Universität Münster

Adaptive Model Hierarchies for Multi-Query Scenarios

MATHMOD 2025 – Minisymposium on “Recent Advances in Model Order Reduction and Data-driven Modelling”

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MM Mathematics Münster Cluster of Excellence

Motivation and general construction

Motivation for model hierarchies

Full order model, reduced model, machine learning surrogate, ...

- Availability of different models with different advantages and disadvantages, such as
  - Full order model
  - Projection-based reduced model
  - Machine learning surrogate
  - ...

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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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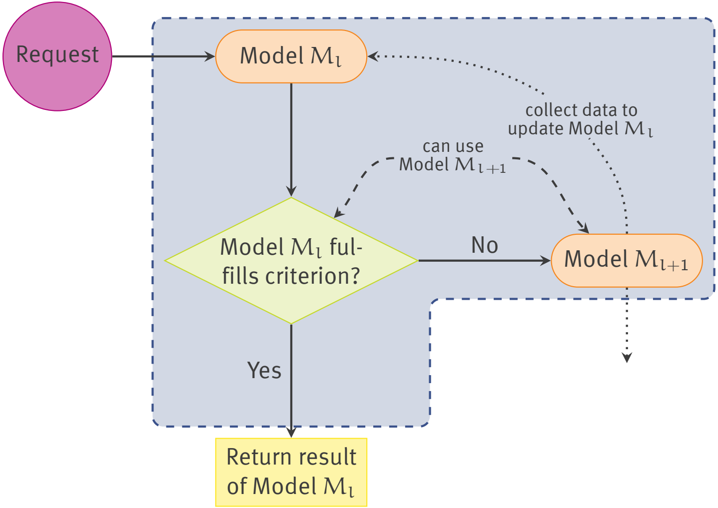
Description of the main building block

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}

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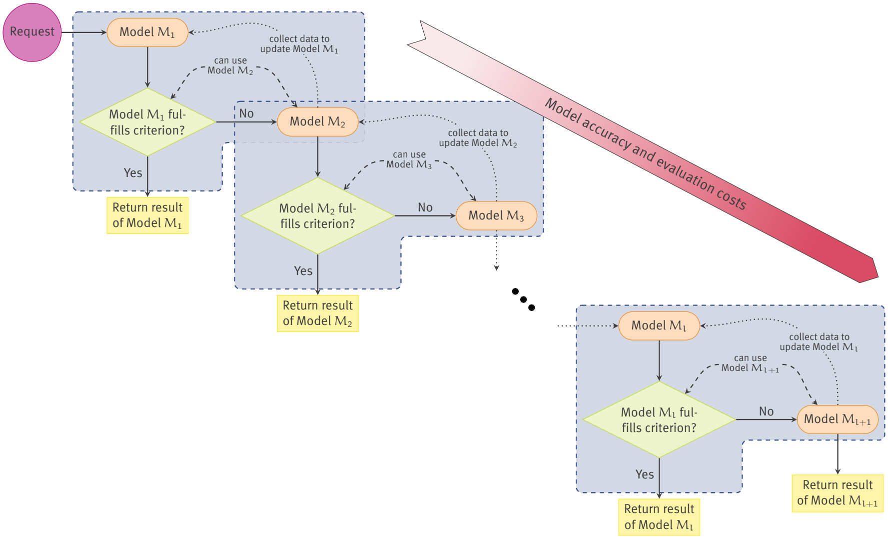
General definition of an adaptive model hierarchy

Combination of several components in multiple stages



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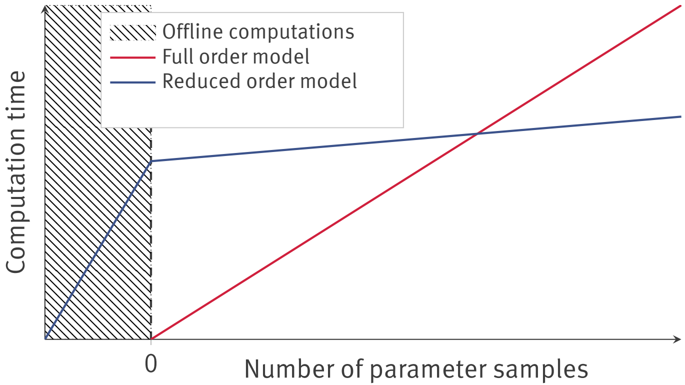
Adaptive model hierarchy for parametrized problems

Adaptivity vs. offline-online decomposition



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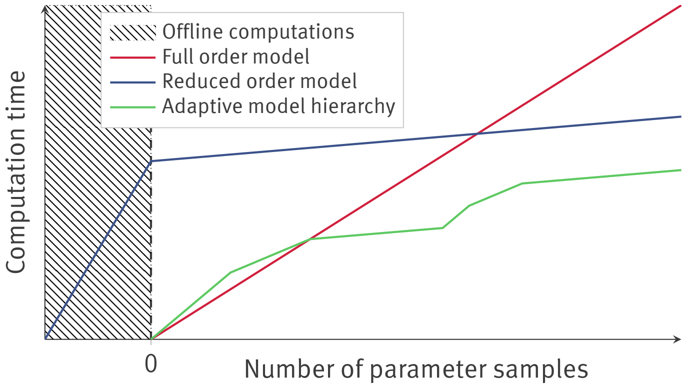


Examples and numerical results

Example 1 – Parametrized parabolic PDEs

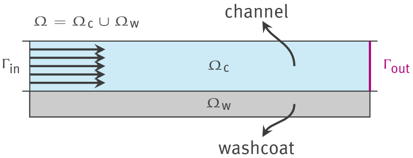
Problem setting – PDE-constrained optimization

Advection-diffusion-reaction equation with parameter $\mu = (\mathrm{Da}, \mathrm{Pe}) \in \mathcal{P} = [0.01, 10] \times [9, 11]$:

$$\partial_t u_\mu - \nabla \cdot (\kappa \nabla u_\mu) + \mathrm{Pe}\, \nabla \cdot (\vec{b}\, u_\mu) + \mathrm{Da}\, \chi_{\Omega_w} u_\mu = 0 \qquad \text{in } (0,T) \times \Omega,$$

$$(\kappa \nabla u_\mu) \cdot n_{\partial\Omega} = 0 \qquad \text{on } \Gamma_{\text{out}},$$

$$\Phi(\mu)(t) = \fint_{\Gamma_{\text{out}}} u_\mu(t)\, ds.$$



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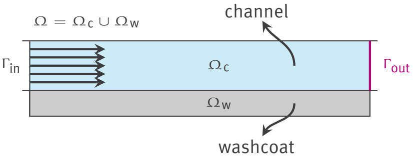

PDE-constrained optimization problem:

$$\min_{\mu \in \mathcal{P}} \mathcal{J}(\mu) := \|\hat{\Phi} - \Phi_{\mathrm{adapt}}(\mu)\|_{L^\infty([0,T])}.$$

Here, $\hat{\Phi} = \Phi(\hat{\mu})$ is a desired break-through curve with $\hat{\mu} = (5.005, 10)$ and $\Phi_{\mathrm{adapt}}(\mu)$ is the output of the adaptive model hierarchy.

M_3: Full order model (FOM)

+ arbitrarily accurate solutions (serves as the reference for error estimators)
– very slow for fine discretizations or many time steps

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Example 1 – Parametrized parabolic PDEs
Three-stage hierarchy

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M_2: Reduced basis ROM (RB-ROM)

- ▶ reduced basis model based on Galerkin projection
- ▶ construction of reduced basis using HaPOD
- + faster than FOM
- + residual-based a posteriori error estimator
- – slow iterative time stepping
- – requires solving dense linear system in each time step

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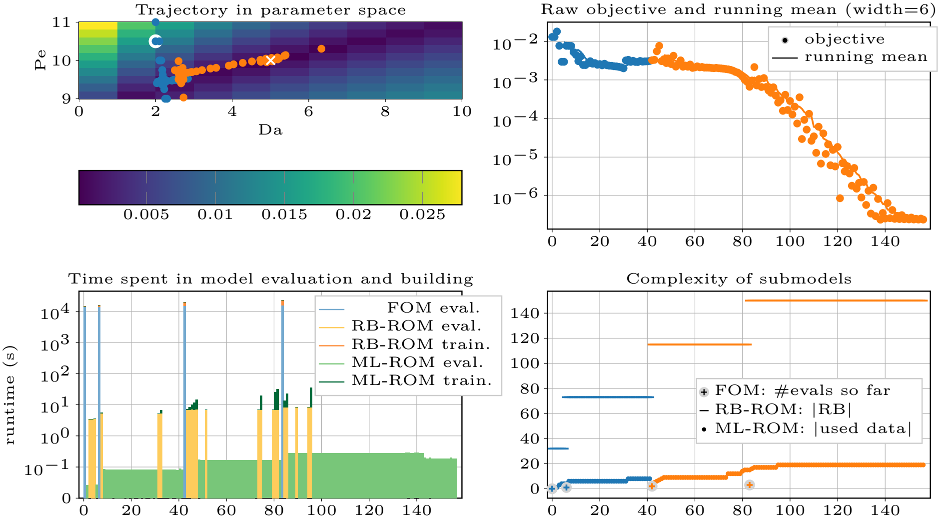
$\mathcal{M}_1$: Machine learning (ML-ROM)

- approximates reduced coefficients of the RB-ROM
- based on the same reduced basis as the RB-ROM

+ faster than RB-ROM
+ parallel evaluation for many time instances possible
+ allows to reuse a posteriori error estimator of RB-ROM
– requires training of machine learning algorithm

Numerical results



Examples 2 and 3

Optimal control of (parametric) systems

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Optimal control of (parametric) systems

Please come to my poster for examples 2 and 3!

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Thank you for your attention!

If you would like to discuss in more detail, come to my poster!

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Example 2 – Parametrized optimal control problems

Problem setting – Monte Carlo simulations

$$\min_{u \in L^2([0,T];U)} \quad \frac{1}{2}\left[\underbrace{\| y_\mu(T) - y_\mu^T \|_Y^2}_{\substack{\text{deviation from target}\\ \text{at final time}}} + \underbrace{\int_0^T \langle u(t), R(t)u(t)\rangle_{U\times U'}\,dt}_{\text{control energy}}\right],$$

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$$\min_{u\in L^2([0,T];U)} \quad \frac{1}{2}\Bigg[\underbrace{\left\| y_\mu(T) - y_\mu^T \right\|_Y^2}_{\text{deviation from target at final time}} + \underbrace{\int_0^T \langle u(t), R(t)u(t)\rangle_{U\times U'}\, dt}_{\text{control energy}}\Bigg],$$

$$\text{such that} \quad \begin{cases} E\frac{d}{dt}x_\mu(t) = A(\mu;t)x_\mu(t) + B(\mu;t)u(t) & \text{for } t\in[0,T], \\ y_\mu(t) = Cx_\mu(t) & \text{for } t\in[0,T], \\ x_\mu(0) = x_\mu^0, & \text{(initial data)} \end{cases}$$

Target output: $y_\mu^T = Cx_\mu^T$

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Theorem (K./Renelt'24)

The optimal state x_μ^**, control* u_μ^* *and adjoint* φ_μ^* *can be characterized as solution to the system:*

$$E\frac{d}{dt}x_\mu(t) = A(\mu;t)x_\mu(t) + B(\mu;t)u_\mu(t), \qquad \textit{(state equation)}$$

$$u_\mu(t) = -R(t)^{-1}B(\mu;t)^*\varphi_\mu(t), \qquad \textit{(control equation)}$$

$$-E_{ad}\frac{d}{dt}\varphi_\mu(t) = A(\mu;t)^*\varphi_\mu(t), \qquad \textit{(adjoint equation)}$$

for almost all $t \in [0,T]$ *with initial condition* $x_\mu(0) = x_\mu^0$ *and terminal condition*

$$\mathcal{R}_X E^*\varphi_\mu(T) = M\left(x_\mu(T) - x_\mu^T\right),$$

where $\mathcal{R}_X \colon X \to X'$ *is the Riesz map,* $E_{ad} \coloneqq \mathcal{R}_X E^* \mathcal{R}_X^{-1}$ *and* $M \coloneqq C^*\mathcal{R}_Y C$.

Example 2 – Parametrized optimal control problems
Linear system for optimal final time adjoints

Lemma (K./Renelt'24)

The optimal final time adjoint $\varphi_\mu^*(T) \in X$ *solves the linear system*

$$\boxed{S(\mu)\varphi_\mu^*(T) = g(\mu)}$$

where

- $S(\mu)$ *involves solving high-dimensional parametric systems,*
- $g(\mu)$ *is a parameter-dependent right hand side.*

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$\Longrightarrow$ Costly to solve!

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$$S(\mu)\varphi_\mu^*(T) = g(\mu) \qquad \Longleftrightarrow \qquad \varphi_\mu^*(T) = \arg\min_{p \in X} \| g(\mu) - S(\mu)p \|_X^2$$

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Example 2 – Parametrized optimal control problems

Four-stage hierarchy

M_4: FOM

Optimal final time adjoint

$$\varphi_\mu^*(T) = \operatorname*{arg\,min}_{p \in X} \| g(\mu) - S(\mu)p \|_X^2$$

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Primal and adjoint systems

$$E \frac{d}{dt} x_\mu(t) = A(\mu; t) x_\mu(t) + B(\mu; t) u_\mu(t)$$

$$-E_{ad} \frac{d}{dt} \varphi_\mu(t) = A(\mu; t)^* \varphi_\mu(t)$$

Four-stage hierarchy

[Lazar/Zuazua'16, K./Lazar/Molinari'24]

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$$\varphi_\mu^*(T) = \arg\min_{p \in X} \| g(\mu) - S(\mu)p \|_X^2$$

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M_3: RB-ROM

Least-squares on reduced subspace

$$\tilde{\varphi}_\mu^N = \arg\min_{p \in X^N} \| g(\mu) - S(\mu)p \|_X^2$$

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[Haasdonk/Ohlberger'11]

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Reduced primal and adjoint systems

$$\hat{E}_{pr} \frac{d}{dt} \hat{x}_\mu(t) = \hat{A}_{pr}(\mu; t) \hat{x}_\mu(t) + \hat{B}_{pr}(\mu; t) u_\mu(t)$$

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$$\tilde{\varphi}_\mu^N = \underset{p \in X^N}{\arg\min} \| g(\mu) - S(\mu)p \|_X^2$$

[Fabrini/Iapichino/Volkwein'18, K./Renelt'24]

M_2: F-ROM

Combination of RB-ROM and system reduction

$$\hat{\varphi}_\mu^{N,\text{red}} = \underset{p \in X^N}{\arg\min} \left\| \hat{g}(\mu) - \hat{S}(\mu)p \right\|_X^2$$

Primal and adjoint systems

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M_1: ML-F-ROM

Approximate $\hat{\varphi}_\mu^{N,\text{red}}$ as a function of the parameter using machine learning

Primal and adjoint systems

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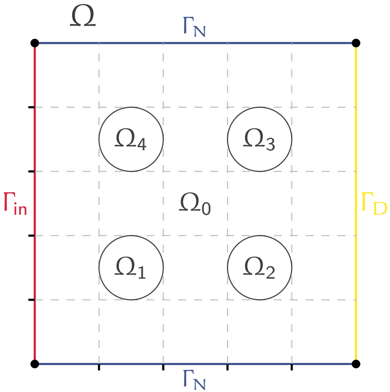
Problem setting



- Heat equation as state system:

$$\partial_t \theta(t;\mu) - \nabla \cdot (\sigma(t;\mu)\nabla\theta(t;\mu)) = 0 \qquad \text{in } \Omega,$$
$$\sigma(t;\mu)\nabla\theta(t;\mu)\cdot\vec{n} = u(t) \qquad \text{on } \Gamma_{in},$$

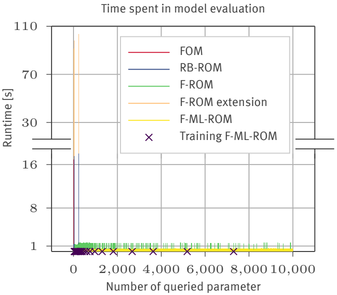
  \+ homogeneous initial, Dirichlet and Neumann conditions

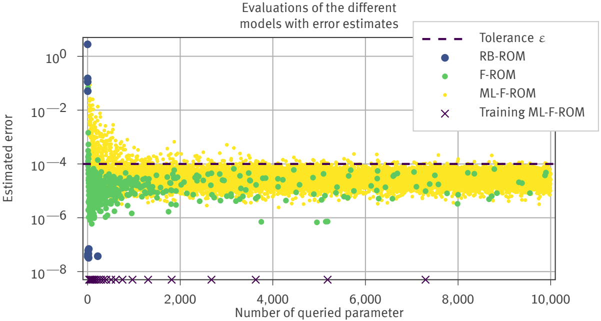
- Parametric and time-dependent diffusivity σ
- Output quantities: Average temperature in the four cookies
- Target state: Prescribed average temperature in all cookies

Example 2 – Parametrized optimal control problems

Numerical results

Model	Number of solves	Number of error estimates	Total time for error est. and solving [s]	Average time for error est. and solving per solve [s]
FOM	4	—	304.95	76.24
RB-ROM	12	16	234.56	19.55
F-ROM	437	453	450.39	1.03
ML-F-ROM	9,547	10,000	5,136.95	0.54





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For more details, see:

- B. Haasdonk, H. Kleikamp, M. Ohlberger, F. Schindler, and T. Wenzel. *A new certified hierarchical and adaptive RB-ML-ROM surrogate model for parametrized PDEs, (2023)*. SIAM J. Sci. Comput., 45(3), A1039–A1065.
- T. Wenzel, B. Haasdonk, H. Kleikamp, M. Ohlberger, and F. Schindler. *Application of Deep Kernel Models for Certified and Adaptive RB-ML-ROM Surrogate Modeling, (2024)*. Proceeding of the LSSC 2023 Conference.
- H. Kleikamp. *Application of an adaptive model hierarchy to parametrized optimal control problems, (2024)*. Proceedings of the Conference Algoritmy, 66–75.
- H. Kleikamp and L. Renelt. *Two-stage model reduction approaches for the efficient and certified solution of parametrized optimal control problems, (2024)* arXiv preprint.

The source code for the papers is available open source:

- Parametrized parabolic PDEs
  - Three-stage hierarchy: `https://github.com/ftschindler/paper-2022-certified-adaptive-RB-ML-ROM-hierarchy`
- Parametrized optimal control problems
  - Three-stage hierarchy: `https://doi.org/10.5281/zenodo.10669855`
  - Four-stage hierarchy: `https://doi.org/10.5281/zenodo.13652744`