Universität Münster

Certified machine learning for model order reduction of parametrized problems

Ulysseus Research Workshop on Mathematics in Machine Learning

Hendrik Kleikamp (University of Münster); based on projects with Bernard Haasdonk, Martin Lazar, Cesare Molinari, Mario Ohlberger, Lukas Renelt, Felix Schindler and Tizian Wenzel.

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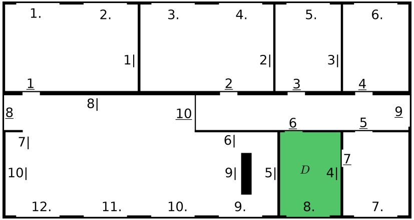
Parametrized problems – Some examples

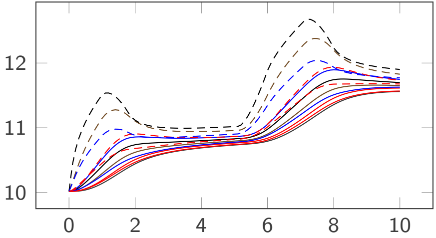
Parametrized problems

Parabolic partial differential equations: Heating of a building

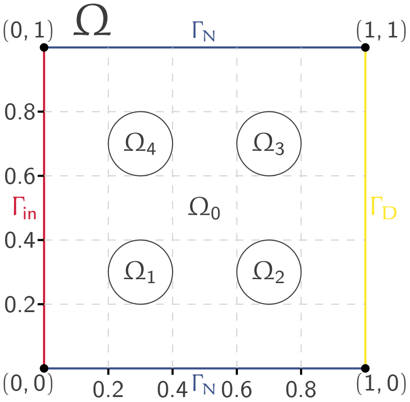
- Parametrized diffusion coefficient and right-hand side (heaters, walls, doors)
- Average temperature in the childcare room D as output
- Goal: Monte Carlo estimation of expectation and variance of output quantity over the parameter space



Outputs for different parameters:



- Parametrized state equation (cookie dough)
- Control acting on the inflow boundary
- Average temperature in cookies as output quantities
- Goal: Find control minimizing sum of distance to a target output and control energy



Computational domain

Reduced basis methods and residual-based error estimates

Projection-based model order reduction

- Linear parametrized problem (after suitable discretization etc.):

$$\boxed{A(\mu)\, y_\mu = f(\mu)} \qquad \longleftarrow \text{ large linear system}$$

where the solution $y_\mu \in X$ is high-dimensional.

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  where the solution $y_\mu \in X$ is high-dimensional.

- Idea: Replace X by low-dimensional subspace $X^N \subset X$ and project system onto X^N:

$$\boxed{\hat{A}(\mu)\,y_\mu^N = \hat{f}(\mu)} \qquad \longleftarrow \quad \text{small linear system}$$

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where the reduced solution $y_\mu^N \in X^N$ comes from a low-dimensional subspace.

- Representation of the reduced solution in a reduced basis $x_1, \dots, x_N \in X^N$:

$$y_\mu^N = \sum_{i=1}^{N} \alpha_i(\mu)\, x_i$$

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A posteriori error estimation

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- Consider residual of the original system for an approximate solution $\tilde{y} \in X^N$:

$$\eta_\mu(\tilde{y}) \coloneqq c \cdot \underbrace{\| A(\mu)\tilde{y} - f(\mu) \|}_{\text{defect in the linear system}}$$

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- Key observation: The estimate works for all $\tilde{y} \in X^N$ and not only for a reduced solution!

Machine learning in model order reduction

Surrogates building on a reduced basis reduced model

- Issue with reduced model: Reduced operator $\hat{A}(\mu)$ and right-hand side $\hat{f}(\mu)$ need to be assembled and reduced system has to be solved!

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Surrogates building on a reduced basis reduced model

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- Observation: Only coefficients are required to characterize the reduced solution!
- Idea [Hesthaven/Ubbiali'18]: Approximate coefficients by machine learning:

$$\tilde{\alpha}_i(\mu) \approx \alpha_i(\mu) \qquad \Longrightarrow \qquad \tilde{y}_\mu^N = \sum_{i=1}^{N} \tilde{\alpha}_i(\mu) x_i \approx y_\mu^N$$

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Certification using a posteriori error estimates

Apply error estimator η_μ of the reduced basis model to machine learning approximation:

$$\| \tilde{y}_\mu^N - y_\mu \| \leqslant \eta_\mu(\tilde{y}_\mu^N)$$

$\Longrightarrow$ Error certification for the machine learning result!

Certification using a posteriori error estimates

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$$\| \tilde{y}_\mu^N - y_\mu \| \leqslant \eta_\mu(\tilde{y}_\mu^N)$$

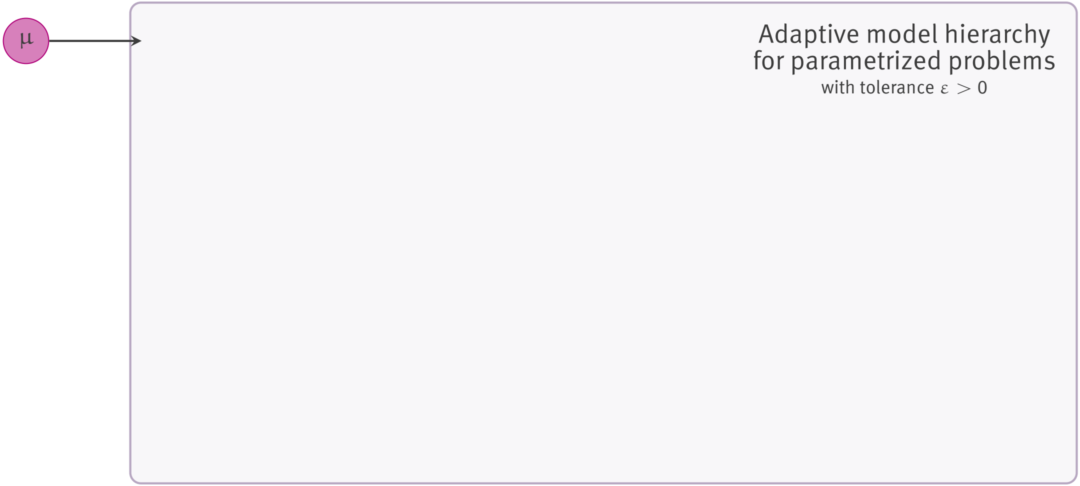
$\Longrightarrow$ Error certification for the machine learning result!

- Different machine learning techniques are applicable, such as deep neural networks, kernel methods, Gaussian process regression, etc.
- Error estimate still holds due to connection to reduced basis model.
- Reduced coefficients serve as training data (no high-dimensional solutions required to obtain training data once reduced basis is built).

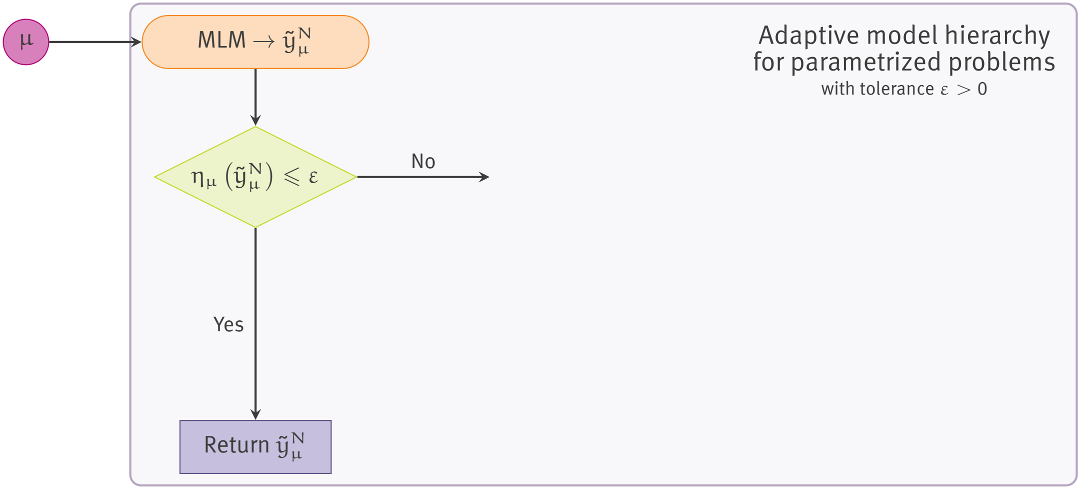
Adaptive model hierarchies combining multiple models

Adaptive model hierarchy for parametrized problems

Three stages: Reduced basis and machine learning models



Adaptive model hierarchy for parametrized problems
Three stages: Reduced basis and machine learning models



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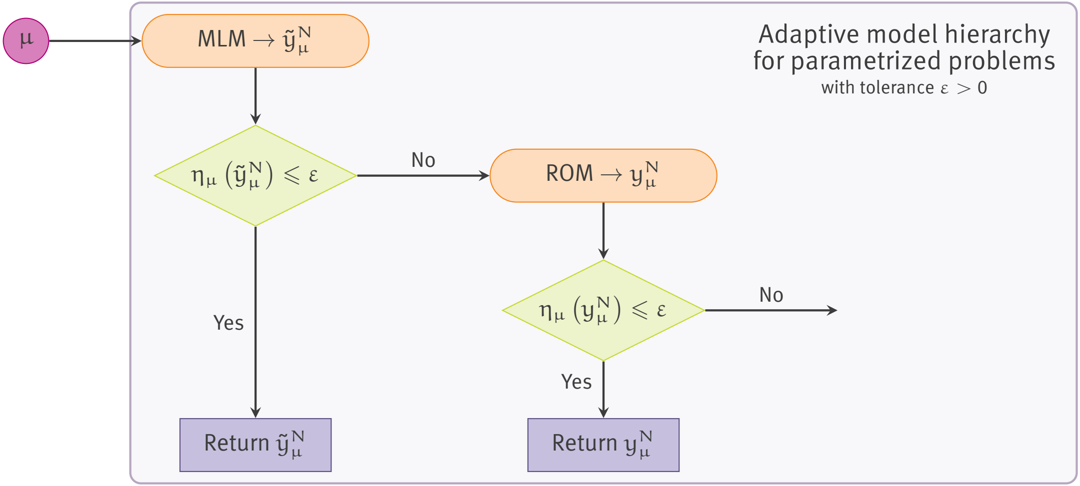
Adaptive model hierarchy for parametrized problems

Three stages: Reduced basis and machine learning models



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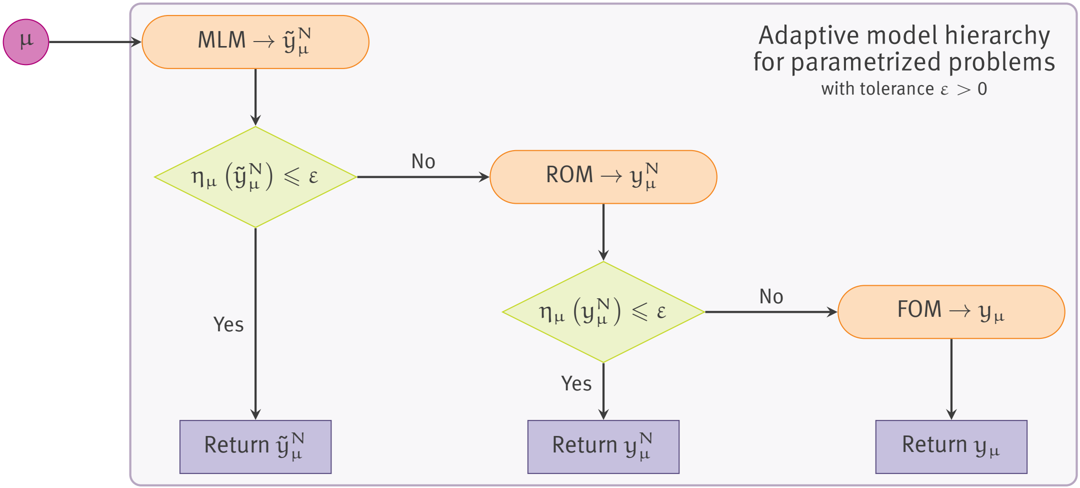
Adaptive model hierarchy for parametrized problems

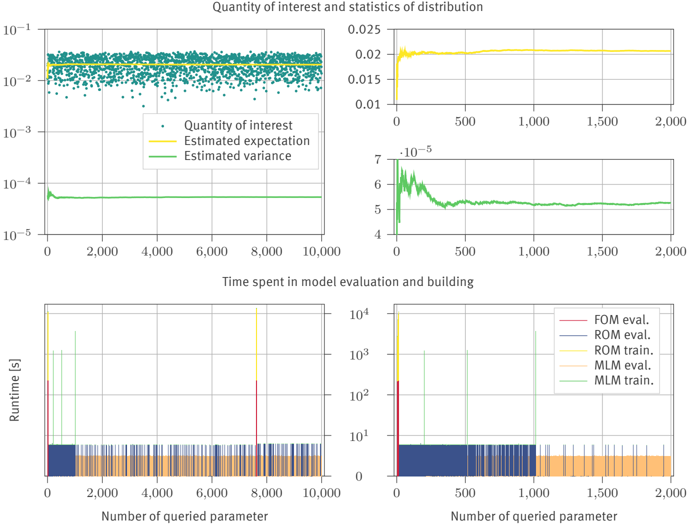
Three stages: Reduced basis and machine learning models



Numerical experiments and results

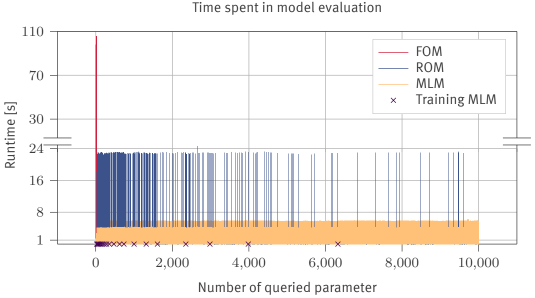
Parabolic partial differential equations: Heating of a building

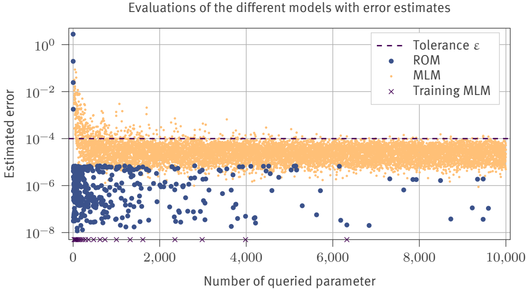
Results of the model hierarchy



Optimal control problems: Baking cookies
Results of the model hierarchy

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	–	330.31	82.58
ROM	412	416	7,653.35	18.58
MLM	9,584	10,000	56,776.25	5.92





Thank you for your attention!

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