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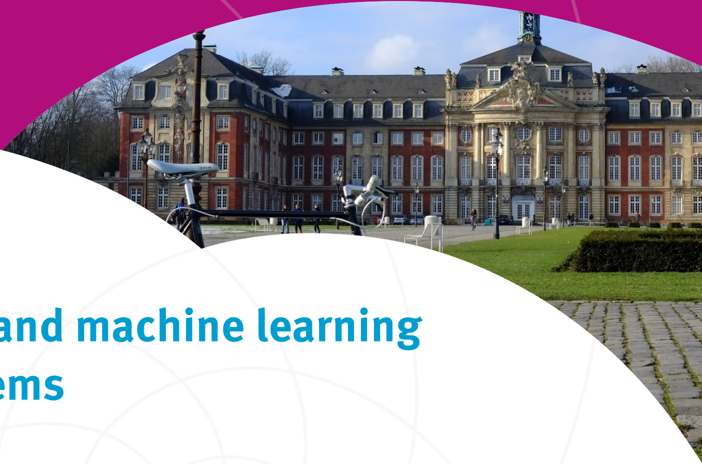

Model order reduction and machine learning for parametrized problems

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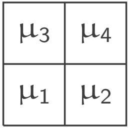
Table of contents

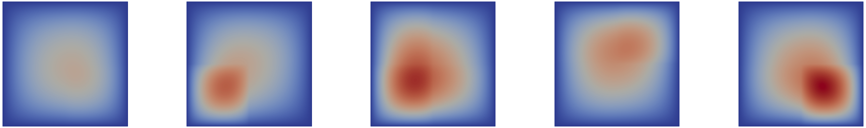
Model order reduction for parametrized problems

Motivation – Parametrized problems

Given:

- Model described by a partial differential equation depending on varying parameters
- Numerical method to solve the PDE for individual parameter values (Full order model)





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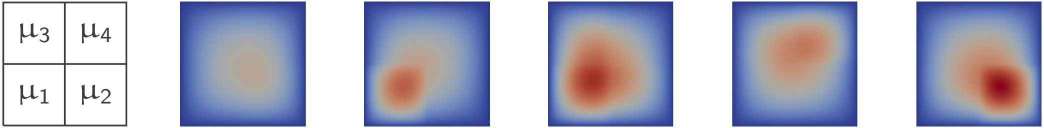

Challenges:

Multi-query context

- Solutions for many different parameter values required, e.g.
  - Parameter studies
  - Optimization

Real-time context

- Solution for specific parameter needed very quickly
- Possibly limited computational resources

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Multi-query context

- Solutions for many different parameter values required, e.g.
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Real-time context

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- Possibly limited computational resources

Main concept:

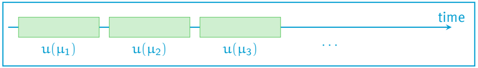
- Build a reduced order model only once

Offline phase

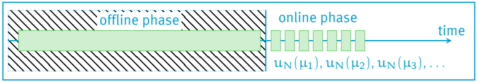
- Compute reduced solutions fast for many different parameter values

Online phase

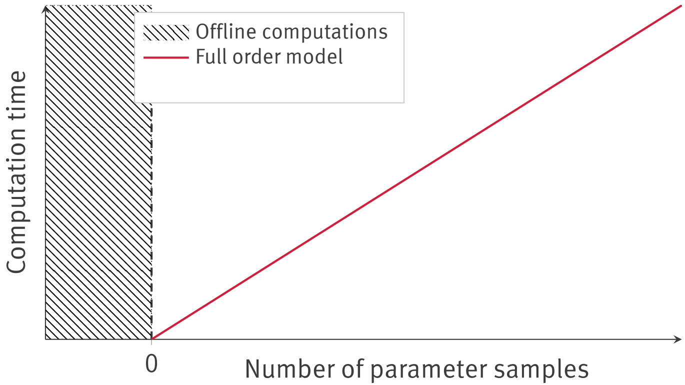
Multi-query scenario using FOM



Multi-query scenario using ROM



Multi-query scenarios
Offline-online decomposition



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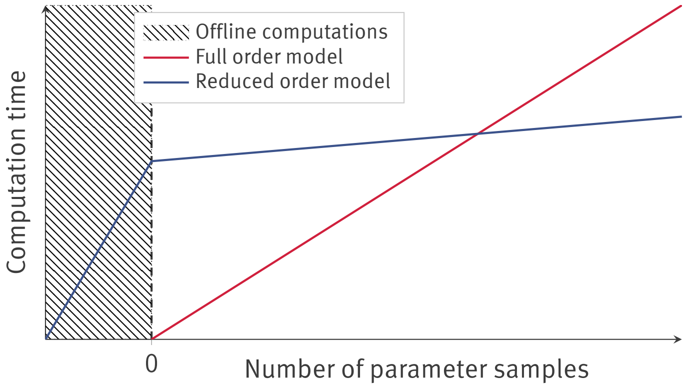

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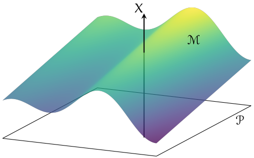
Reduced basis methods

The reduced basis model
Approximation theory

- Denote by $\mu \in \mathcal{P} \subset \mathbb{R}^p$ the parameter value.
- For each $\mu \in \mathcal{P}$, the solution to the PDE is denoted by $u(\mu) \in X$, where the solution space X is infinite or high dimensional.
- Define the solution manifold $\mathcal{M} \coloneqq \{u(\mu) : \mu \in \mathcal{P}\} \subset X$.

Assumption: $\mathcal{M}$ can be approximated well by a low dimensional linear space $X_N \subset X$.



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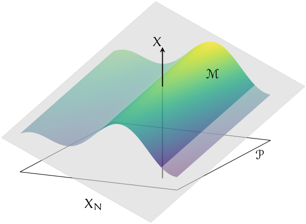
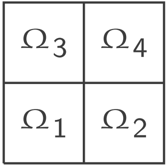


Reduced basis (RB) method:

- Precompute snapshots $u(\mu_i), i = 1, \ldots, n$
- Build $X_N \subseteq \mathrm{span}\{u(\mu_i) : i = 1, \ldots, n\}$
- Compute reduced solutions $u_N(\mu) \in X_N$ as approximation to $u(\mu) \in \mathcal{M}$



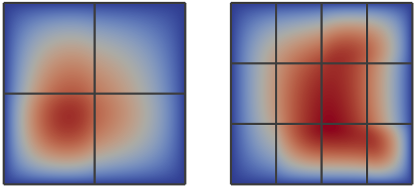
- Stationary (steady-state) heat conduction
- Domain Ω consists of blocks Ω_i, $i = 1, \dots, p$, of materials with different heat conductivity $\mu_i \in [\mu_{\min}, \mu_{\max}]$
- Parameter values define different conductivities, i.e. $\mathcal{P} := [\mu_{\min}, \mu_{\max}]^p$

Partial differential equation:

$$\begin{aligned} -\nabla \cdot \left(\kappa(x;\mu)\nabla u(x;\mu)\right) &= 1, \quad x \in \Omega, \\ u(x;\mu) &= 0, \quad x \in \Gamma = \partial\Omega, \end{aligned}$$

with heat-conductivity

$$\kappa(x;\mu) := \sum_{q=1}^{p} \mu_q \chi_{\Omega_q}(x).$$



Weak formulation

Problem

For $\mu \in \mathcal{P}$ we seek the solution $u(\mu) \in X$ of

$$a(u(\mu), v; \mu) = f(v; \mu) \qquad \text{for all } v \in X.$$

Weak formulation

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Abstract formulation

X real separable Hilbert space

Thermal block problem

$X \coloneqq H_0^1(\Omega)$

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Abstract formulation

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$\mathcal{P} \subset \mathbb{R}^p$ parameter domain

Thermal block problem

$$X := H_0^1(\Omega)$$

$$\mathcal{P} := [\mu_{\min}, \mu_{\max}]^p$$

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Abstract formulation

X real separable Hilbert space

$\mathcal{P} \subset \mathbb{R}^p$ parameter domain

$a(\cdot\,, \cdot\,; \mu) \colon X \times X \to \mathbb{R}$ bilinear form

Thermal block problem

$$X \coloneqq H_0^1(\Omega)$$

$$\mathcal{P} \coloneqq [\mu_{\min}, \mu_{\max}]^p$$

$$a(u, v; \mu) \coloneqq \int_\Omega \kappa(x; \mu) \nabla u(x; \mu) \cdot \nabla v(x)\, dx$$

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Abstract formulation	**Thermal block problem**
X real separable Hilbert space	$X \coloneqq H_0^1(\Omega)$
$\mathcal{P} \subset \mathbb{R}^p$ parameter domain	$\mathcal{P} \coloneqq [\mu_{\min}, \mu_{\max}]^p$
$a(\,\cdot\,, \,\cdot\,; \mu)\colon X \times X \to \mathbb{R}$ bilinear form	$a(u, v; \mu) \coloneqq \int_\Omega \kappa(x; \mu) \nabla u(x; \mu) \cdot \nabla v(x)\, dx$
$f(\,\cdot\,; \mu)\colon X \to \mathbb{R}$ linear functional	$f(v; \mu) \coloneqq \int_\Omega v(x)\, dx$

Galerkin projection

- Approximation in a subspace $\bar{X} \subset X$ of X.
- Galerkin projection: $\bar{u}(\mu) \in \bar{X}$ is given by

$$a(\bar{u}(\mu), v; \mu) = f(v; \mu) \qquad \text{for all } v \in \bar{X}.$$

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- **Standard numerical analysis:**
  - X infinite dimensional space (e.g. Sobolev space)
  - $\bar{X} = X^h$ discrete space with high dimension (e.g. finite element space)

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- **Standard numerical analysis:**
  - X infinite dimensional space (e.g. Sobolev space)
  - $\bar{X} = X^h$ discrete space with high dimension (e.g. finite element space)
- **Reduced basis method:**
  Usually: Assume that X^h is “good enough” so that the discretization error can be neglected.
  - $X = X^h$ high dimensional “truth” space
  - $\bar{X} = X_N$ low dimensional reduced basis space

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Reduced solution

Given an RB space $X_N \subset X$, define the reduced solution $u_N(\mu) \in X_N$ such that

$$a(u_N(\mu), v_N; \mu) = f(v_N; \mu) \quad \text{for all } v_N \in X_N.$$

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Standard theory for Galerkin projections:

- Well-posedness: Lax-Milgram (continuity and coercivity is directly inherited from X to X_N)

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Standard theory for Galerkin projections:

- Well-posedness: Lax-Milgram (continuity and coercivity is directly inherited from X to X_N)
- A priori error estimate using Céa's lemma:

$$\|u(\mu) - u_N(\mu)\|_X \leqslant \frac{\gamma(\mu)}{\alpha(\mu)} \inf_{v_N \in X_N} \|u(\mu) - v_N\|_X$$

  - Quasi-optimality of the solution
  - Approximation error determined by approximation quality (w.r.t. $\mathcal{M}$) of the reduced space X_N
  - Reproduction of solutions: $u(\mu) \in X_N \implies u_N(\mu) = u(\mu)$

Computation of the reduced solution

- Given: Reduced basis $\Phi_N = \{\varphi_1, \dots, \varphi_N\} \subset X$ such that $X_N = \operatorname{span}\{\varphi_1, \dots, \varphi_N\}$.

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Computation of the reduced solution

- Given: Reduced basis $\Phi_N = \{\varphi_1, \dots, \varphi_N\} \subset X$ such that $X_N = \operatorname{span}\{\varphi_1, \dots, \varphi_N\}$.
- For a parameter $\mu \in \mathcal{P}$, compute system matrix

$$\mathbf{A}_N(\mu) \coloneqq [a(\varphi_j, \varphi_i; \mu)]_{i,j=1}^N \in \mathbb{R}^{N \times N}$$

  and right-hand side vector

$$\mathbf{f}_N(\mu) \coloneqq [f(\varphi_i; \mu)]_{i=1}^N \in \mathbb{R}^N.$$

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- Solve small linear system

$$\mathbf{A}_N(\mu)\mathbf{u}_N(\mu) = \mathbf{f}_N(\mu)$$

  for reduced coefficients $\mathbf{u}_N(\mu) \in \mathbb{R}^N$.

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- Solve small linear system

$$\mathbf{A}_N(\mu)\mathbf{u}_N(\mu) = \mathbf{f}_N(\mu)$$

  for reduced coefficients $\mathbf{u}_N(\mu) \in \mathbb{R}^N$.
- **Issue:** Assembling $\mathbf{A}_N(\mu)$ requires high dimensional computations!

Assumption: We have

$$a(u, v; \mu) = \sum_{q=1}^{Q_a} \theta_q^a(\mu) a_q(u, v) \qquad \text{for all } u, v \in X, \mu \in \mathcal{P},$$

$$f(v; \mu) = \sum_{q=1}^{Q_f} \theta_q^f(\mu) f_q(v) \qquad \text{for all } v \in X, \mu \in \mathcal{P}$$

with “small” Q_a, Q_f.

- Fulfilled for the thermal block problem.
- Necessary for efficient offline-online decomposition.
- Can be approximated for non-affine problems (empirical interpolation).

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Offline-online decomposition

- **Offline phase:**
  - Generate reduced space X_N with basis $\{\varphi_i\}_{i=1}^N$.

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Offline-online decomposition

- **Offline phase:**
  - Generate reduced space X_N with basis $\{\varphi_i\}_{i=1}^N$.
  - Precompute parameter-independent quantities:

$$\begin{aligned} \mathbf{A}_{N,q} &\coloneqq [a_q(\varphi_j,\varphi_i)]_{i,j=1}^N \in \mathbb{R}^{N\times N}, && q=1,\dots,Q_a, \\ \mathbf{f}_{N,q} &\coloneqq [f_q(\varphi_i)]_{i=1}^N \in \mathbb{R}^N, && q=1,\dots,Q_f. \end{aligned}$$

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- **Online phase:**
  - Assemble parameter-dependent system:

$$\mathbf{A}_N(\mu) = \sum_{q=1}^{Q_a} \theta_q^a(\mu)\,\mathbf{A}_{q,N}, \qquad \mathbf{f}_N(\mu) = \sum_{q=1}^{Q_f} \theta_q^f(\mu)\,\mathbf{f}_{q,N}.$$

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  - Reduced solution:
    1. Solve $\mathbf{A}_N(\mu)\mathbf{u}_N(\mu) = \mathbf{f}_N(\mu)$ with $\mathbf{u}_N(\mu) = [\alpha_i(\mu)]_{i=1}^N \in \mathbb{R}^N$.
    2. Set $u_N(\mu) = \sum_{i=1}^N \alpha_i(\mu)\,\varphi_i$.

A posteriori error estimation

- Consider the error $e(\mu) \coloneqq u(\mu) - u_N(\mu) \in X$.
- Define the residual $r(\,\cdot\,;\mu) \in X'$ via

$$r(v;\mu) \coloneqq f(v;\mu) - a(u_N(\mu), v; \mu) \qquad \text{for } v \in X.$$

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- Error-residual relation:

$$a(e(\mu), v;\mu) = r(v;\mu) \qquad \text{for all } v \in X.$$

- A posteriori error bound:

$$\|u(\mu) - u_N(\mu)\|_X \leqslant \Delta(\mu) \coloneqq \frac{\|r(\,\cdot\,;\mu)\|_{X'}}{\alpha(\mu)}.$$

  - X infinite dim. (standard FEM theory): $\|\cdot\|_{X'}$ is not computable
  - $X = X^h$ (finite dim.): $\|\cdot\|_{(X^h)'}$ is computable

Weak greedy algorithm

- **Main idea:** Use $X_N = \text{span}\{u(\mu_i)\}$, but choose “the right” snapshots $u(\mu_i)$ to incorporate into the reduced space.
- “Greedy” procedure: Iteratively choose worst approximated snapshot and add it to the reduced basis.
- Use a posteriori error estimator to determine next parameter for which to compute the snapshot.

Basis generation

Weak greedy algorithm

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Proper orthogonal decomposition

- Widely used method for "compression" of data sets.
- In other contexts known as *Karhunen-Loève Decomposition*, *Principal Component Analysis* or *Truncated Singular Value Decomposition*.
- **Main idea:** Represent a given (large) data set by a smaller orthonormal basis which is optimal in a least-squares sense.

Machine learning and model order reduction

Surrogates based on machine learning

Learning the map from parameters to reduced coefficients [Hesthaven/Ubbiali'18]

- Recall: Representation of the reduced solution in a reduced basis $\varphi_1, \dots, \varphi_N \in X$:

$$u_N(\mu) = \sum_{i=1}^{N} \boxed{\alpha_i(\mu)}\, \varphi_i$$

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- **Observation:** Only coefficients are required to characterize the reduced solution!

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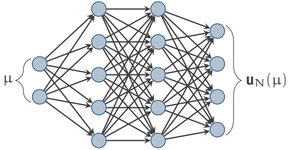
- Hesthaven/Ubbiali'18: Approximate coefficients $\mathbf{u}_N(\mu) = [\alpha_i(\mu)]_{i=1}^N$ by machine learning:



$$\tilde{\alpha}_i(\mu) \approx \alpha_i(\mu) \quad \Longrightarrow \quad \tilde{u}_N(\mu) \coloneqq \sum_{i=1}^{N} \tilde{\alpha}_i(\mu)\, \varphi_i \approx u_\mu^N(\mu)$$

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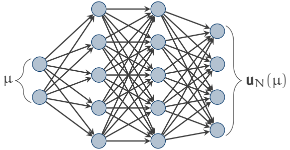

$$\tilde{\alpha}_i(\mu) \approx \alpha_i(\mu) \qquad \Longrightarrow \qquad \tilde{u}_N(\mu) := \sum_{i=1}^{N} \tilde{\alpha}_i(\mu)\, \varphi_i \approx u_\mu^N(\mu)$$

- Error estimation possible using the error estimator of the RB model ($\tilde{u}_N(\mu) \in X_N$).

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Adaptive model hierarchies

Adaptive model hierarchies[1]

Breaking the traditional offline-online splitting

- Availability of different models with different advantages and disadvantages, such as
  - Full order model
  - Reduced basis model
  - Machine learning surrogate
  - ...

[1] Joint work with Bernard Haasdonk, Mario Ohlberger, Felix Schindler and Tizian Wenzel

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- **Idea:** Train surrogates adaptively and try to leverage their advantages.

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- **Idea:** Train surrogates adaptively and try to leverage their advantages.

$\Longrightarrow$ Combine all available models in an adaptive and certified hierarchy!

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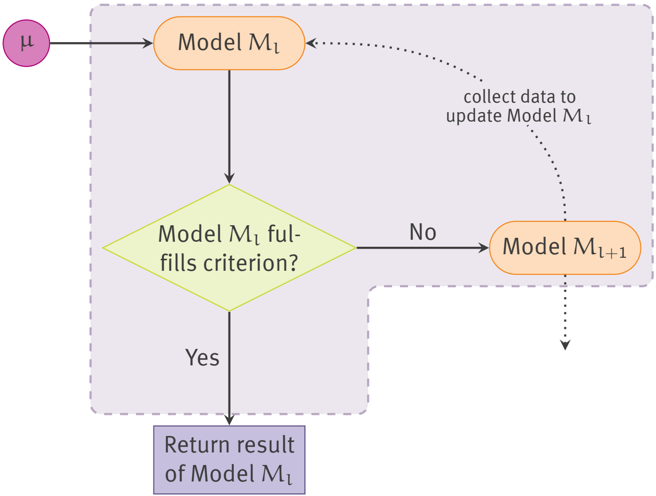
Description of the main building block
Multi-fidelity assumptions

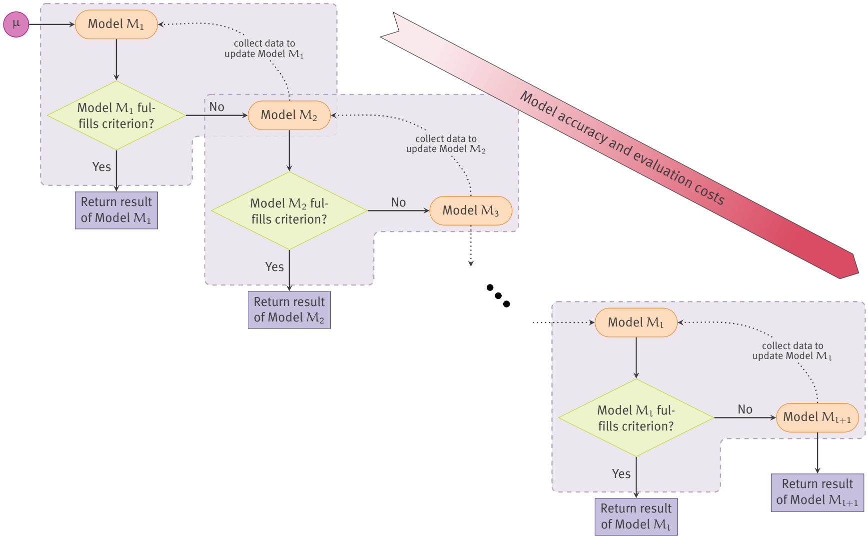
Assumptions:

- Model M_l can be solved faster than Model M_{l+1}
- Model M_{l+1} is more accurate than Model M_l
- Model M_l can be improved by means of information from Model M_{l+1}



General definition of an adaptive model hierarchy

Combination of several components in multiple stages



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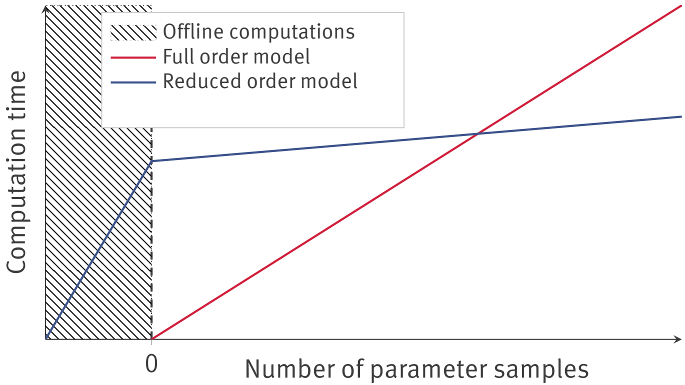
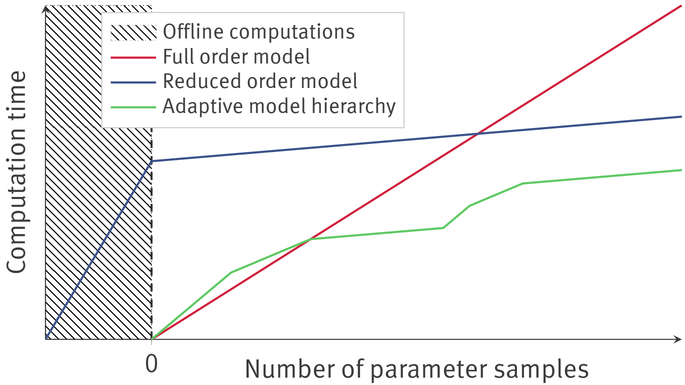
Adaptive model hierarchy for parametrized problems

Adaptivity vs. offline-online decomposition



Adaptive model hierarchy for parametrized problems
Adaptivity vs. offline-online decomposition



Live Demo

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Thank you for your attention!

Links to papers on
adaptive model hierarchies

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