \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \end{array}$$

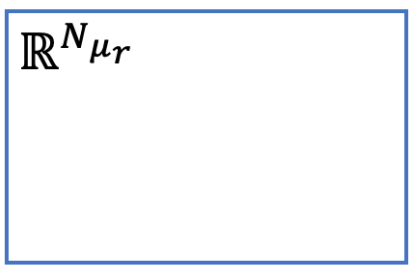


Greedy *feasible* sampling algorithm

- Compute the ROB $\mathbf{V}_{\boldsymbol{\mu}} \in \mathbb{R}^{N_{\boldsymbol{\mu}} \times N_{\boldsymbol{\mu}_r}}$ representing the AS, where the AS dimension is $N_{\boldsymbol{\mu}_r}$
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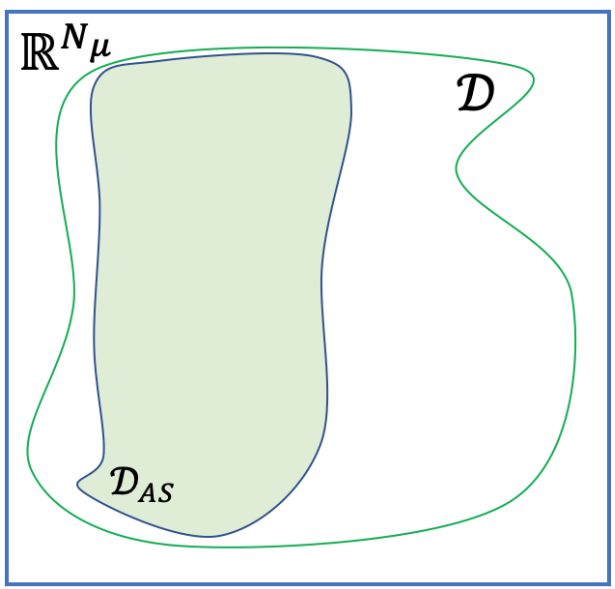


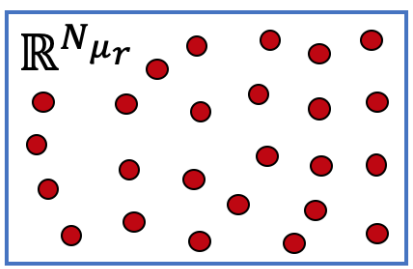


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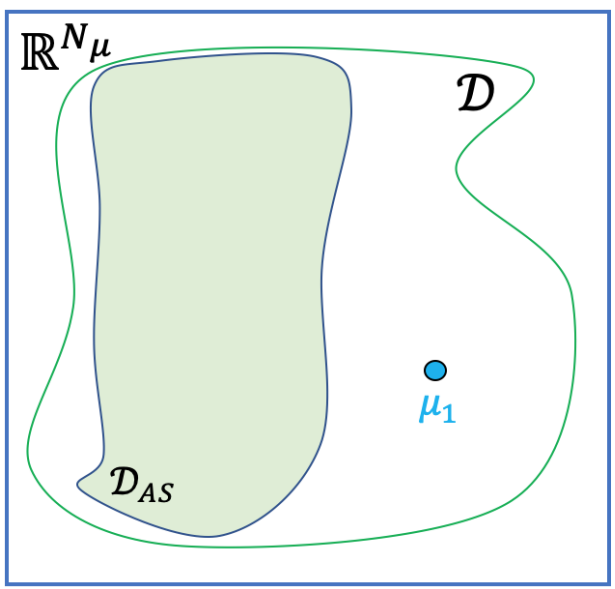
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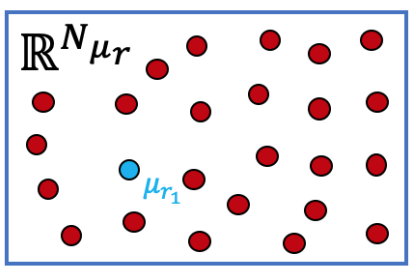




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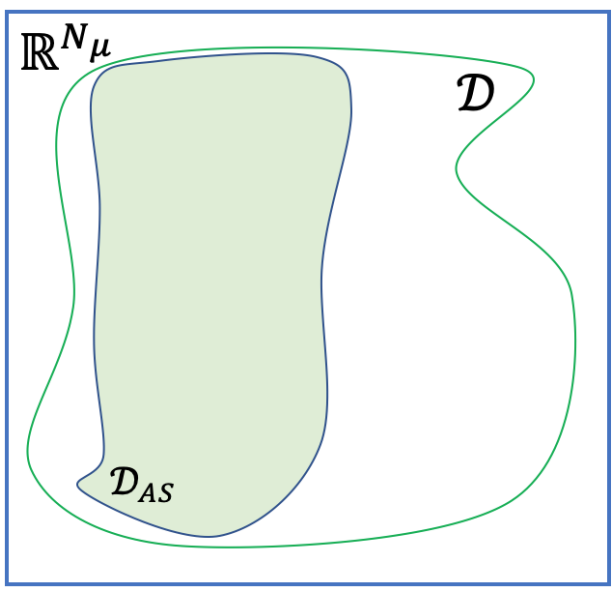
$$\boldsymbol{\mu}_i{}^{\star} = \begin{array}{ll} \min\limits_{\boldsymbol{\mu} \in \mathbb{R}^{N_\mu}} & \mathbf{0}^{\mathsf{T}}\boldsymbol{\mu} \\ \text{s.t.} & \mathbf{V}_{\mu}^{\mathsf{T}}\boldsymbol{\mu} = (\mathbf{V}_{\mu}^{\mathsf{T}}\boldsymbol{\mu}_{\text{ref}} + \boldsymbol{\mu}_{r_i}) \\ & \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \end{array}$$

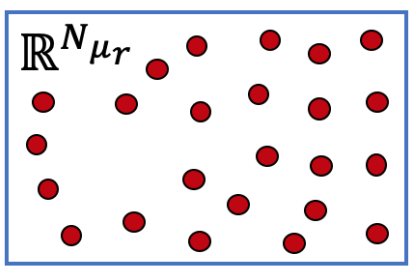




- Compute the ROB $\mathbf{V}_{\boldsymbol{\mu}} \in \mathbb{R}^{N_{\boldsymbol{\mu}} \times N_{\boldsymbol{\mu}_r}}$ representing the AS, where the AS dimension is $N_{\boldsymbol{\mu}_r}$
- Train PROMs in the **feasible** active subspace $\mathcal{D}_{AS}$
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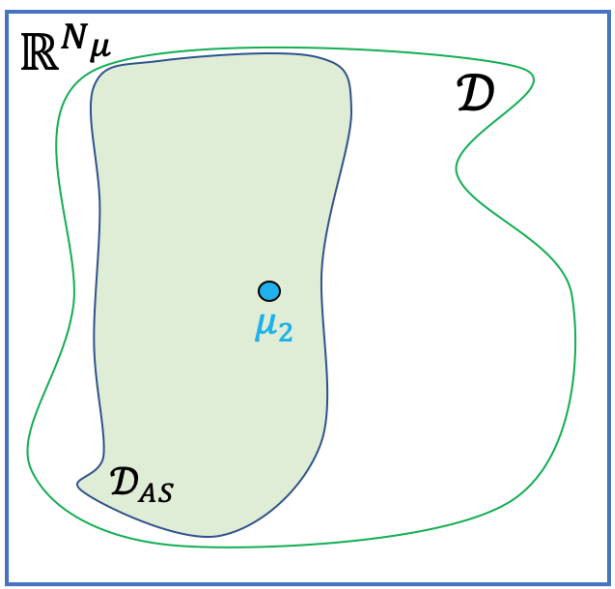
$$\boldsymbol{\mu}_i{}^{\star} = \begin{aligned} & \min_{\boldsymbol{\mu} \in \mathbb{R}^{N_\mu}} && \mathbf{0}^{\intercal}\boldsymbol{\mu} \\ & \text{s.t.} && \mathbf{V}_{\mu}^{\intercal}\boldsymbol{\mu} = (\mathbf{V}_{\mu}^{\intercal}\boldsymbol{\mu}_{\text{ref}} + \boldsymbol{\mu}_{r_i}) \\ & && \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \end{aligned}$$

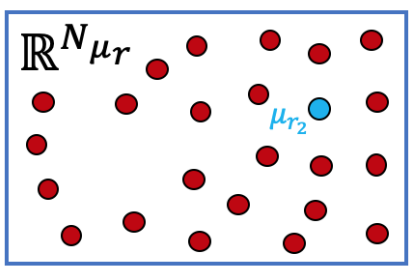




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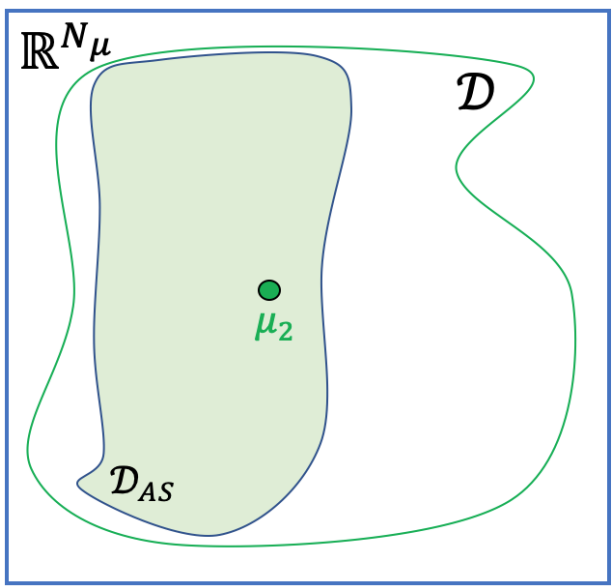
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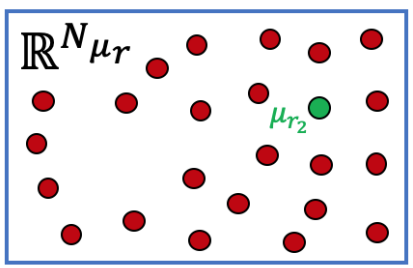




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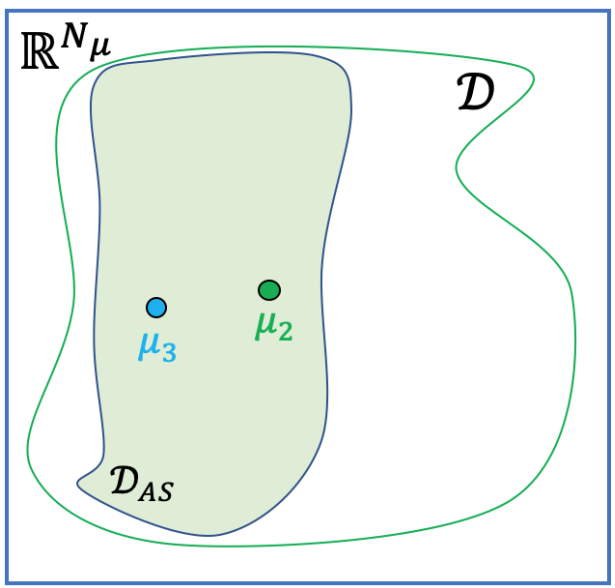
$$\boldsymbol{\mu}_i^{\star} = \begin{aligned} & \min_{\boldsymbol{\mu} \in \mathbb{R}^{N_\mu}} && \mathbf{0}^{\intercal}\boldsymbol{\mu} \\ & \text{s.t.} && \mathbf{V}_{\mu}^{\intercal}\boldsymbol{\mu} = (\mathbf{V}_{\mu}^{\intercal}\boldsymbol{\mu}_{\text{ref}} + \boldsymbol{\mu}_{r_i}) \\ & && \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \end{aligned}$$

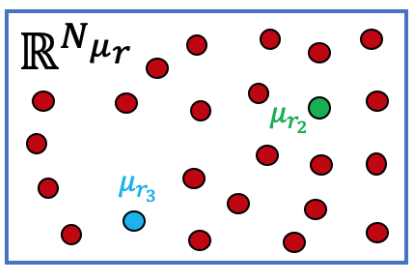




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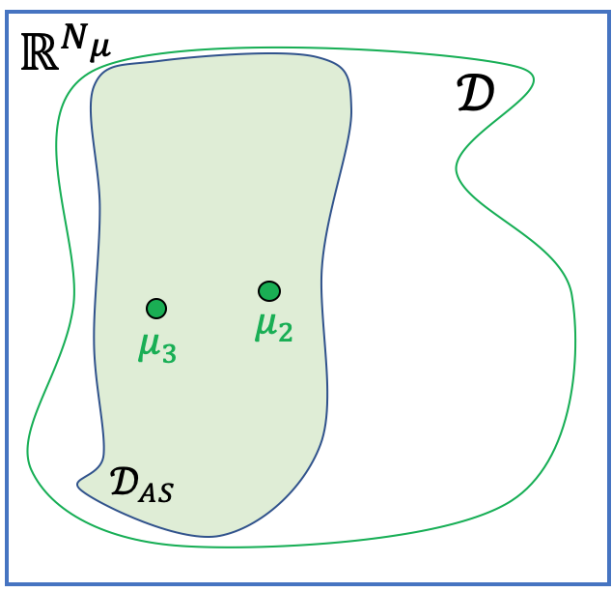
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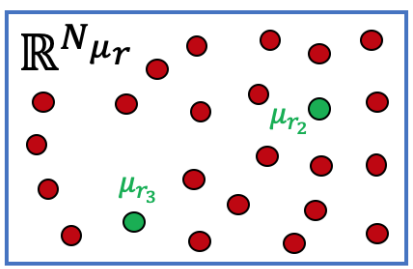




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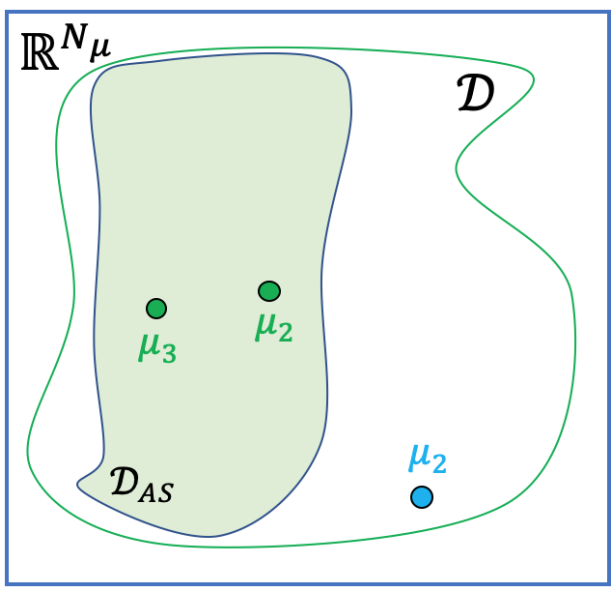
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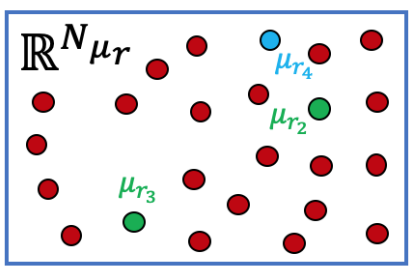




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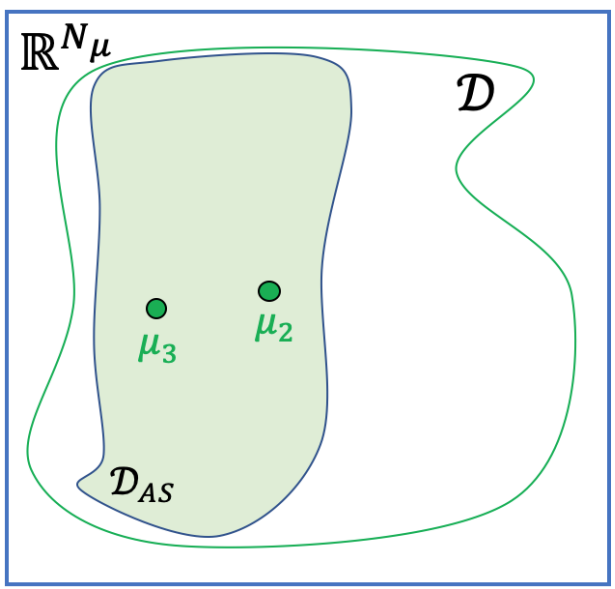
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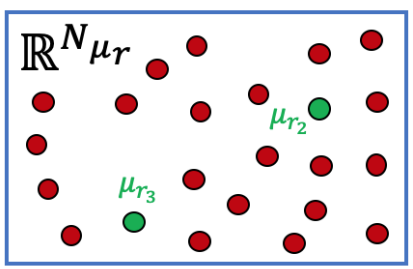




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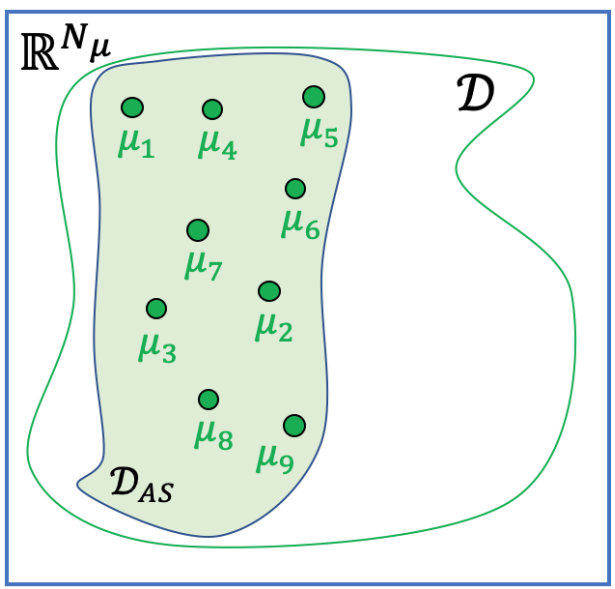
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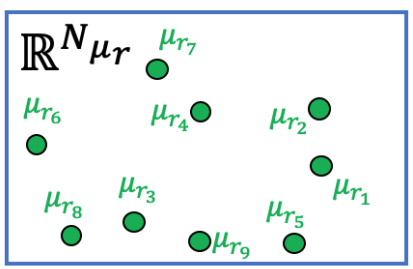




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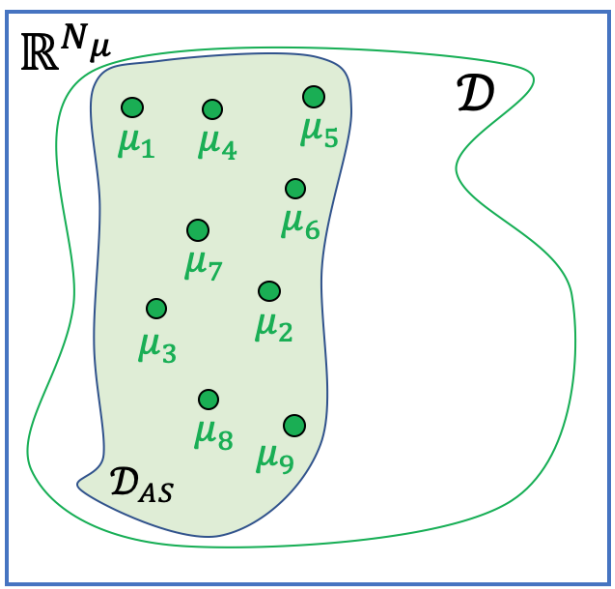


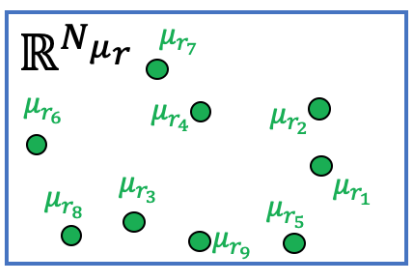


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  2. use greedy algorithm on set of feasible candidate points to sample snapshots of the PDE and train PROMs

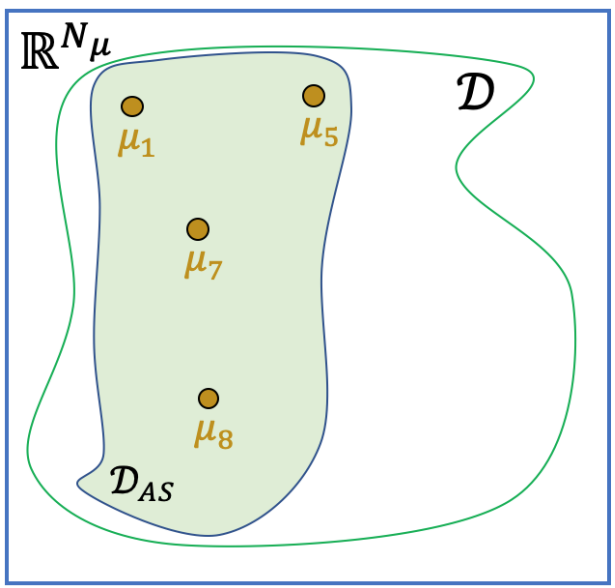


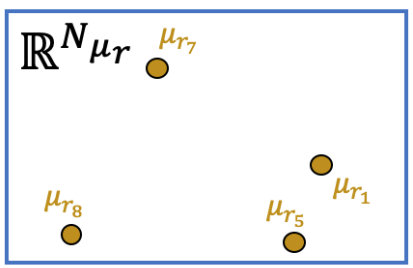


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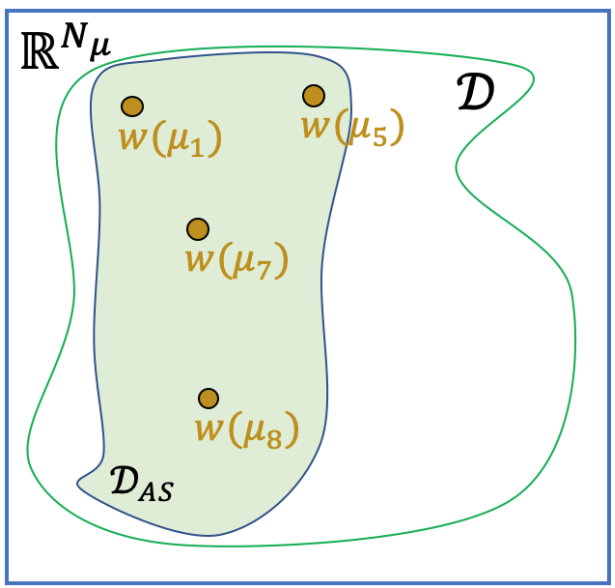


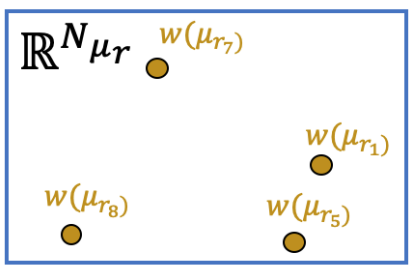


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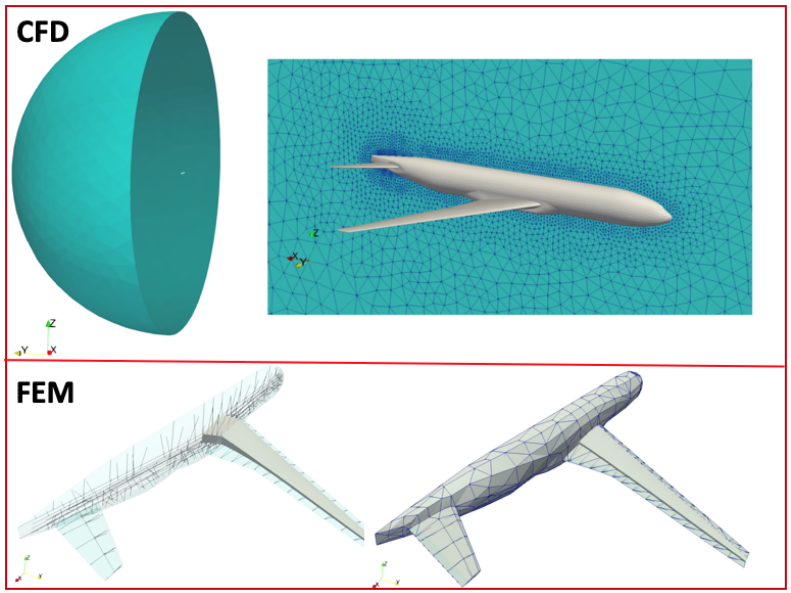
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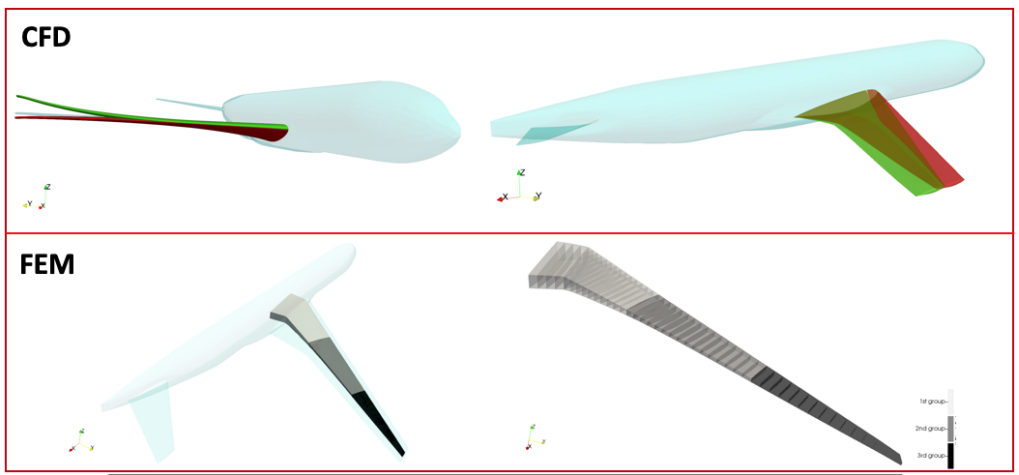


Shape optimization under flutter constraint (case 1)



- NASA's Common Research Model (**CRM**)
- **Flow**: $M_\infty = 0.85, \alpha = 1.823^\circ$
- Inviscid (**CFD**) grid with 740,248 grid points
- Finite element structural model (**FEM**) with beam and shell elements and 58,888 DOF

- Parametric model[6], $\boldsymbol{\mu} \in \mathbb{R}^6$



- **Shape parameters**: dihedral angle (μ_s^1, μ_s^2) and sweep angle μ_s^3
- **Structural parameters**: 3 thickness increments $(\mu_m^1, \mu_m^2, \mu_m^3)$ for 3 different groups of stiffeners

[6] Gabriele Boncoraglio, Charbel Farhat, and Charbel Bou-Mosleh. "Model reduction framework with a new take on active subspaces for optimization problems with linearized fluid-structure interaction constraints". In: International Journal for Numerical Methods in Engineering (2020).

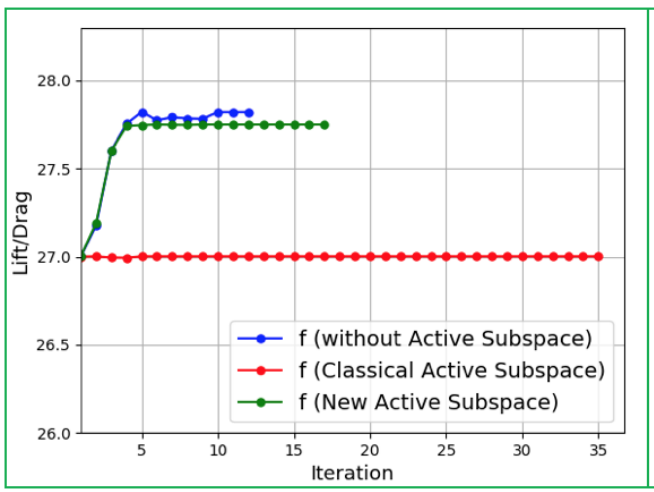
- Optimization problem

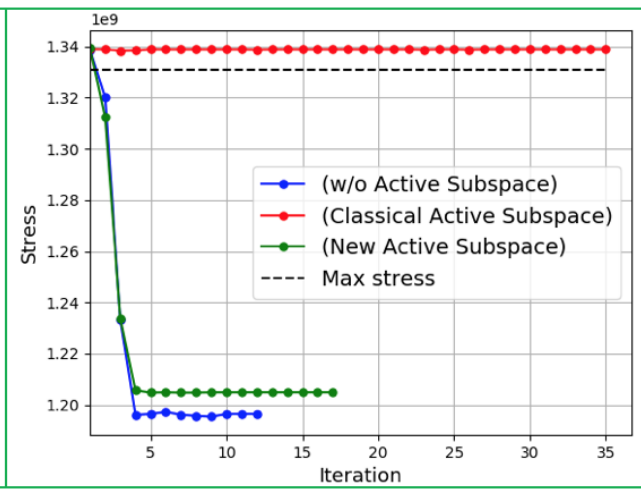
$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^6}{\text{maximize}} \quad & \frac{L(\boldsymbol{\mu})}{D(\boldsymbol{\mu})} \\ \text{subject to} \quad & \sigma_{\text{VM}}(\boldsymbol{\mu}) \leqslant \sigma_{\text{ub}} \\ & \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \\ & \boldsymbol{\zeta}(\boldsymbol{\mu}) \geqslant \mathbf{1}\zeta_{\text{lb}} \end{aligned}$$

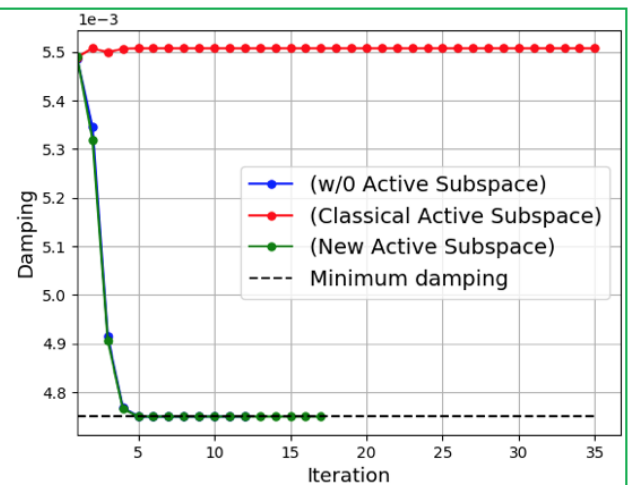
  - L: lift, D: drag, σ_{VM}: von Mises stress, $\boldsymbol{\zeta}$: damping ratios
  - $\boldsymbol{\zeta}$ computed using database of local linear PROMs
- Offline phase: training of PROMs

Method	$N_{\boldsymbol{\mu}}$	m	Wall-clock time computing $\mathbf{V}_\mu$	$N_{\mathcal{D}B}$	Wall-clock time greedy procedure	Wall-clock time total offline
w/o AS	6	N.A.	N.A.	119	120.87 hrs	120.87 hrs
Classical AS	3	47	14.06 hrs	61	61.95 hrs	76.01 hrs
Alternative AS	3	17	5.83 hrs	62	62.97 hrs	68.80 hrs

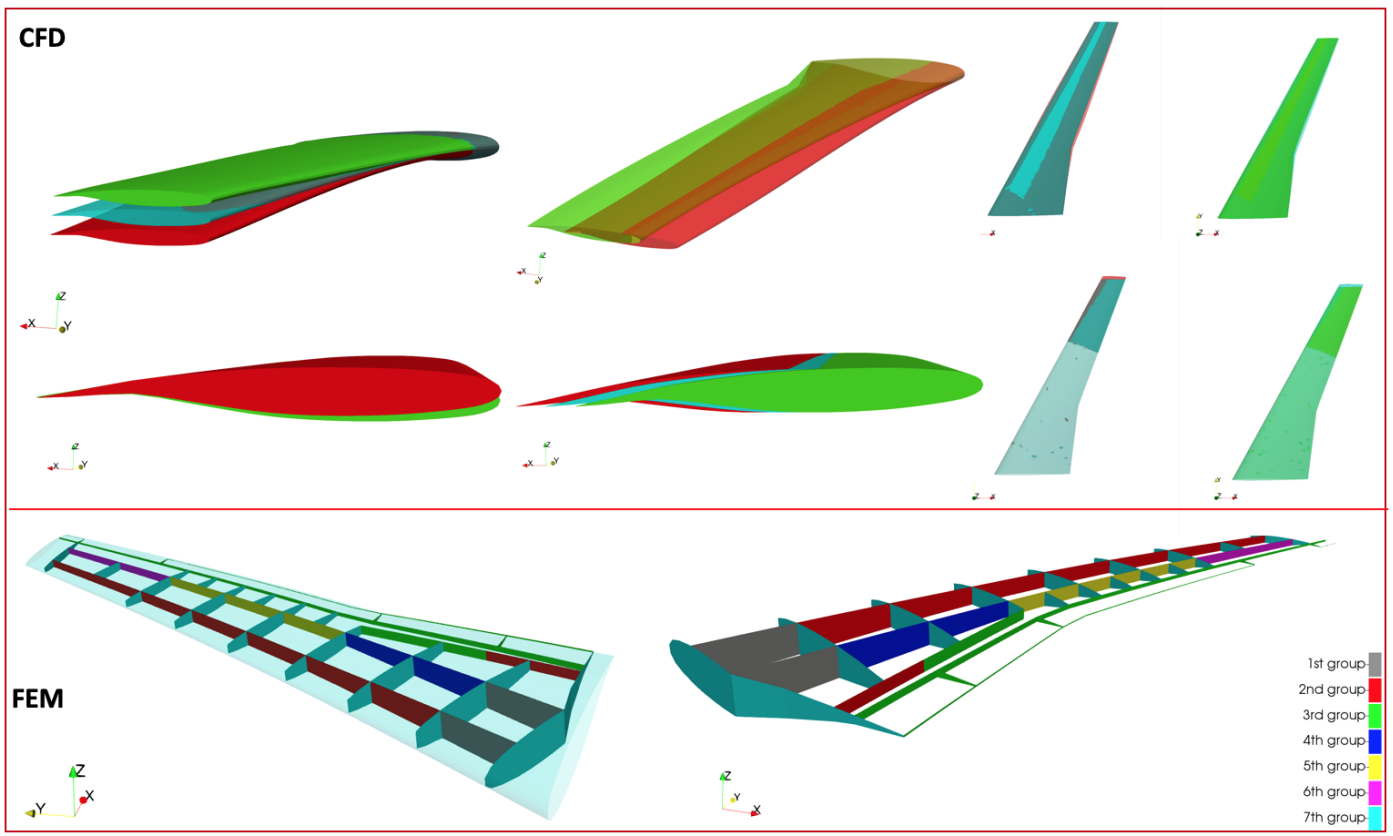
- Online phase







- NASA's ARW-2 aeroelastic model
- Parametric model[6], $\boldsymbol{\mu} \in \mathbb{R}^{15}$
  - **shape parameters**: wingspan stretching μ_s^1, twist angle (μ_s^2, μ_s^3), dihedral angle (μ_s^4, μ_s^5), backsweep angle μ_s^6, wingspan taper μ_s^7, and chord stretching μ_s^8
  - **structural parameters**: 7 thickness increments $(\mu_m^1, \cdots, \mu_m^7)$ for 7 different groups of stiffeners



[6] Gabriele Boncoraglio, Charbel Farhat, and Charbel Bou-Mosleh. "Model reduction framework with a new take on active subspaces for optimization problems with linearized fluid-structure interaction constraints". In: International Journal for Numerical Methods in Engineering (2020).

Shape optimization under flutter constraint (case 2)

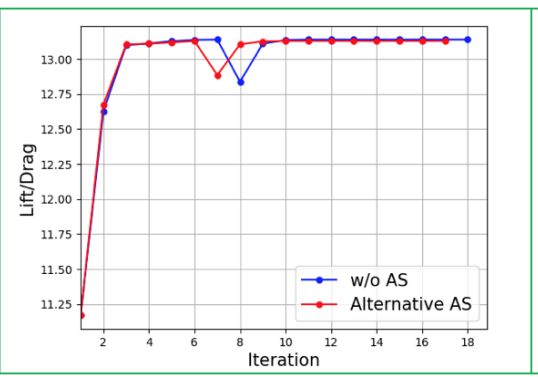
- Optimization problem

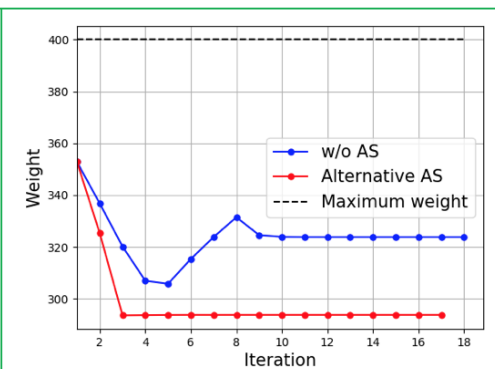
$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{15}}{\text{maximize}} \quad & \frac{L(\boldsymbol{\mu})}{D(\boldsymbol{\mu})} \\ \text{subject to} \quad & W(\boldsymbol{\mu}) \leqslant W_{\text{ub}} \\ & \sigma_{\text{VM}}(\boldsymbol{\mu}) \leqslant \sigma_{\text{ub}} \\ & \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \\ & \boldsymbol{\zeta}(\boldsymbol{\mu}) \geqslant \mathbf{1}\zeta_{\text{lb}} \end{aligned}$$

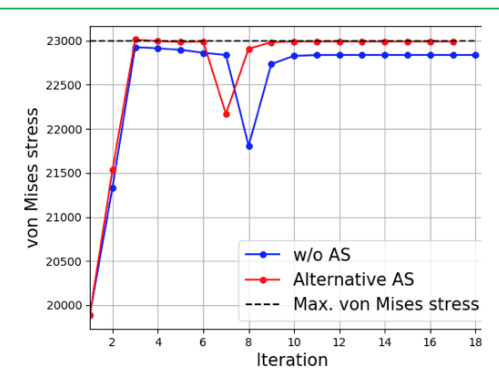
  - L: lift, D: drag, W: weight, σ_{VM}: von Mises stress, $\boldsymbol{\zeta}$: damping ratios
  - $\boldsymbol{\zeta}$ computed using database of local linear PROMs
- Offline phase: training of PROMs

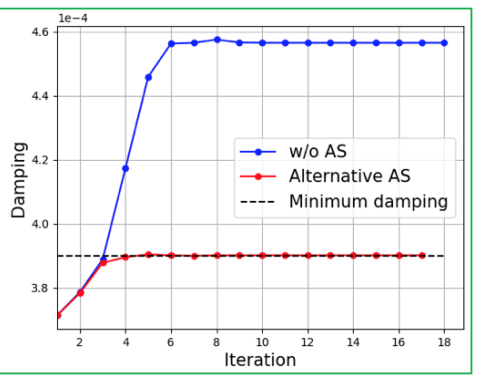
Method	$N_{\boldsymbol{\mu}}$	m	Wall-clock time computing $\mathbf{V}_\mu$	$N_{\mathcal{DB}}$	Wall-clock time greedy procedure	Wall-clock time total offline
w/o AS	15	N.A.	N.A.	415	93.2 hrs	93.2 hrs
Alternative AS	7	20	1.77 hrs	203	38.5 hrs	40.27 hrs

- Online phase

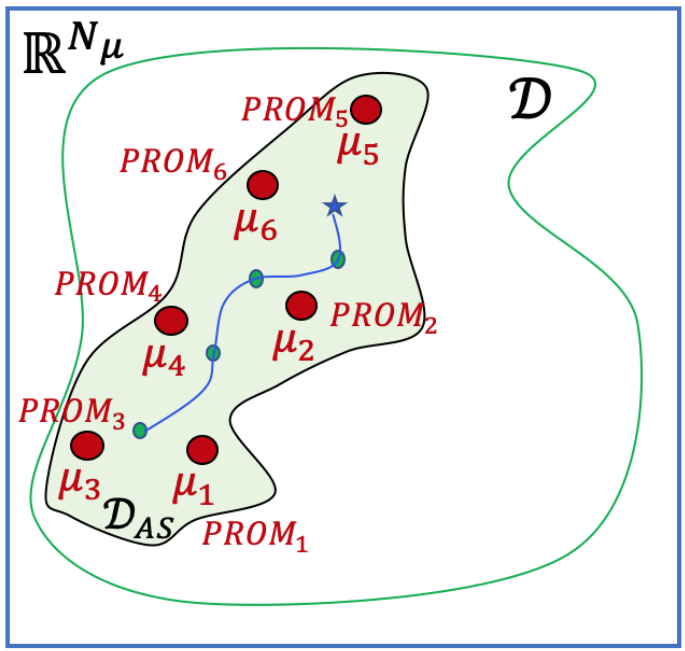




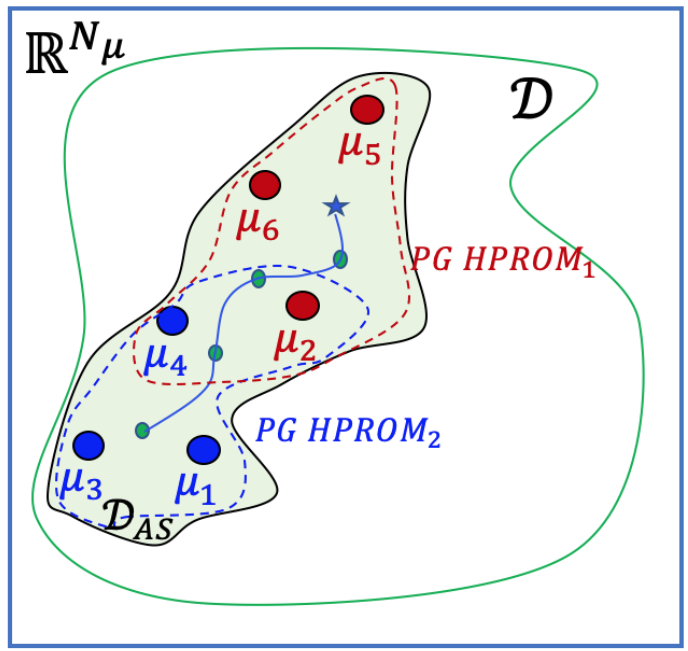




- Train/exploit linear, local PROMs and nonlinear, piecewise-global HPROMs, and solve optimization problem in $\mathcal{D}_A \subset \mathcal{D}$

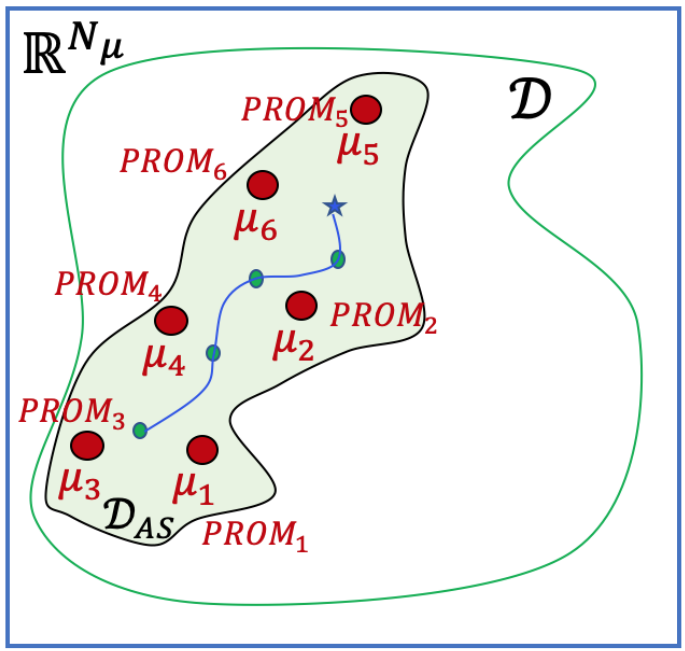


Database $\mathcal{DB}$ of local linear PROMs

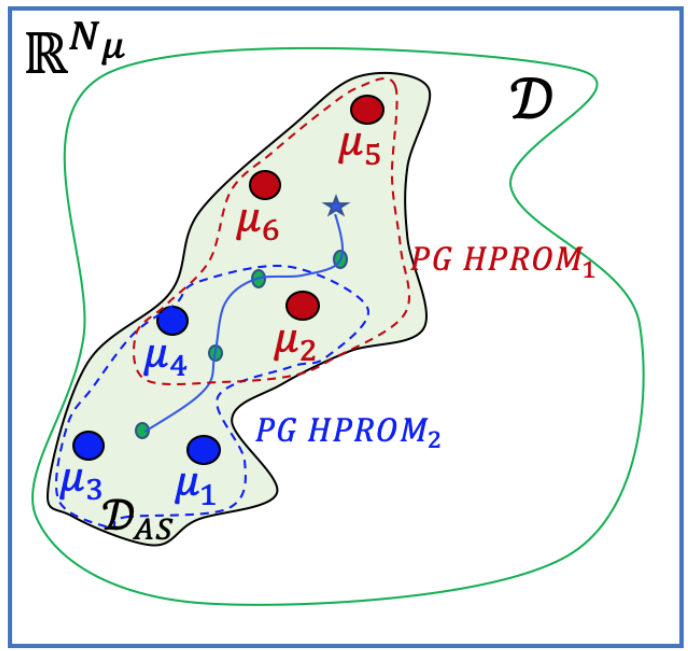


Piecewise-Global nonlinear HPROMs

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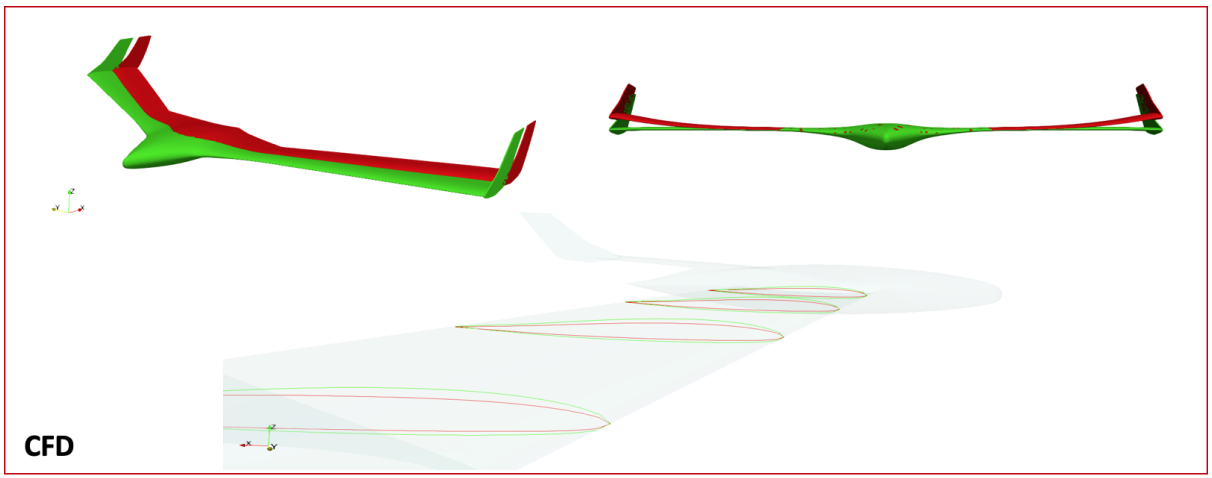
Database $\mathcal{DB}$ of local linear PROMs



Piecewise-Global nonlinear HPROMs



- mAEWing2 flying aircraft
- Parametric model, $\boldsymbol{\mu} \in \mathbb{R}^{33}$



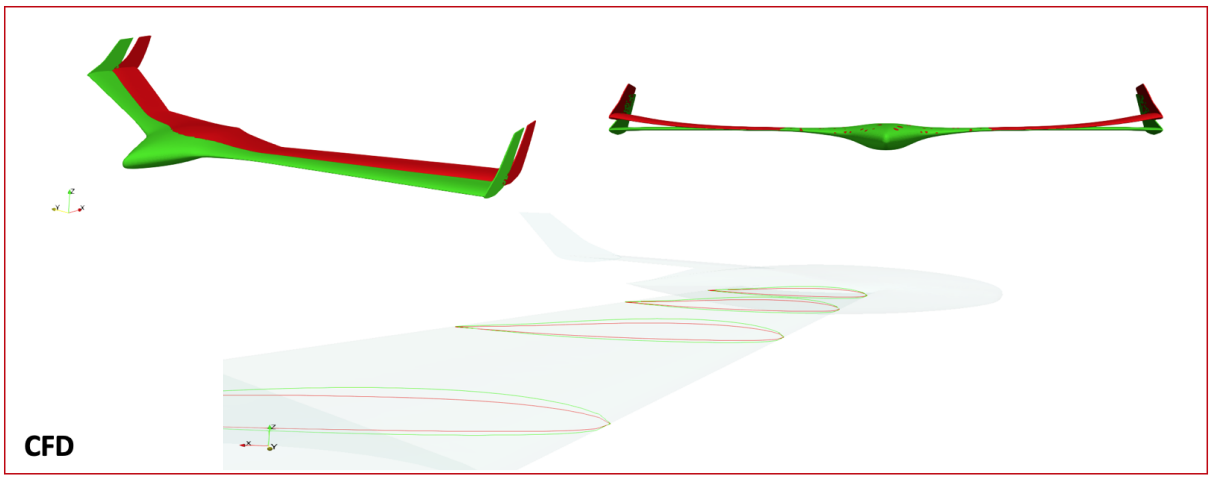
- **Shape parameters**: dihedral angle (μ_s^1, μ_s^2), sweep angle μ_s^3, and airfoil shape $(\mu_s^4, \cdots, \mu_s^{33})$

- Global optimization problem using Basin-hopping algorithm

$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{33}}{\text{maximize}} \quad & \frac{L(\boldsymbol{\mu})}{D(\boldsymbol{\mu})} \\ & L(\boldsymbol{\mu}) \geqslant 0.9 L_0 \\ & \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \end{aligned}$$

[7] Gabriele Boncoraglio and Charbel Farhat. "Optimization in High-Dimensional Parameter Spaces Using Piecewise-Global Nonlinear Hyperreduced Models and Active Subspaces". In: Submitted. 2021.

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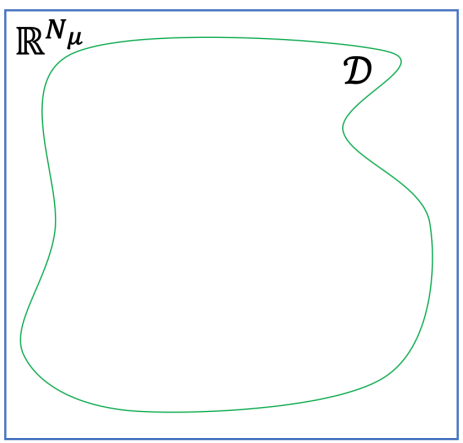
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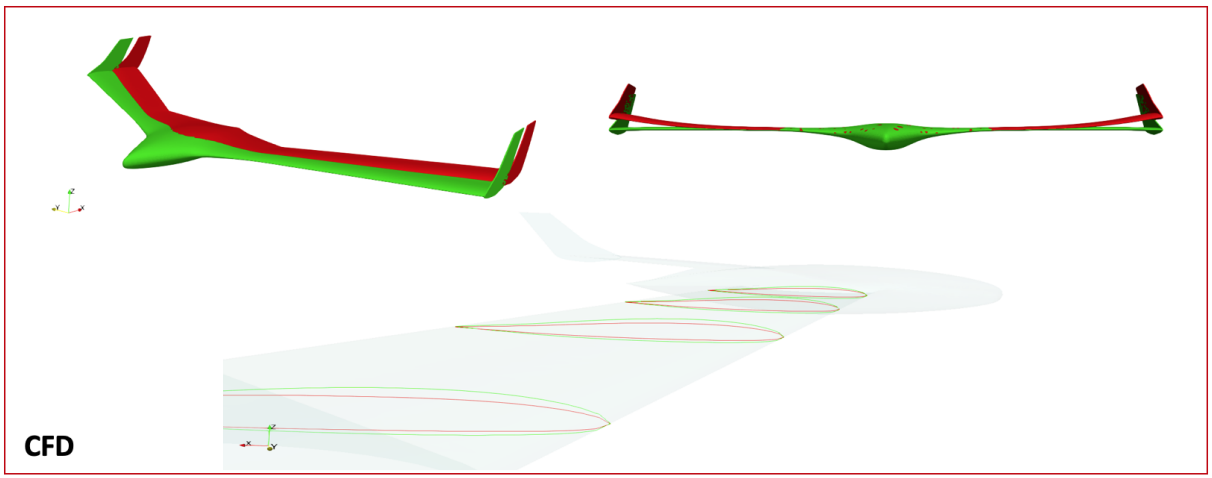
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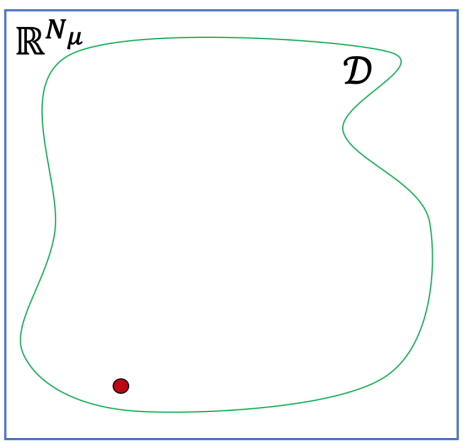
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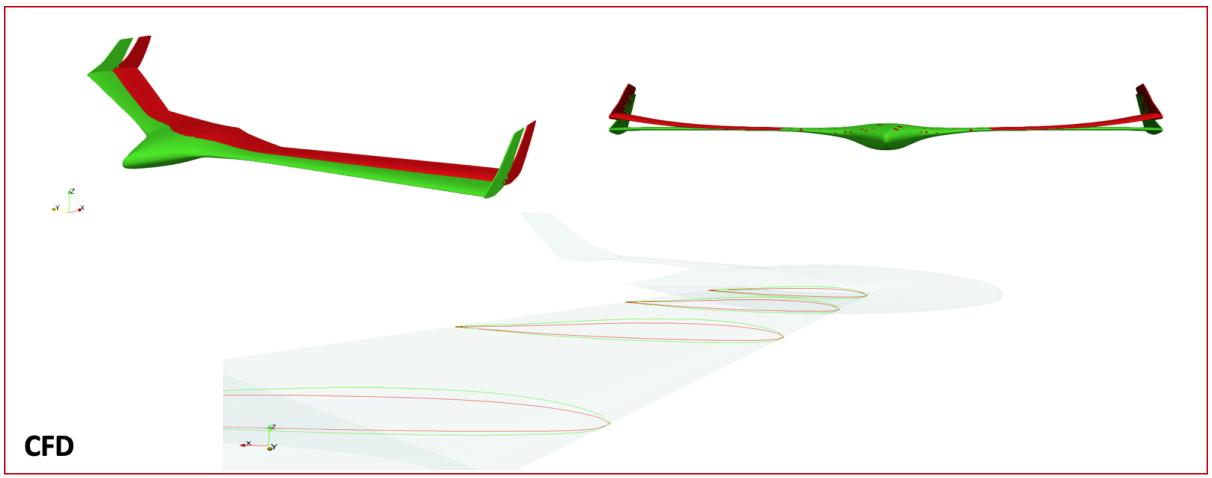


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Global shape optimization of a flying wing

- mAEWing2 flying aircraft
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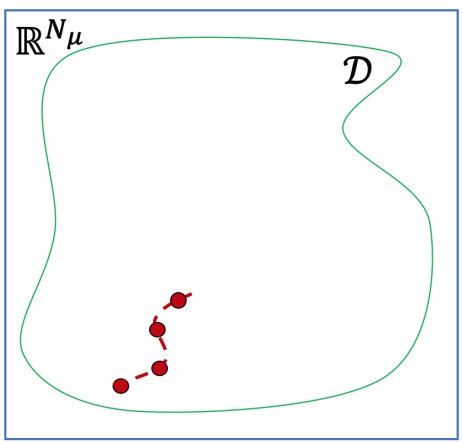
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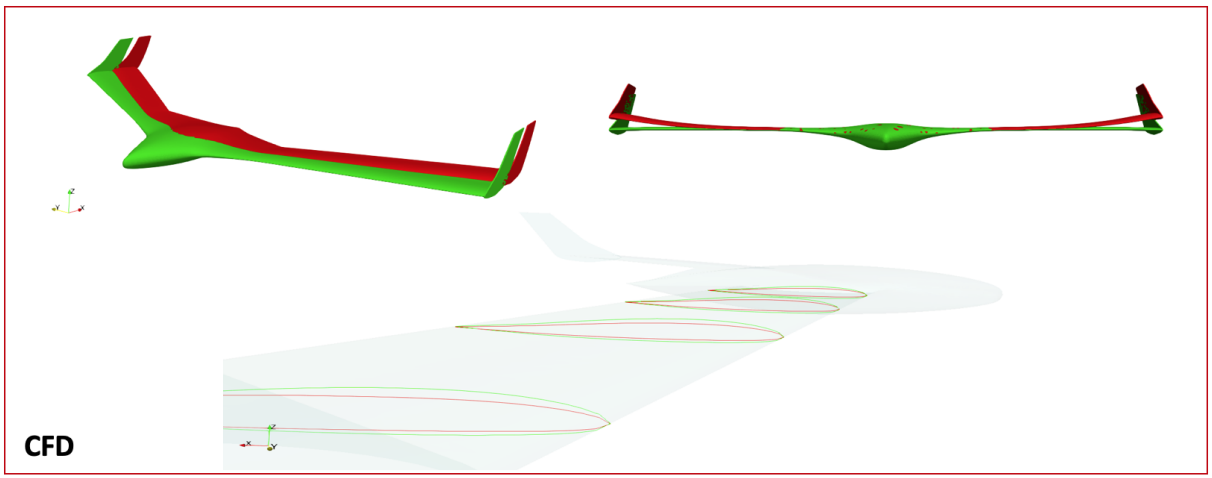


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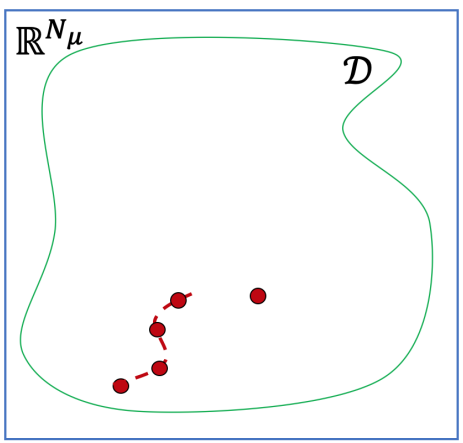
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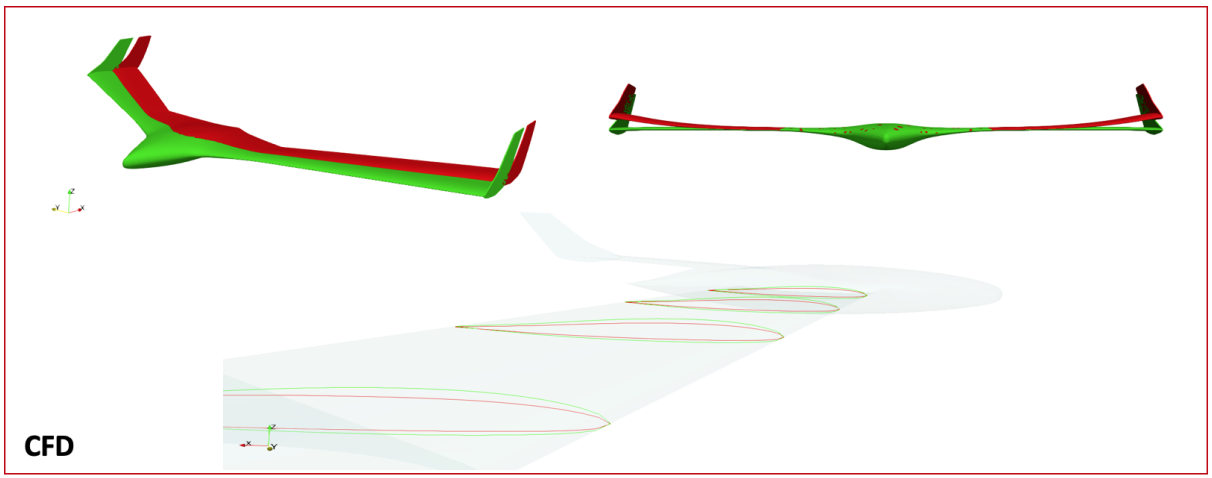
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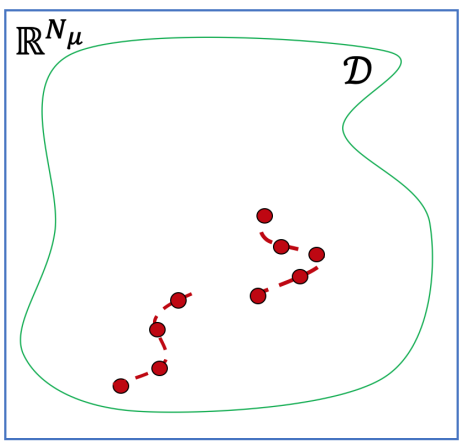
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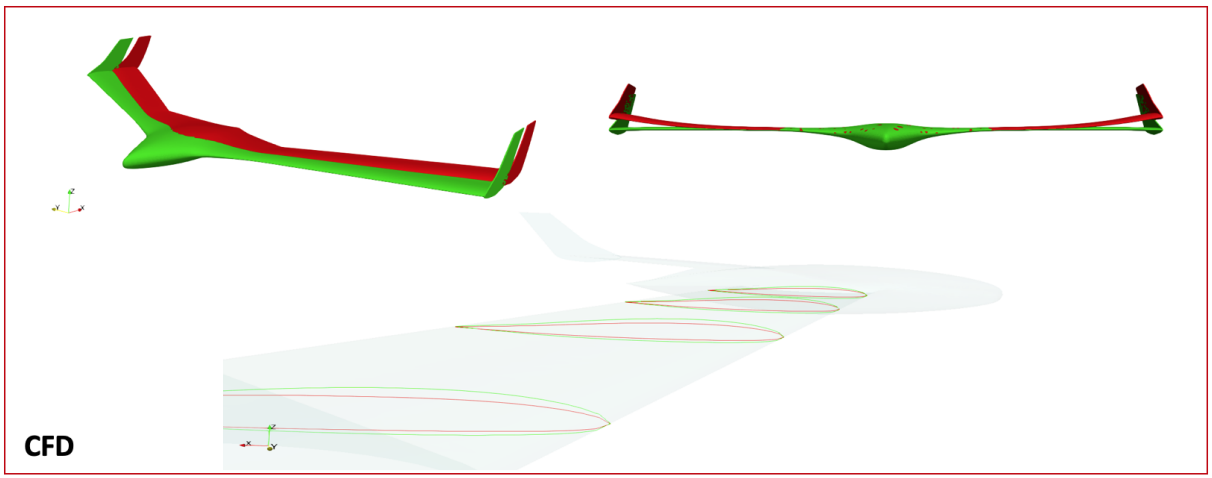
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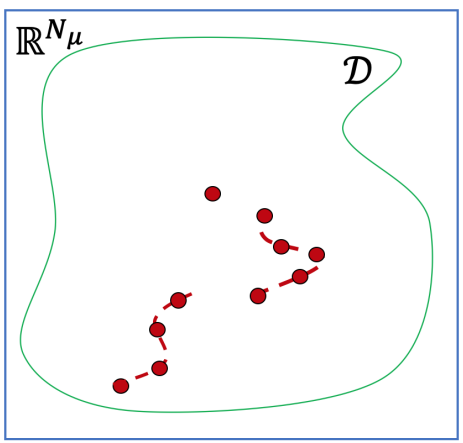
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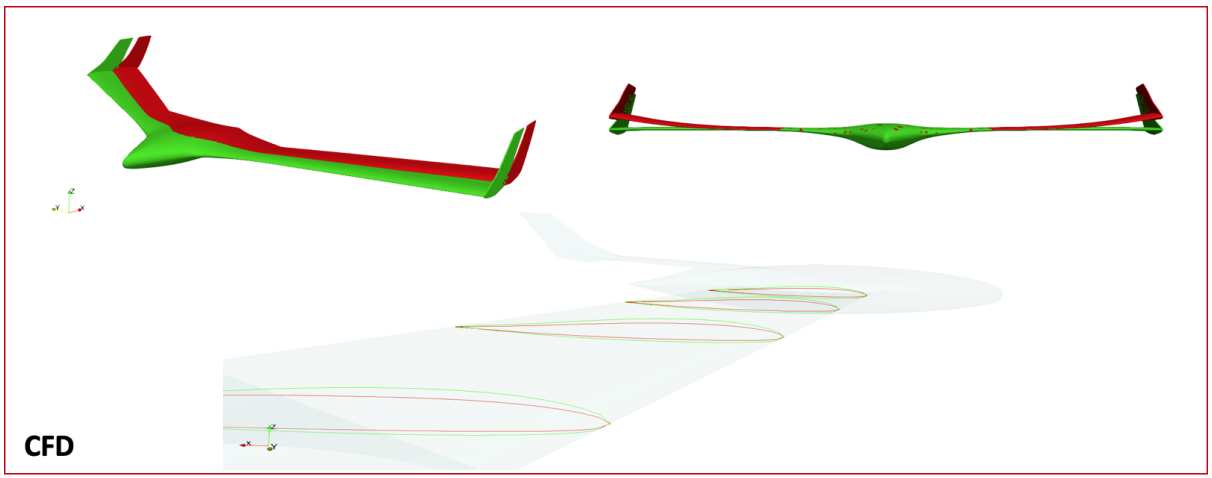
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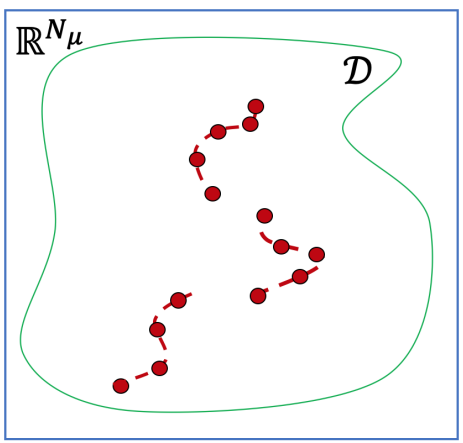
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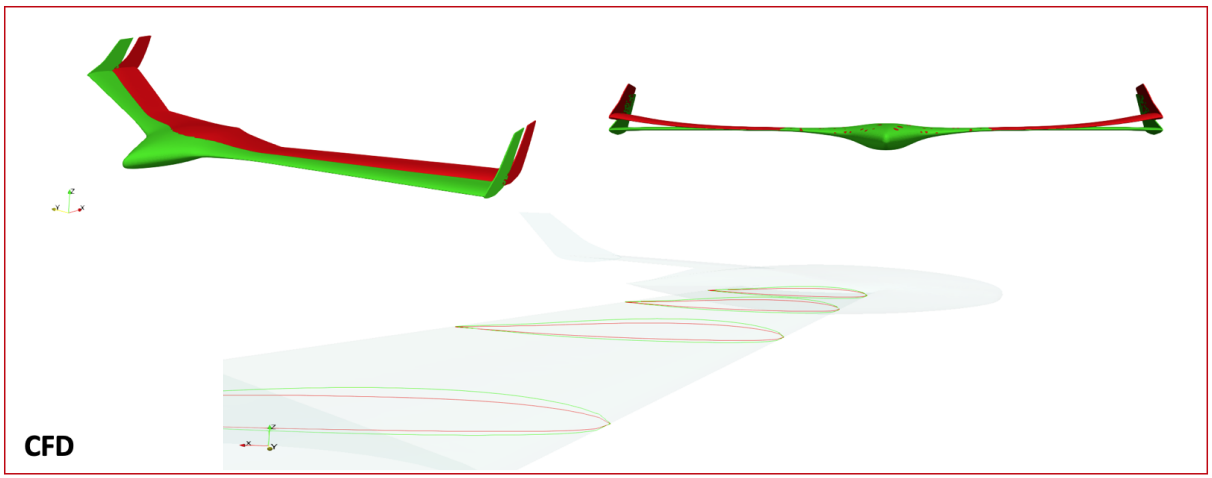
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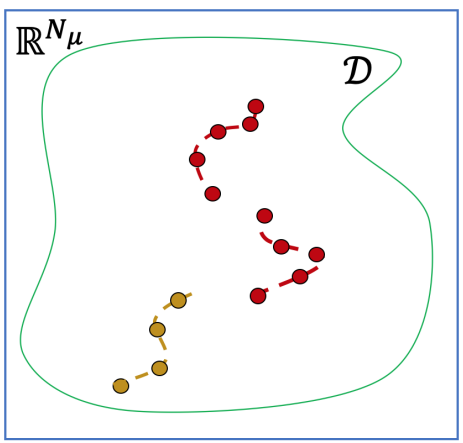
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Basin-hopping algorithm

- AS computed using one instance of the local optimization problems: dimension AS = 15; $L(\boldsymbol{\mu})$ and $D(\boldsymbol{\mu})$ computed using HPROMs[7]

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Global shape optimization of a flying wing

- 1 Global HPROM
  - dimension global ROB $\mathbf{V_w} = 1{,}179$
  - size sampled mesh = 28.8% of size original mesh
- Database of 17 P-G HPROMs
  - average dimension P-G ROB $\mathbf{V}_{\mathbf{w}}^{i} = 130$
  - average sampled mesh size = 5.5% of size original mesh

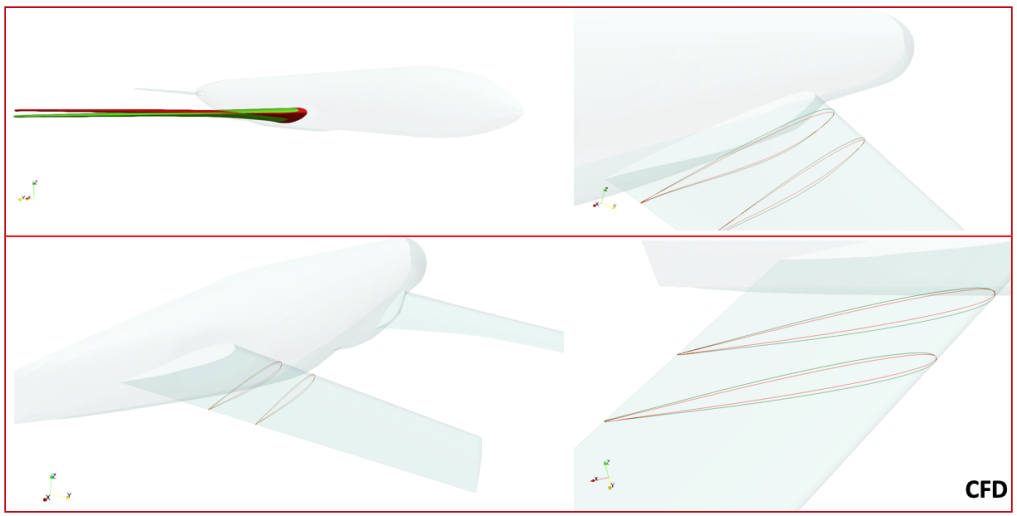
- Optimization results

	HDM	Global HPROM	Piecewise-global HPROMs
$\frac{L_0}{D_0}$	6.835	6.835	6.835
$\frac{L(\boldsymbol{\mu}^*)}{D(\boldsymbol{\mu}^*)_1}$	8.406	8.408	8.411
$\frac{L(\boldsymbol{\mu}^*)}{D(\boldsymbol{\mu}^*)_2}$	8.398	8.371	8.347
$\frac{L(\boldsymbol{\mu}^*)}{D(\boldsymbol{\mu}^*)_3}$	8.396	8.316	8.198

- Performance comparison

Computational problem	**HDM** (wall clock time)	**Global HPROM** (wall clock time)	**P-G HPROMs** (wall clock time)
Construction AS	-	30.41 hrs	30.41 hrs
Construction HPROM/s	-	20.59 hrs	19.04 hrs
Optimization problem	253.97 hrs	34.38 hrs	1.29 hrs
Optimization problem (**speedup**)	1	**7.43**	**196.95**
Overall	253.97 hrs	85.38 hrs	50.74 hrs
Overall (**speedup**)	1	**2.97**	**5.00**

- NASA's Common Research Model (CRM)
- Parametric model, $\boldsymbol{\mu} \in \mathbb{R}^{54}$



- Multi-objective optimization problem using ϵ-constraint method

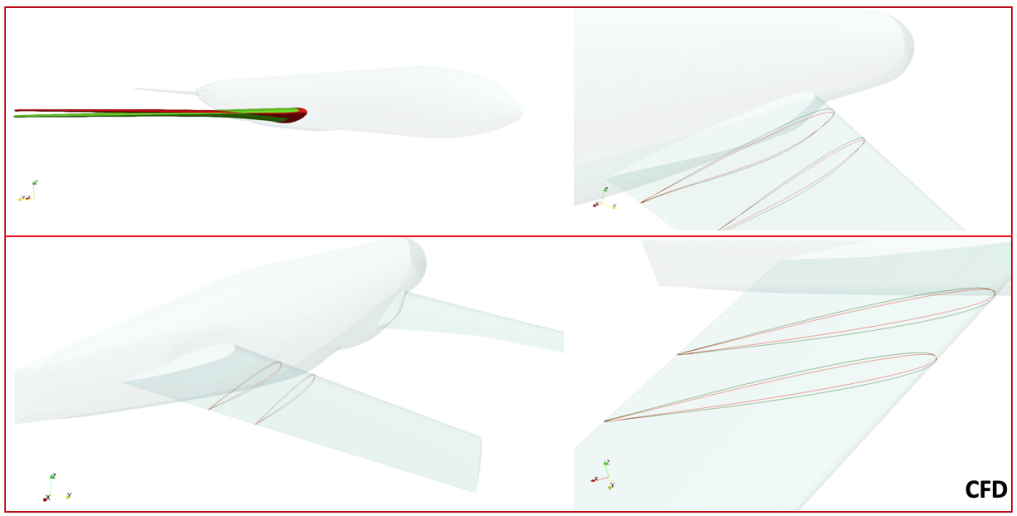
$$\max_{\boldsymbol{\mu} \in \mathcal{D}} \quad \left\{ \frac{\frac{L(\boldsymbol{\mu})}{D(\boldsymbol{\mu})} - \frac{L_0}{D_0}}{\frac{L_0}{D_0}}, \quad L(\boldsymbol{\mu}) \right\}$$

$$\text{s.t} \qquad \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}}$$

- **Shape parameters**:
  dihedral angle and wing airfoil shape $(\mu_s^1, \cdots, \mu_s^{34})$;
  tailplane airfoil shape $(\mu_s^{35}, \cdots, \mu_s^{54})$

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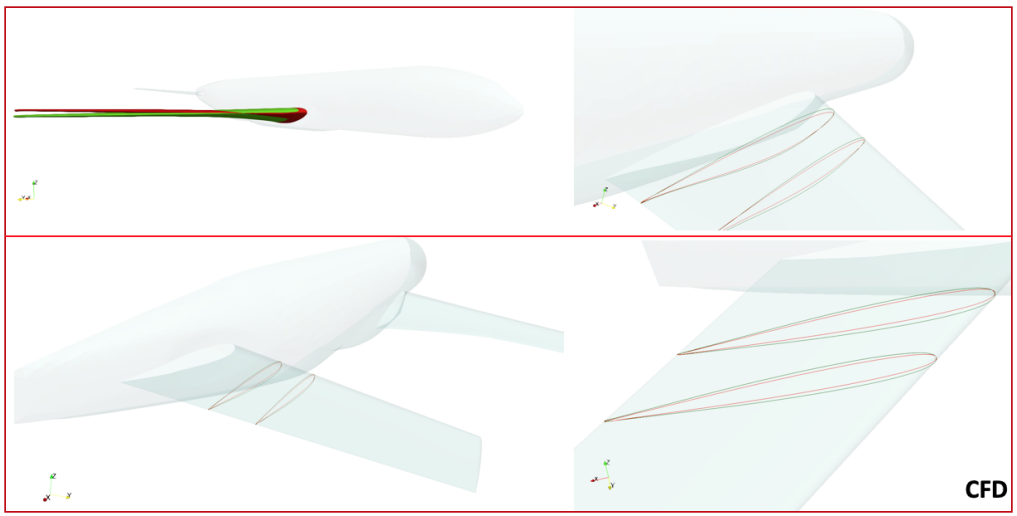
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$$\text{s.t} \quad \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \qquad \text{s.t.} \quad L(\boldsymbol{\mu}) \geqslant \epsilon, \quad \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}}$$

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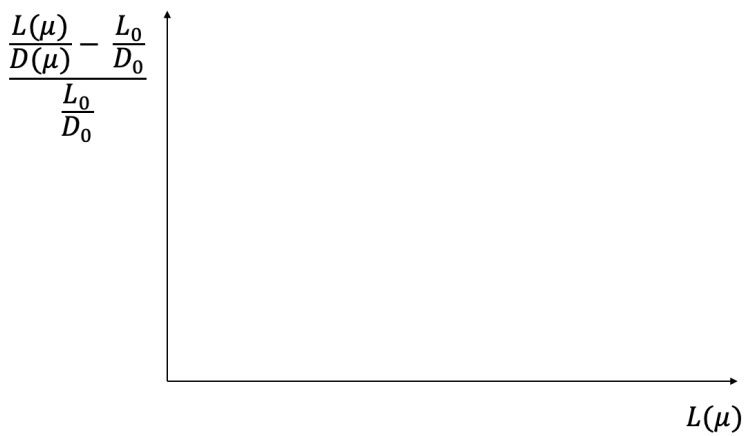


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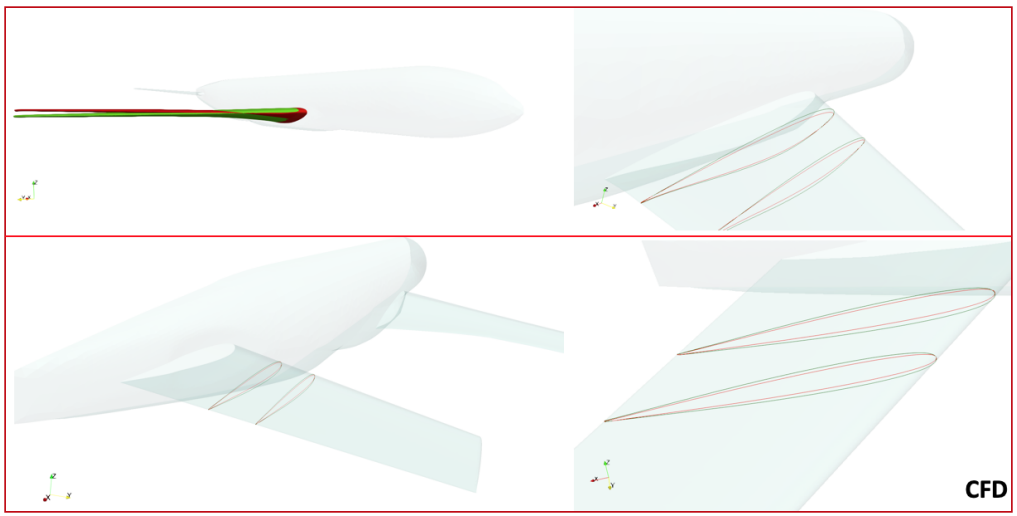
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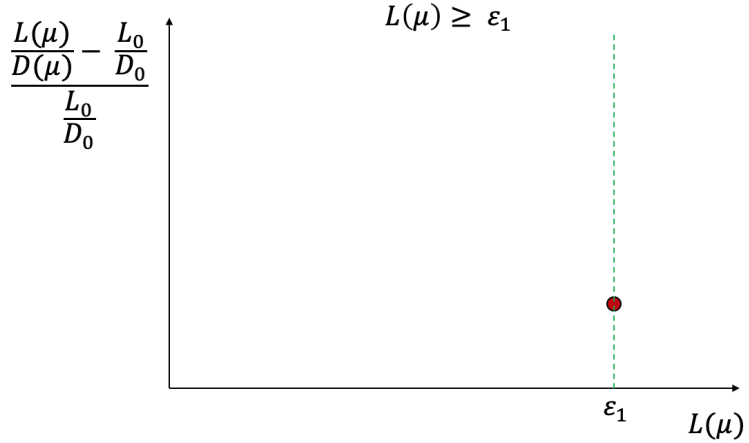


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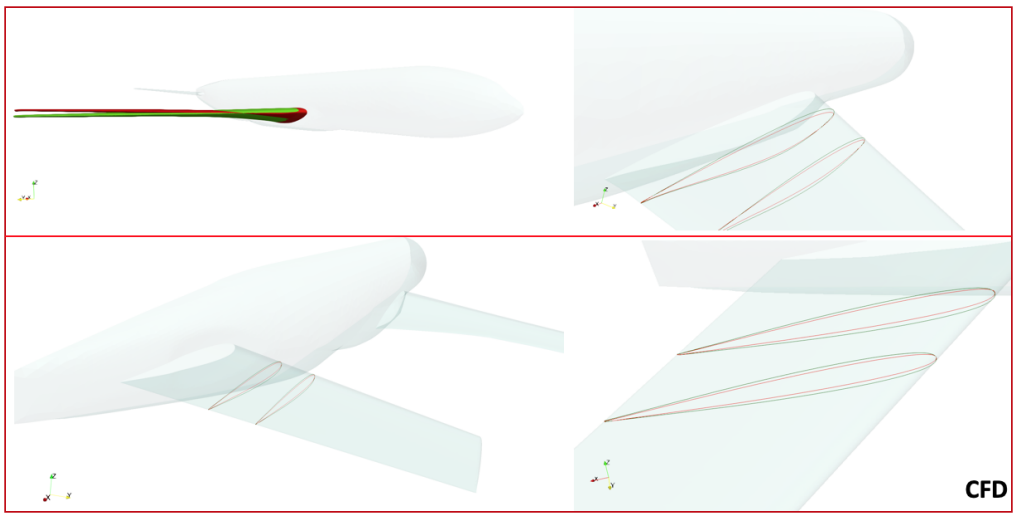
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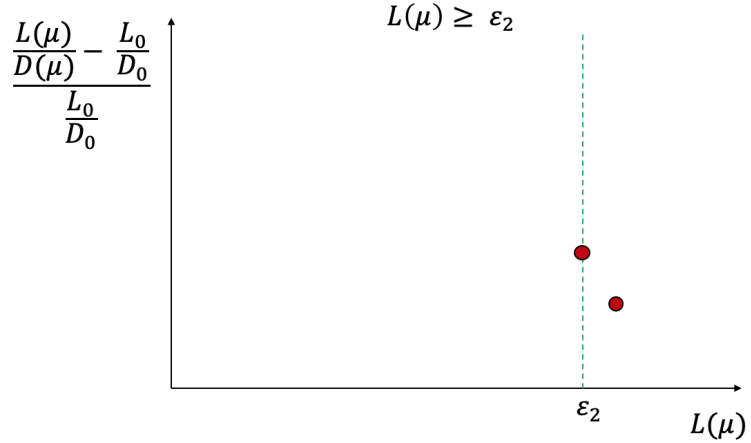


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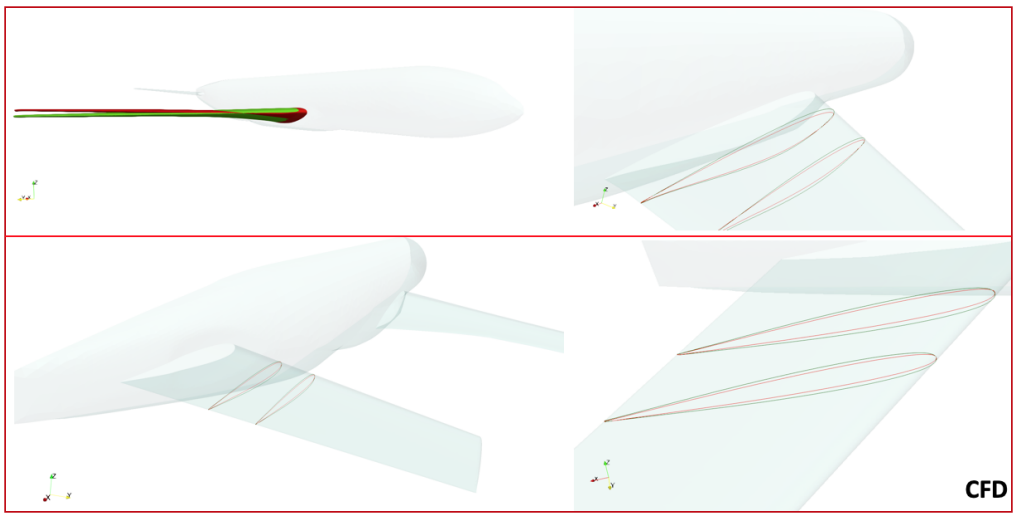
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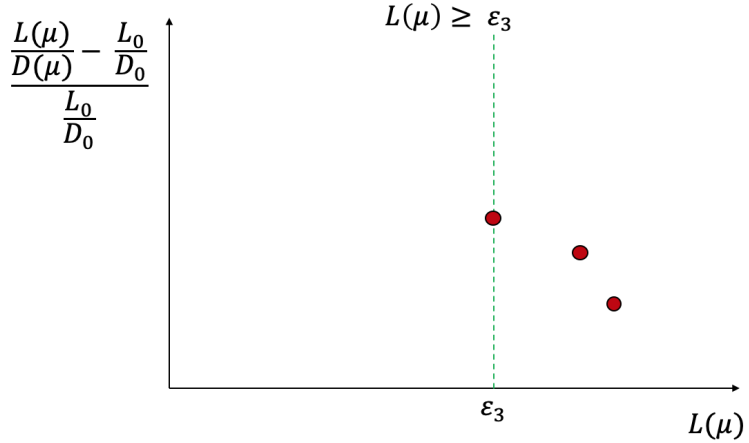


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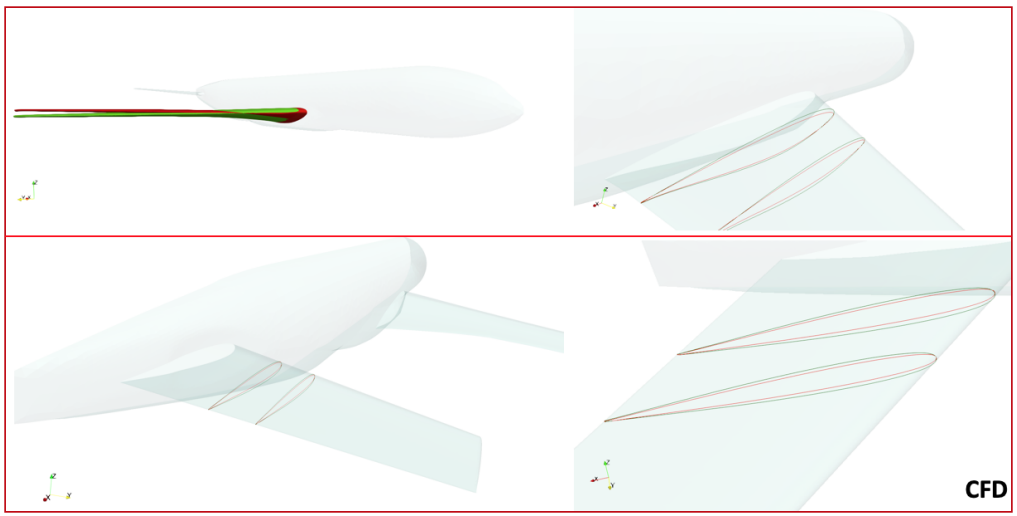
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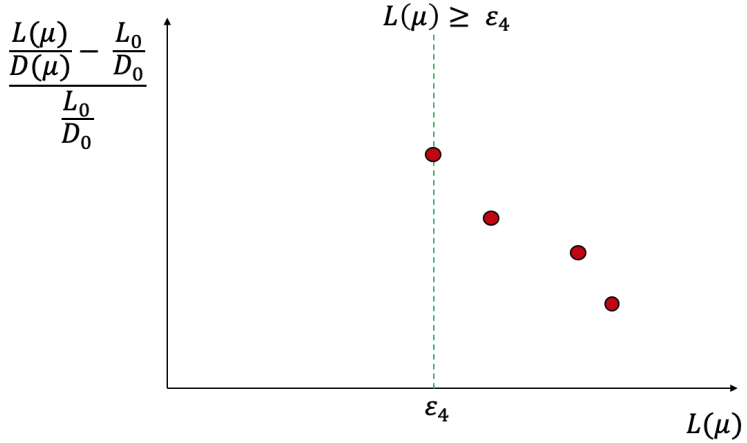


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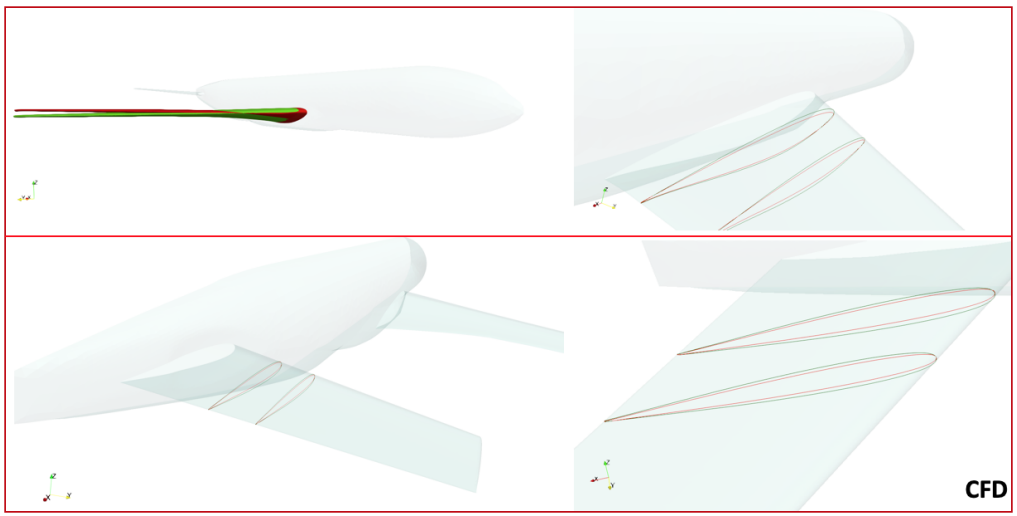
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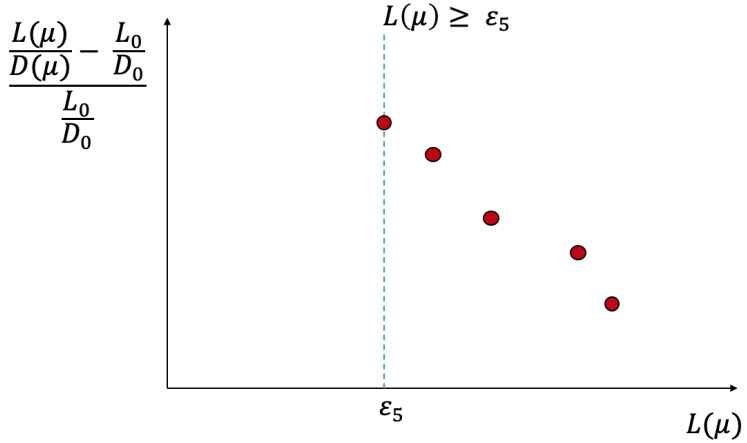


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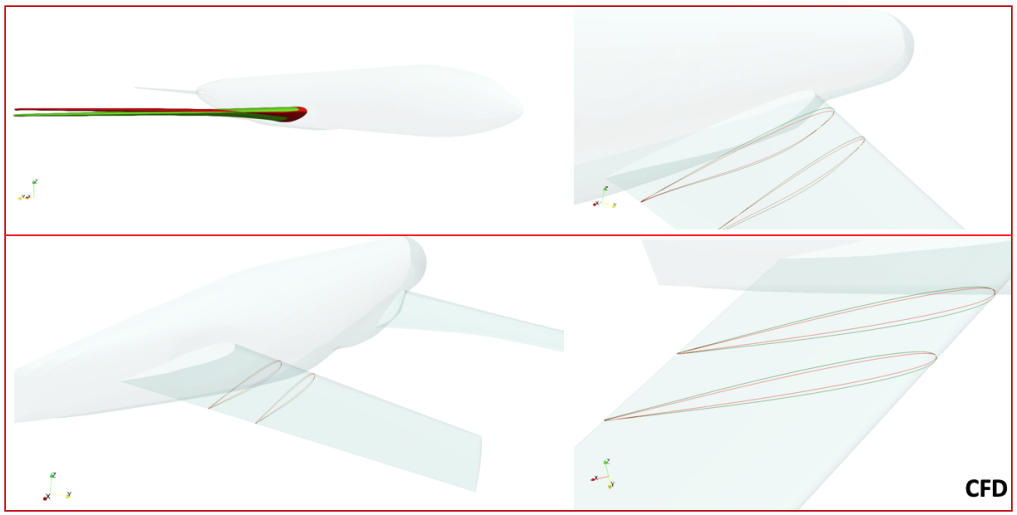
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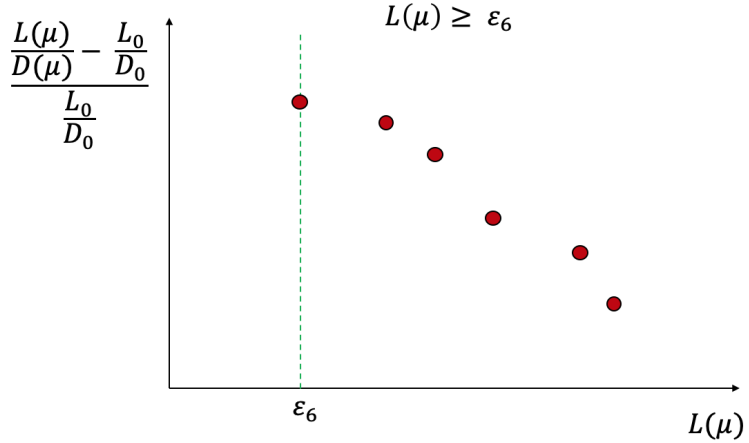


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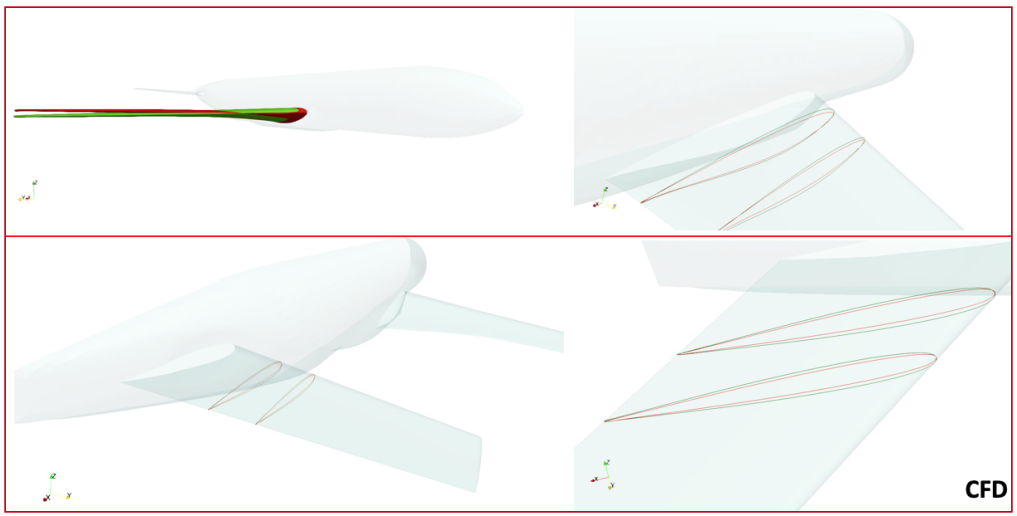
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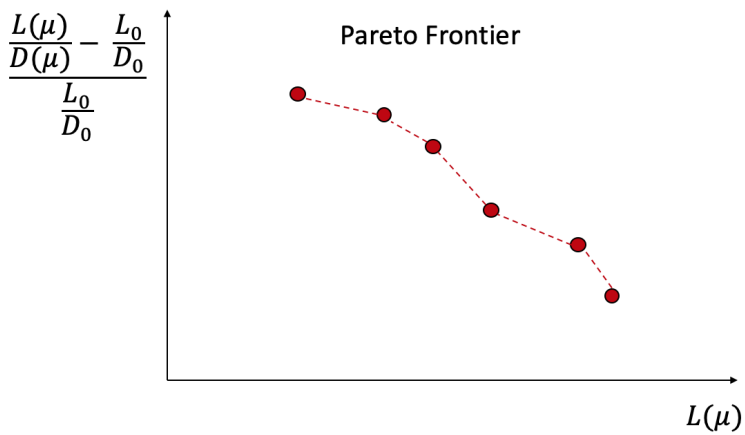


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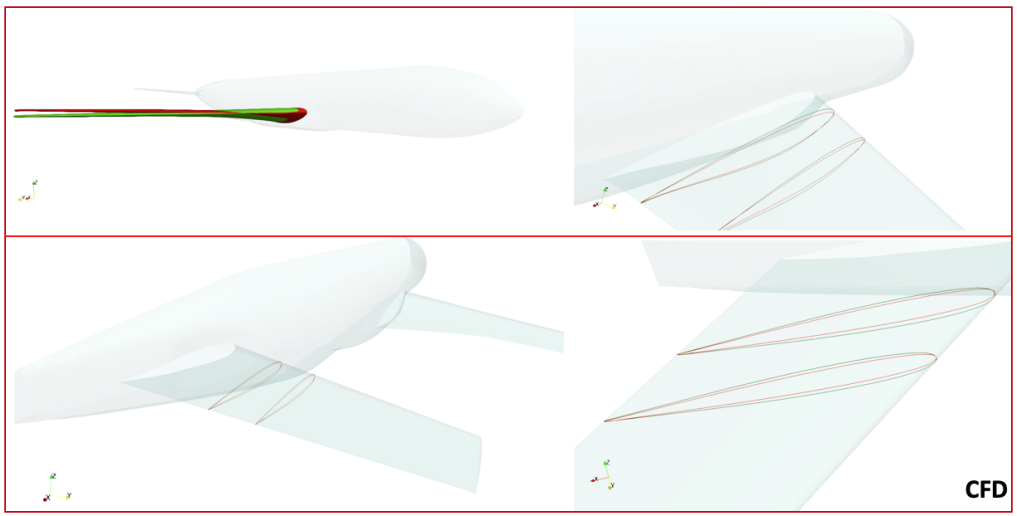
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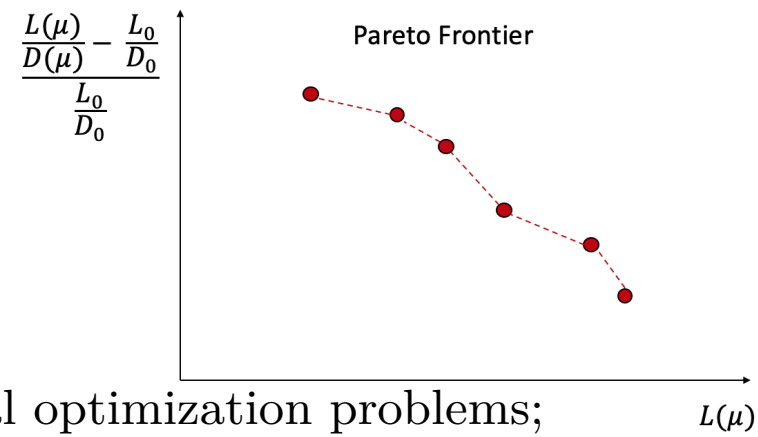


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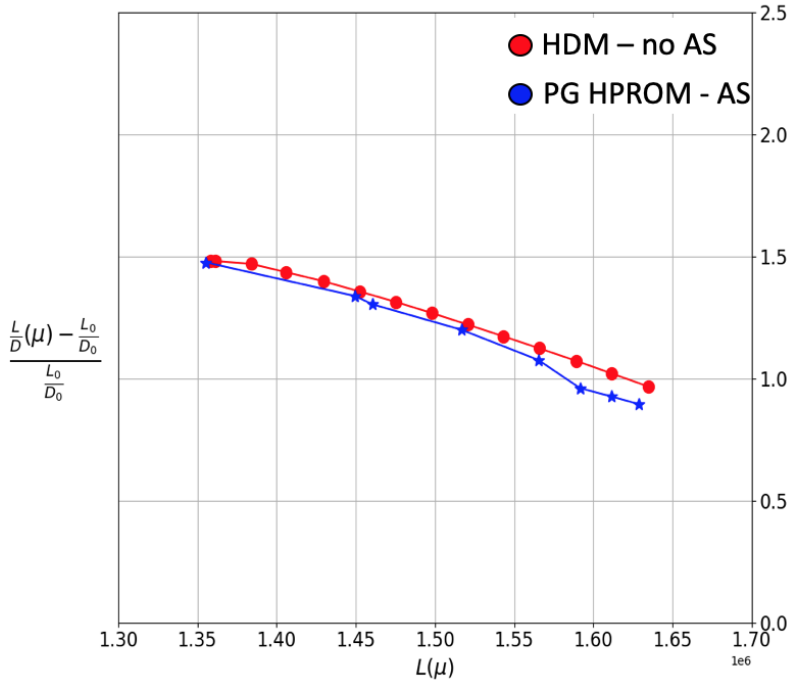
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- AS computed using one instance of the local optimization problems; dimension AS = 10; $L(\boldsymbol{\mu})$ and $D(\boldsymbol{\mu})$ computed using P-G HPROMs[7]

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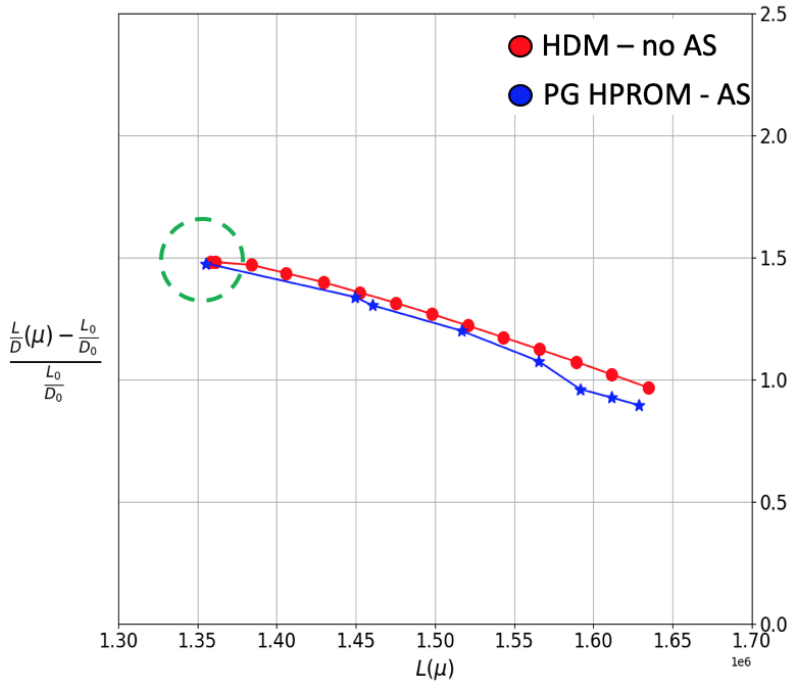
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    - size sampled mesh = 0.9% of size original mesh
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- Performance comparison

Computational problem	**HDM** (wall clock time)	**P-G HPROMs** (wall clock time)	**Speedup** (wall clock time)
Construction AS	-	38.70 hrs	-
Construction database HPROMs	-	44.73 hrs	-
Optimization problem	776.70 hrs	0.76 hrs	**1,022.0**
Overall	776.70 hrs	84.19 hrs	**9.2**

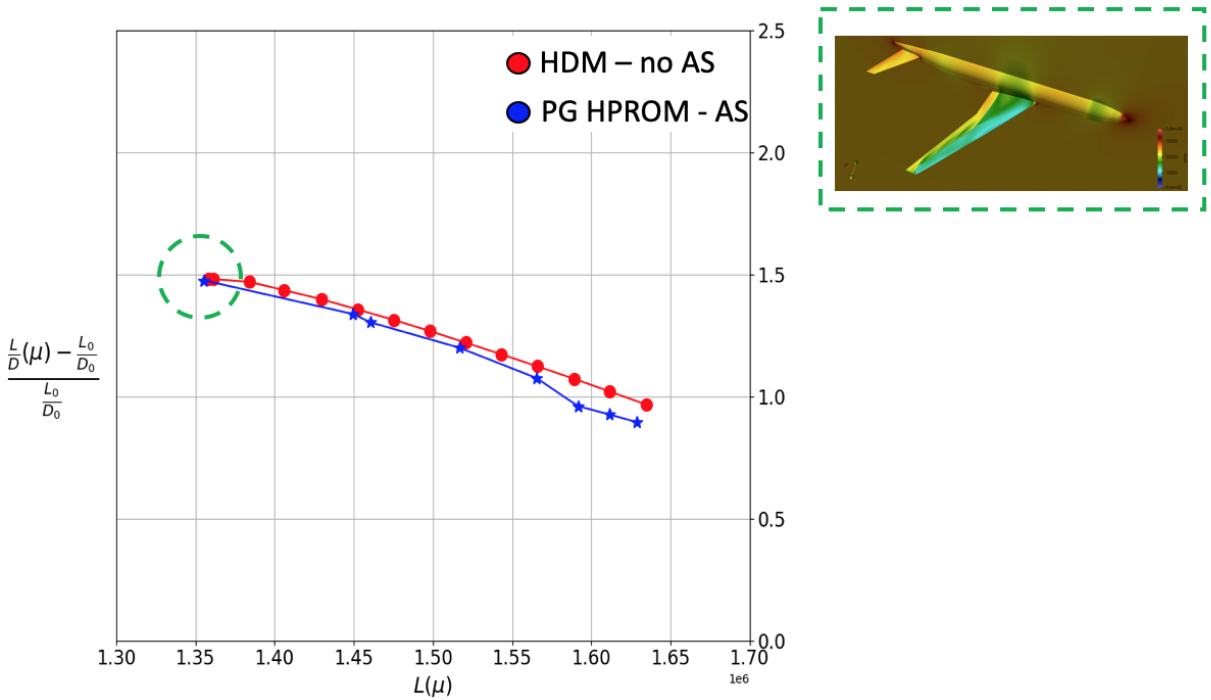
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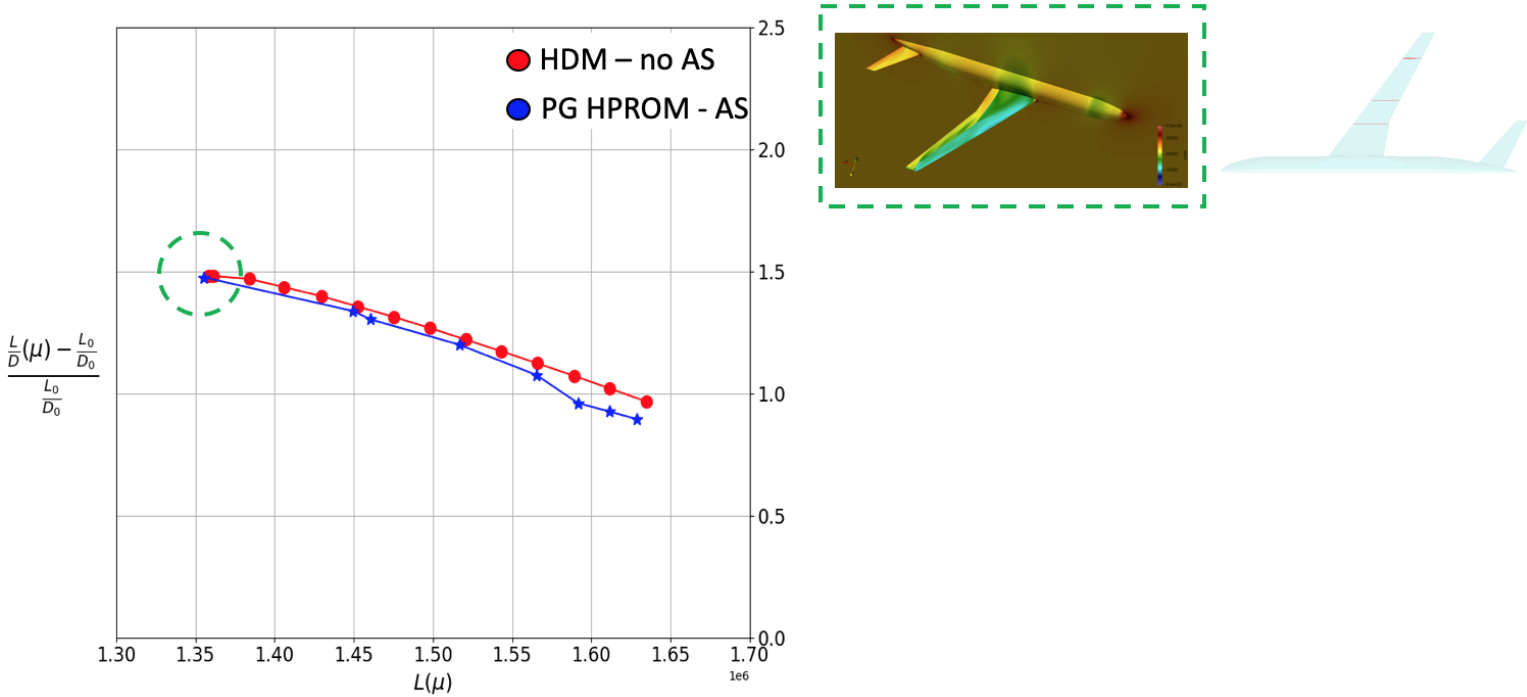
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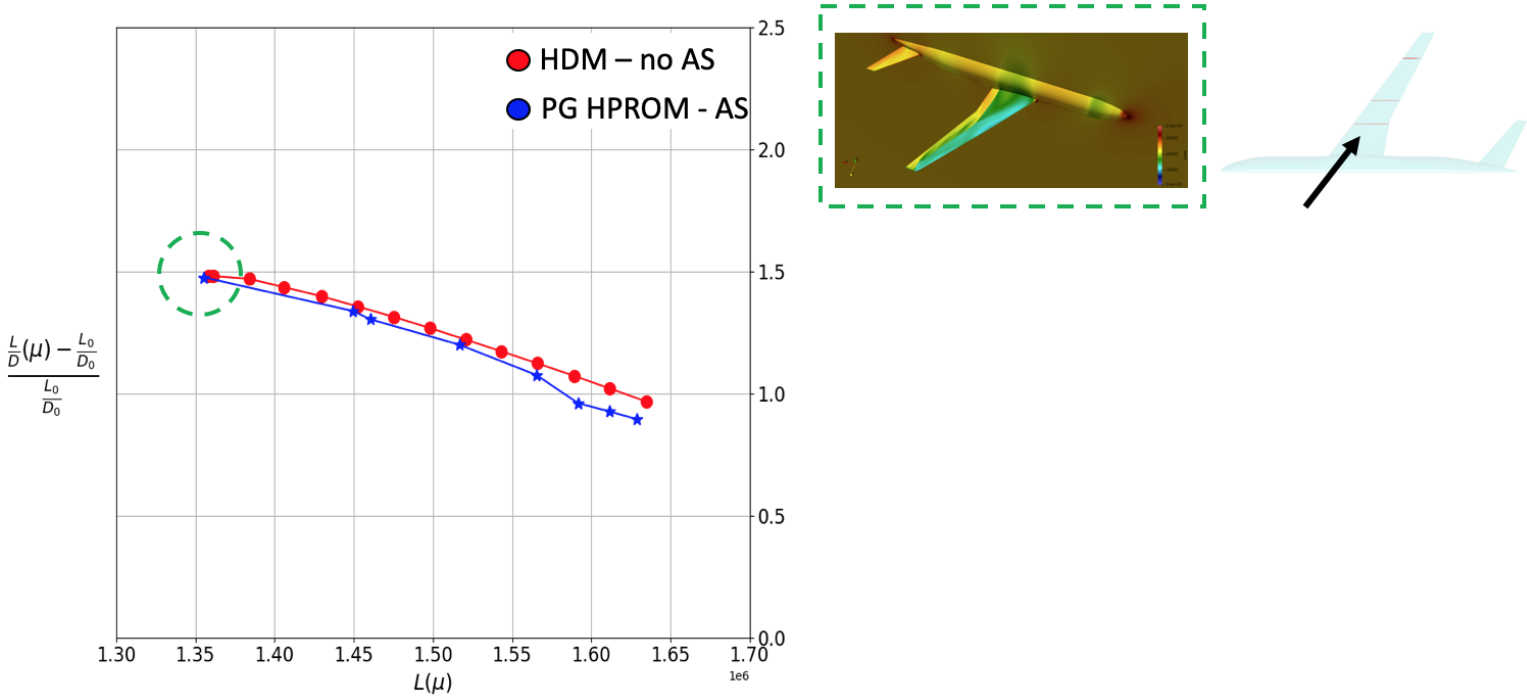
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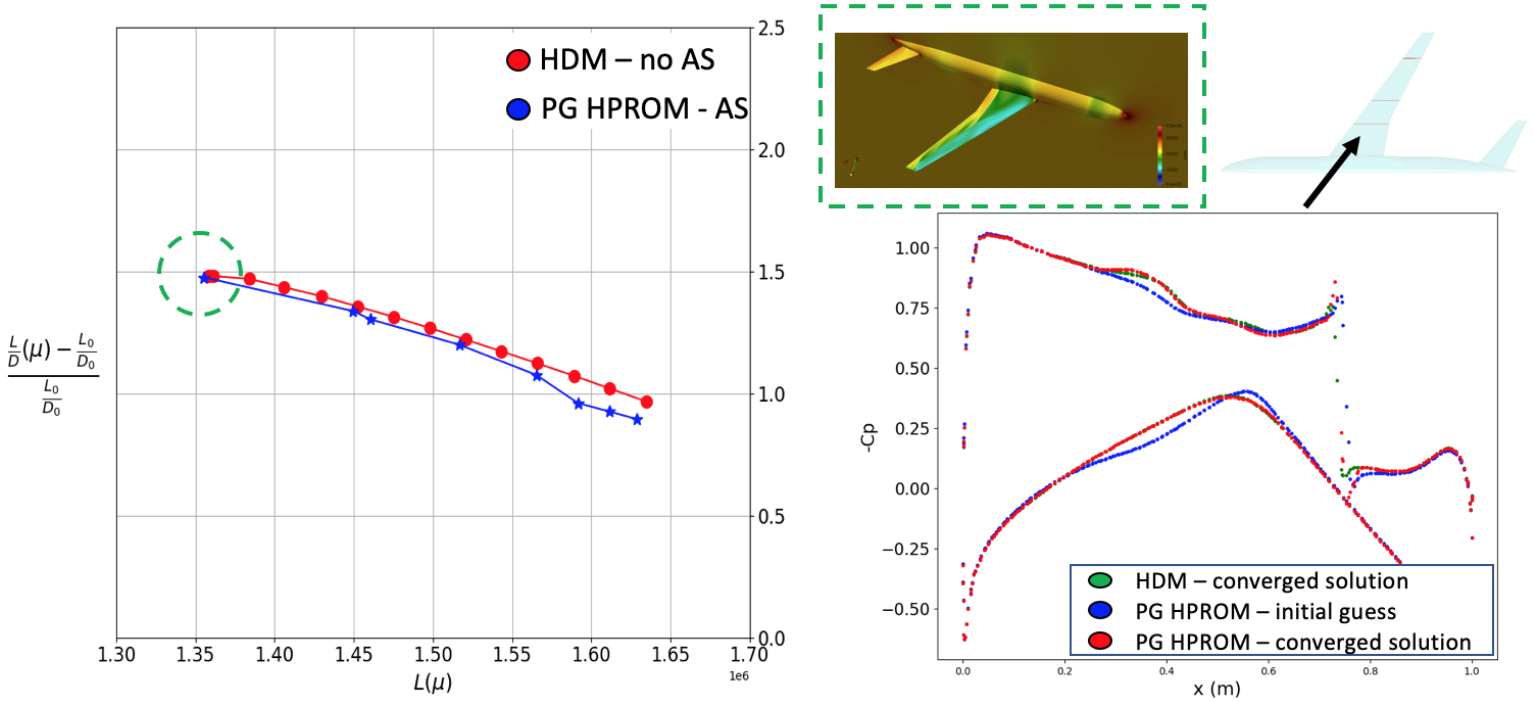
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is an **affine** approximation

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$$\boldsymbol{\mu} = \boldsymbol{\mu}_{\text{ref}} + \mathbf{g}_{\mu}(\boldsymbol{\mu}_{r})$$

is a **nonlinear** approximation

- PDE-constrained optimization problem

$$\begin{aligned} &\min_{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{N_{\boldsymbol{\mu}}}} && f(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}), \\ &\text{subject to} && \mathbf{c}(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}) \geqslant 0, \end{aligned} \tag{$\star$}$$

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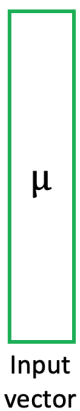
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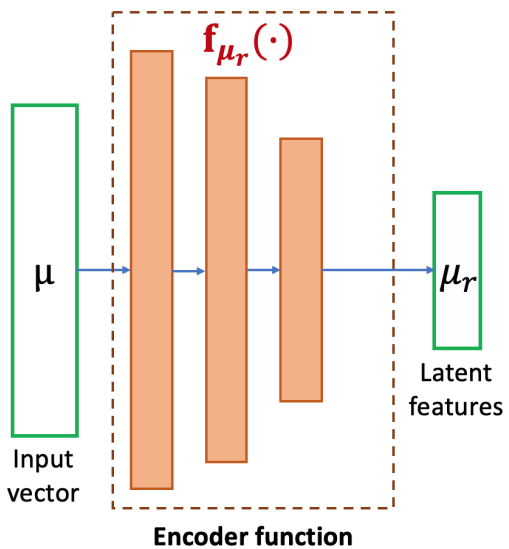
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$$\begin{aligned} &\min_{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{N_{\boldsymbol{\mu}}}} && f(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}), \\ &\text{subject to} && \mathbf{c}(\mathbf{w}(\boldsymbol{\mu}); \boldsymbol{\mu}) \geqslant 0, \end{aligned} \tag{$\star$}$$

- Solution of problem $(\star)$ is contained in the AM, i.e., $\mathcal{D}_{AM} \subset \mathcal{D}$
- Each design parameter vector $\boldsymbol{\mu} \in \mathcal{D}_{AM} \subset \mathcal{D}$

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{\text{ref}} + \mathbf{g}_{\boldsymbol{\mu}}(\boldsymbol{\mu}_r)$$

  - $\mathbf{g}_{\mu} : \mathbb{R}^{N_{\boldsymbol{\mu}_r}} \rightarrow \mathbb{R}^{N_{\boldsymbol{\mu}}}$ is a **nonlinear function** $(N_{\boldsymbol{\mu}} \gg N_{\boldsymbol{\mu}_r})$
  - $\boldsymbol{\mu}_r \in \mathbb{R}^{N_{\boldsymbol{\mu}_r}}$ are the latent coordinates of $\boldsymbol{\mu}$
- $\mathbf{g}_{\boldsymbol{\mu}}(\cdot)$ is built using a feed-forward autoencoder



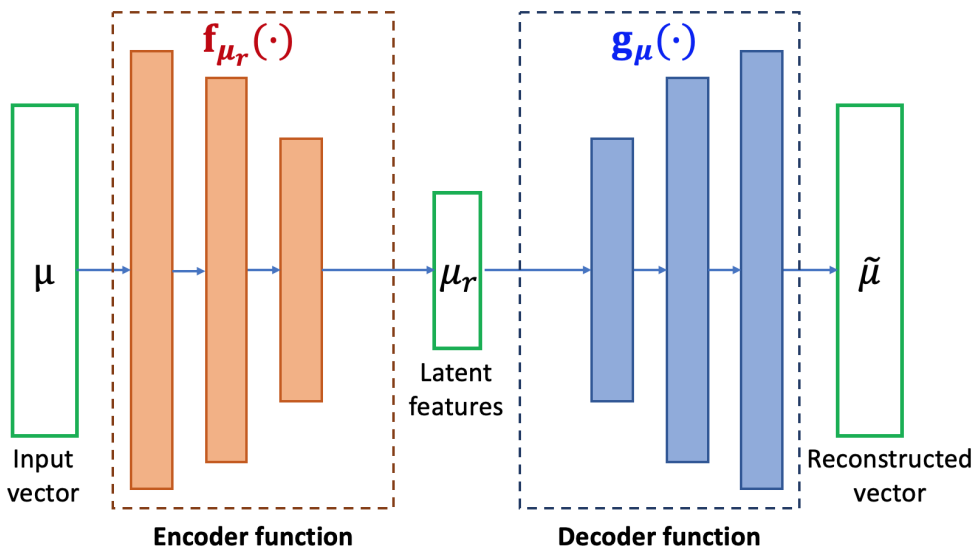
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  - same as AS training data, i.e. $\{\boldsymbol{\mu}_k + \Delta\boldsymbol{\mu}_k - \boldsymbol{\mu}_{\text{ref}}\}_{k=1}^{N_{\mathcal{S}}}$
  - **augmented with**, for each snapshot $\mathbf{x}_k = \boldsymbol{\mu}_k + \Delta\boldsymbol{\mu}_k - \boldsymbol{\mu}_{\text{ref}}$

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1. find set of feasible candidate points
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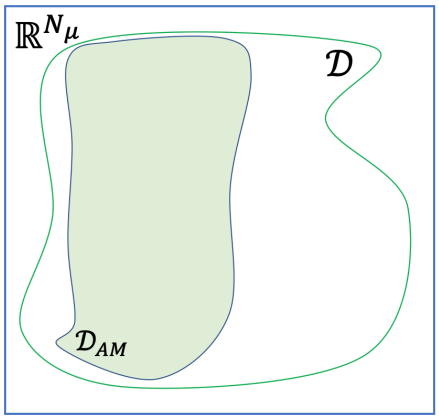
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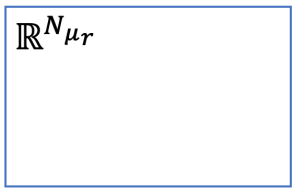
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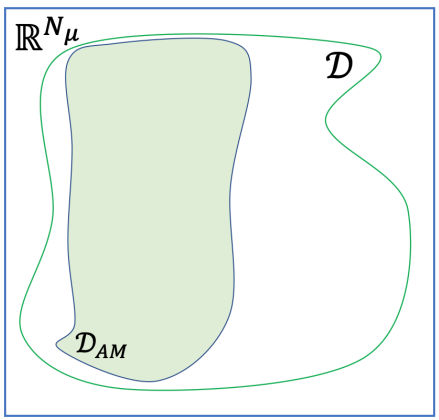
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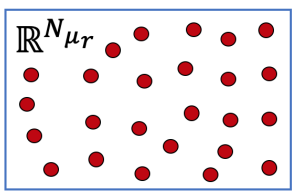
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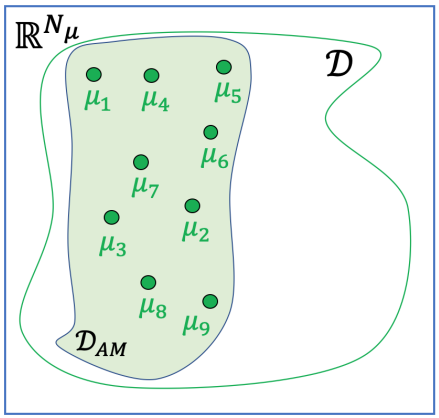
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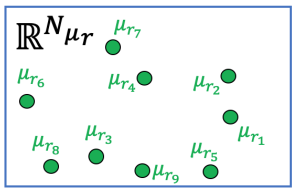
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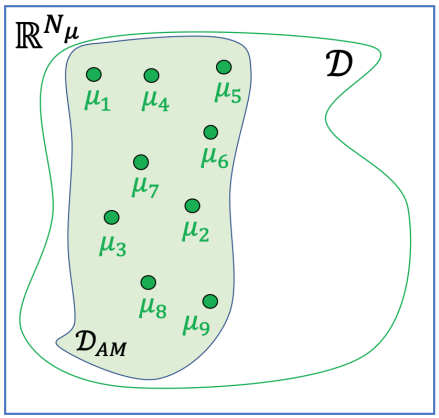
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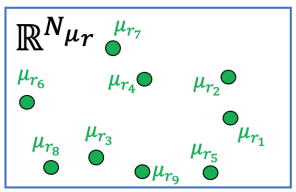
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  2. use greedy algorithm to train PROMs





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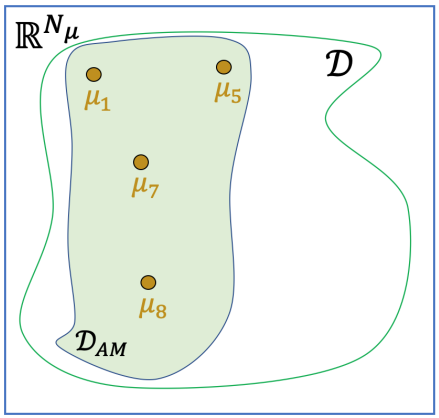
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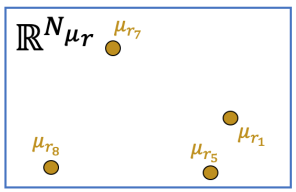
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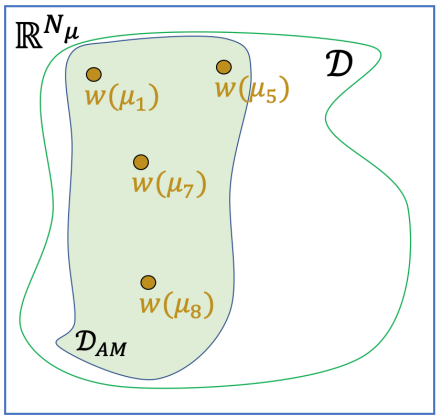
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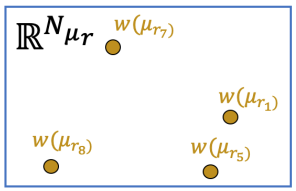
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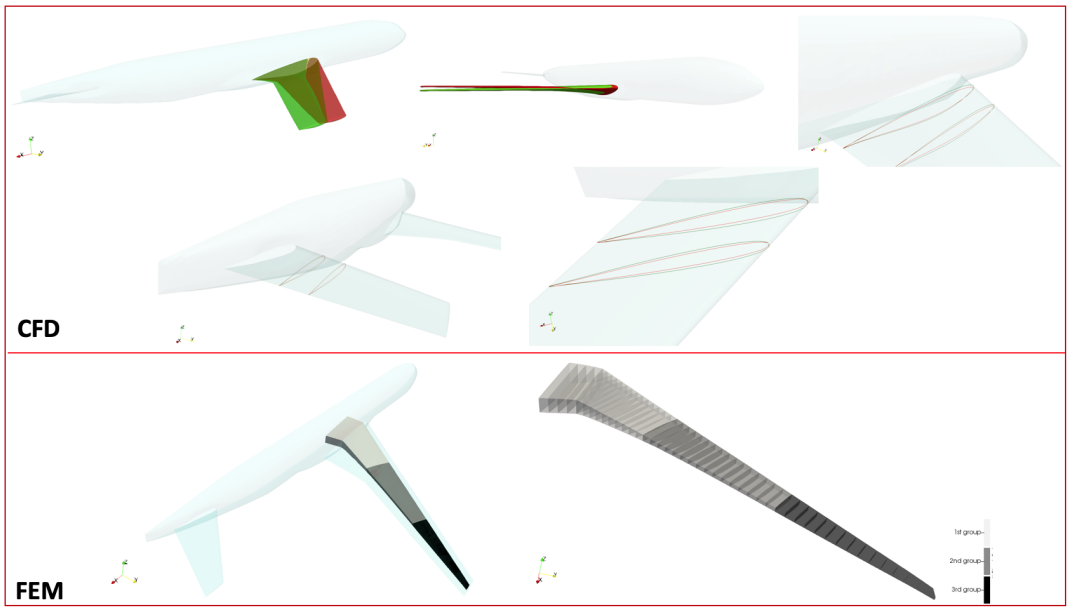
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2. use greedy algorithm to train PROMs





- NASA's Common Research Model (CRM)
- Parametric model[8], $\boldsymbol{\mu} \in \mathbb{R}^{58}$



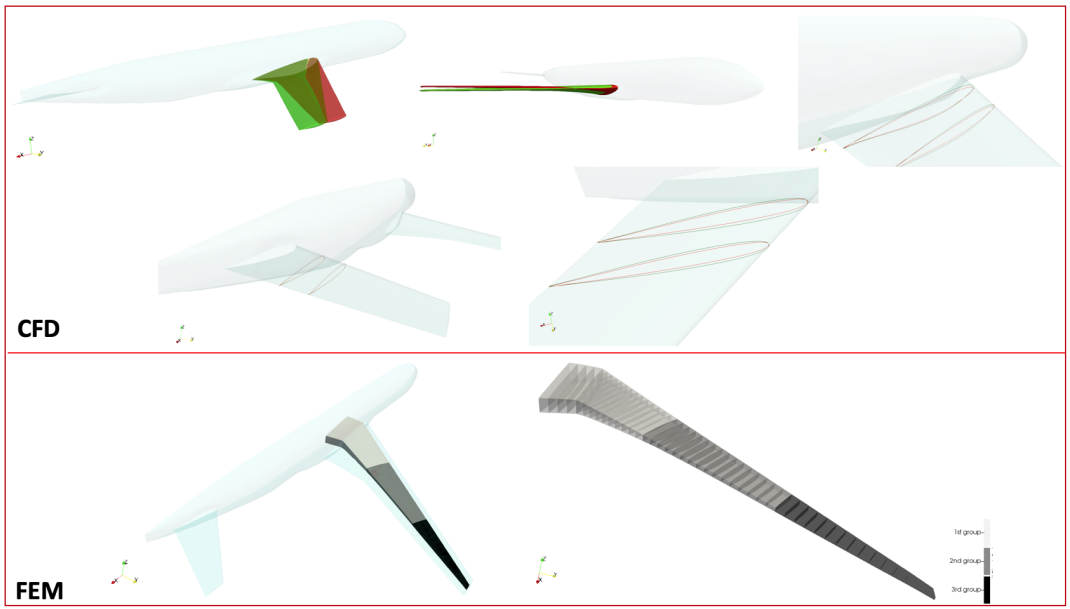
- **Shape parameters**: sweep angle, dihedral angle, and wing airfoil shape $(\mu_s^1, \cdots, \mu_s^{35})$;
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- **Structural parameters**: 3 thickness increments $(\mu_m^1, \mu_m^2, \mu_m^3)$ for 3 groups of stiffeners

- Optimization problem

$$\begin{aligned} \underset{\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^{58}}{\text{maximize}} \quad & \frac{L(\boldsymbol{\mu})}{D(\boldsymbol{\mu})} \\ \text{subject to} \quad & \frac{L(\boldsymbol{\mu}) - L_{\text{lb}}}{L_{\text{lb}}} \geqslant 0 \\ & \boldsymbol{\mu}_{\text{lb}} \leqslant \boldsymbol{\mu} \leqslant \boldsymbol{\mu}_{\text{ub}} \\ & \boldsymbol{\zeta}(\boldsymbol{\mu}) \geqslant \mathbf{1}\zeta_{\text{lb}} \end{aligned}$$

[8] Gabriele Boncoraglio and Charbel Farhat. "Active Manifold and Model Reduction for Multidisciplinary Analysis and Optimization". In: AIAA journal (2021).

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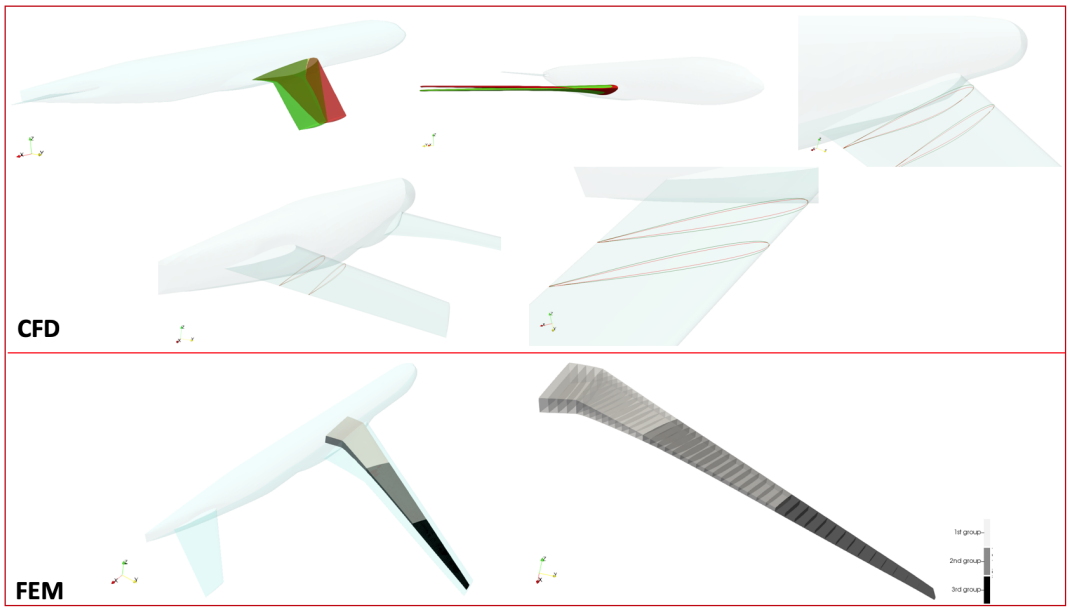
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- Optimization problem → auxiliary optimization problem

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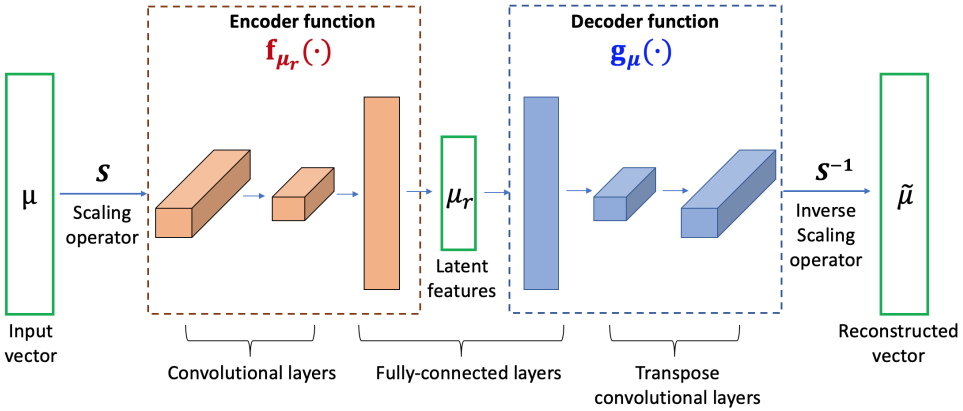
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- lift L and drag D computed using nonlinear HPROM
- damping ratios $\boldsymbol{\zeta}$ computed using database of linear PROMs

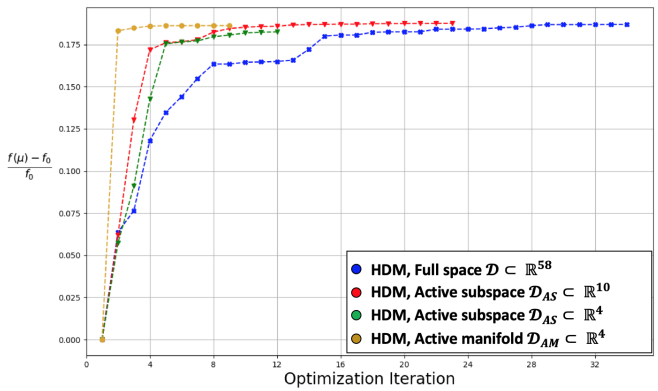
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- Comparison of AM and AS

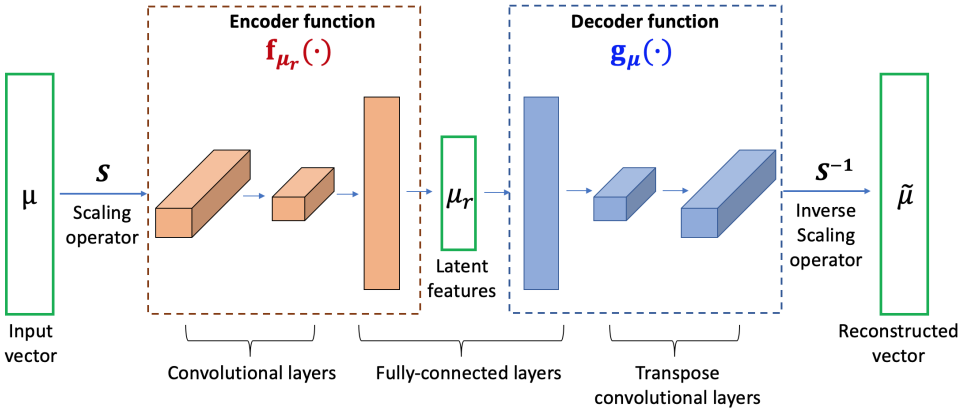


- **Active manifold**: deep convolutional autoencoder $\mathbf{g}_{\boldsymbol{\mu}} : \mathbb{R}^4 \to \mathbb{R}^{58}$ with $\mathcal{D}_{AM} \subset \mathbb{R}^4$
- **Active subspace**: optimal ROB $\mathbf{V}_{\boldsymbol{\mu}} \in \mathbb{R}^{58\times 10}$ with $\mathcal{D}_{AS_1} \subset \mathbb{R}^{10}$ for comparison, computed ROB $\mathbf{V}_{\boldsymbol{\mu}} \in \mathbb{R}^{58\times 4}$ with $\mathcal{D}_{AS_2} \subset \mathbb{R}^4$

- Optimal AM of dimension equal to 4 outperforms optimal AS of same dimension

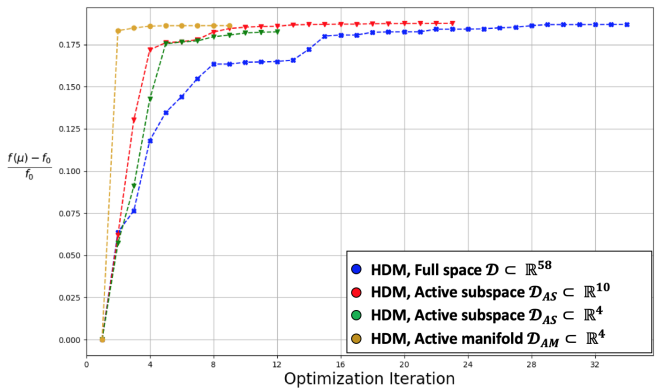


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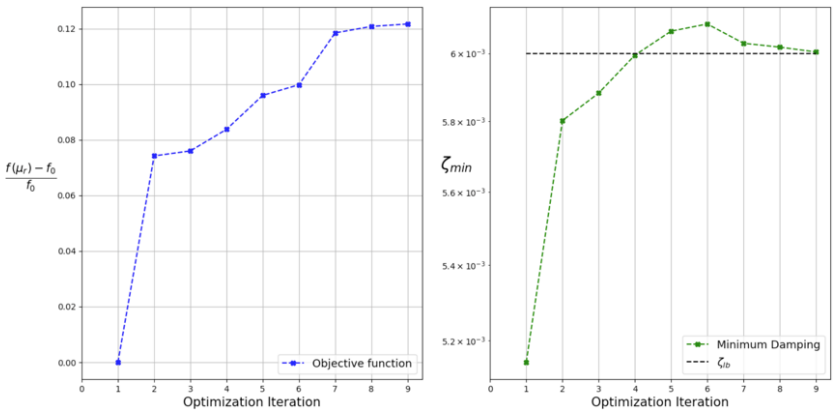
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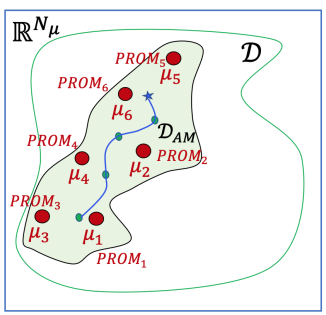
- Offline ($\approx$ 70 hrs) and online ($\approx$ 0.4 hrs) phase with AM method

Wall-clock time computing $\mathbf{g}_{\mu}$ and $\mathbf{f}_{\mu_r}$	Wall-clock time greedy procedure $\mathcal{DB}$ of linear aeroelastic PROMs	Wall-clock time greedy procedure global nonlinear HPROM	Wall-clock time total offline phase
43.1 hours	**27.8 hours**	20.0 hours	**70.85 hours**

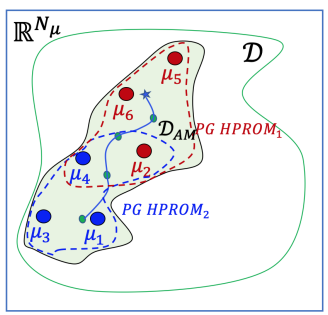


- Innovative framework for accelerating the solution of PDE-constrained optimization problems *in higher-dimensional parameter spaces*
  - ⋆ parametric nonlinear **piecewise-global HPROMs** are efficient
    30× speedup for aircraft design problem over global HPROM
  - ⋆ intensive PROM training avoided by using the concept of an **active manifold**
    optimal AM of a certain dimension **outperforms** new take AS of same dimension
  - ⋆ **sampling strategy** for computing the active design space by solving an auxiliary optimization problem
    3× speedup of the construction of classical AS for an aicraft MDAO problem (but classical AS approach failed to solve the MDAO problem)

- Applied to variety of problems in computational mechanics and outperforms state-of-the-art methods
  - **1, 000**× speedup of online phase of multi-shape and multi-objective aircraft design optimization problems and **10**× overall speedup (including offline training costs)



Database $\mathcal{DB}$ of local linear PROMs



Piecewise-Global nonlinear HPROMs

