Universität Münster

Adaptive model hierarchies for solving parametrized optimal control problems in multi-query scenarios

Seminar Talk – Università di Genova

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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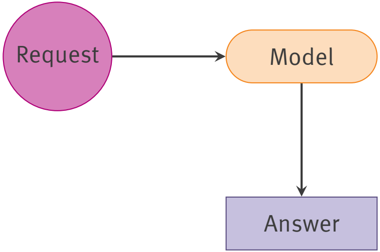
MM Mathematics Münster Cluster of Excellence

Adaptive model hierarchies

What is a model?

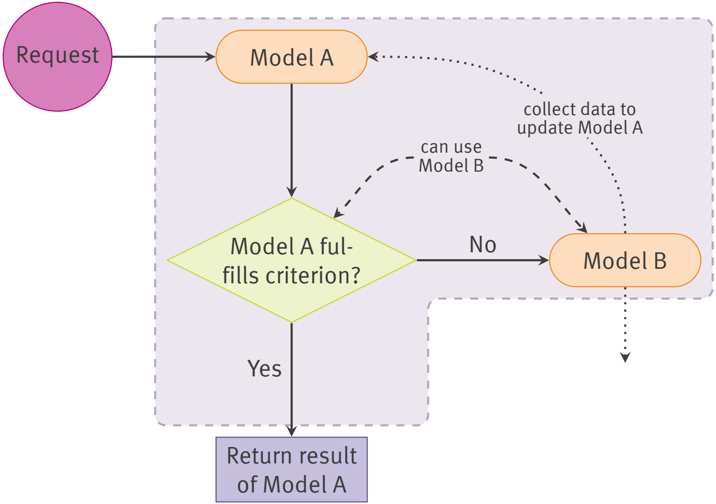
Assumptions:

- A model can handle requests and produces associated outputs.
- There is a notion of accuracy of a model and its output.
- There is a notion of computational effort or speed of a model.



Model hierarchies for multi-query problems [Haasdonk et al.'23]

The main building block

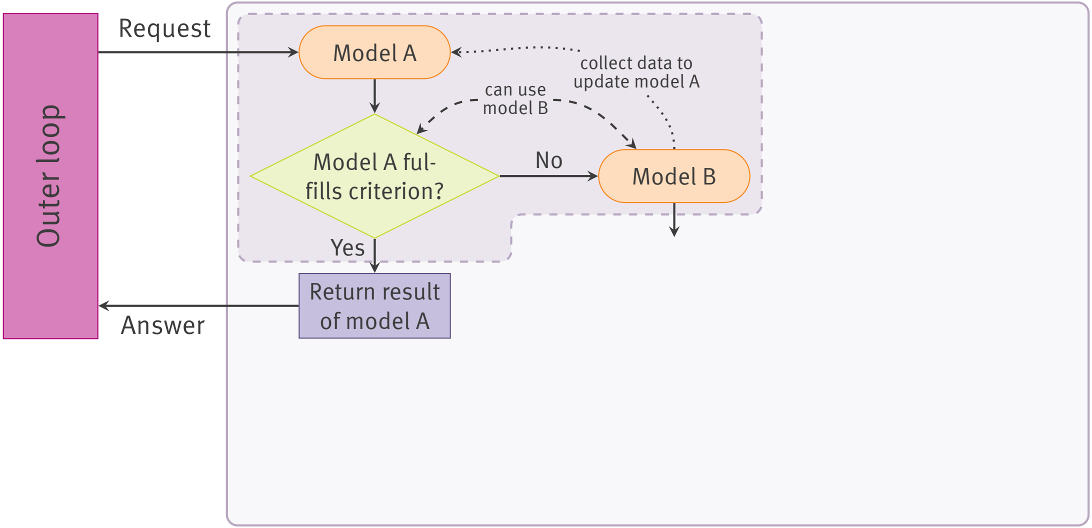


Assumptions:

- Model A can be solved faster than Model B.
- Model B is more accurate than Model A.
- Model A can be improved by means of information from Model B.

Model hierarchies for multi-query problems

Application within an outer loop



Model hierarchies for multi-query problems
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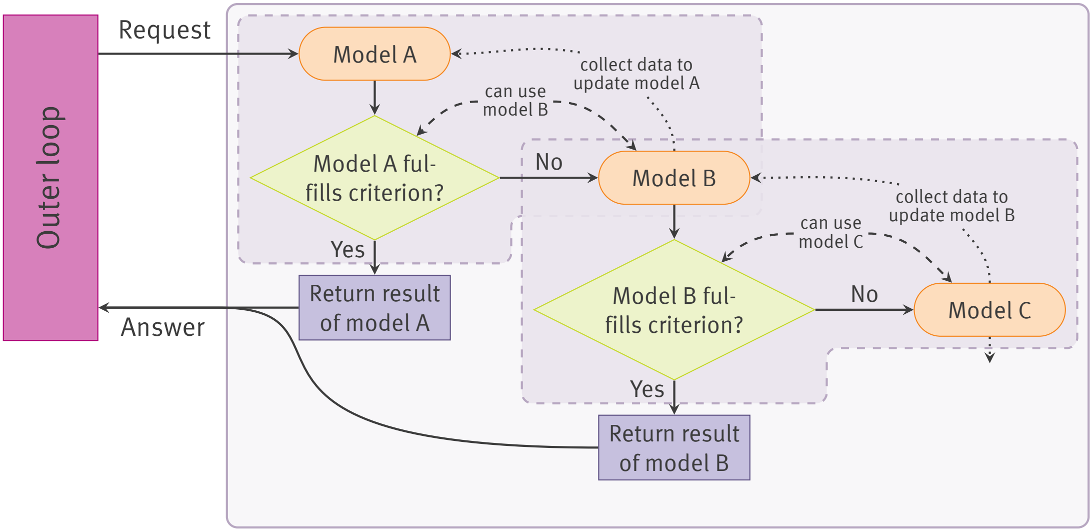

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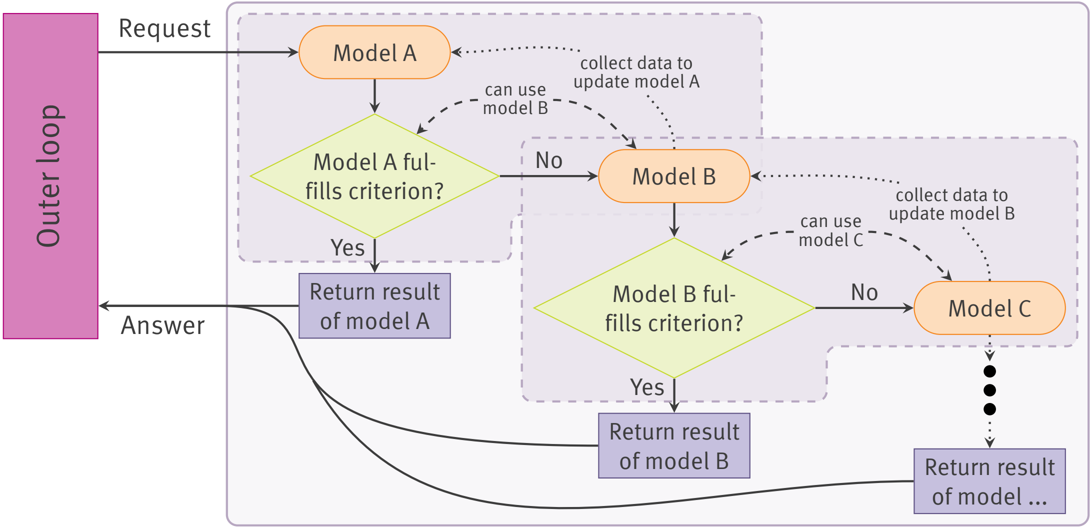

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Model hierarchies for multi-query problems
Key points and ideas

- No offline training phase required

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Model hierarchies for multi-query problems
Key points and ideas

- No offline training phase required
- Certified answers to all requests
- Returns sufficiently accurate results as fast as possible
- Adaptive refinement of models using data that is computed anyways

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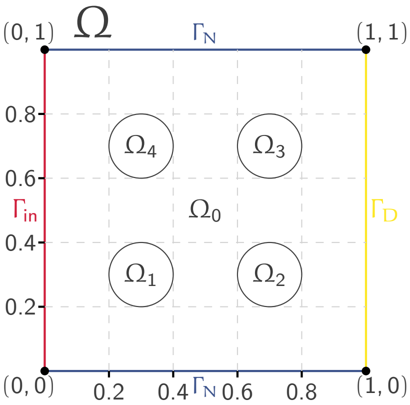
Parametrized optimal control problems

The cookie baking example [Rave/Saak'21]

Problem setting



Computational domain

- State equation:

$$\partial_t \theta(t,\xi;\mu) - \nabla \cdot (\sigma(t,\xi;\mu)\nabla\theta(t,\xi;\mu)) = 0$$
$$\sigma(t,\xi;\mu)\nabla\theta(t,\xi;\mu)\cdot\vec{n}(\xi) = u(t), \quad \xi \in \Gamma_{in},$$

\+ homogeneous initial, Dirichlet and Neumann conditions

The cookie baking example [Rave/Saak'21]

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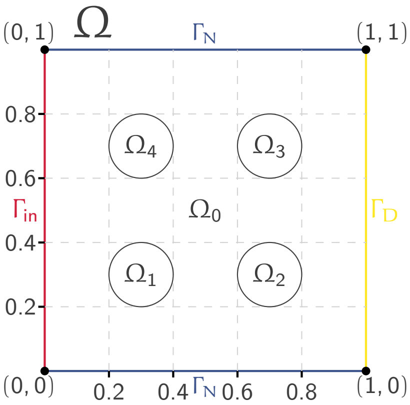

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+ homogeneous initial, Dirichlet and Neumann conditions

- Parametric and time-dependent diffusivity:

$$\sigma(t,\xi;\mu) := \begin{cases} 14\cdot(t-0.25)^2 + 0.125, & \text{for } \xi \in \Omega_0, \\ \mu_1, & \text{for } \xi \in \Omega_1 \cup \Omega_3, \\ \mu_2, & \text{for } \xi \in \Omega_2 \cup \Omega_4. \end{cases}$$

The cookie baking example [Rave/Saak'21]

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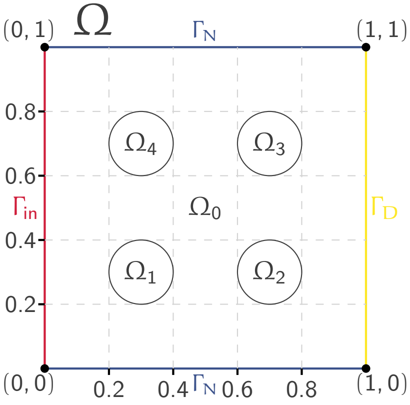

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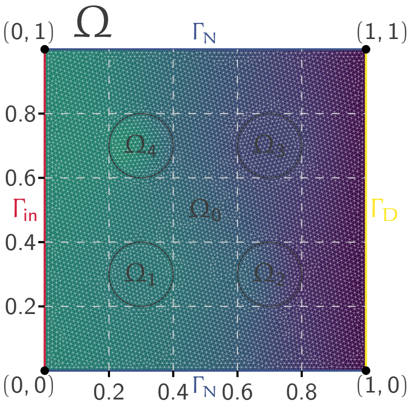
- Output quantities:

$$y_i(t;\mu) := \frac{1}{|\Omega_i|}\int_{\Omega_i}\theta(t,\xi;\mu)\,d\xi \qquad \text{for } i=1,\dots,4.$$

The cookie baking example
Problem setting

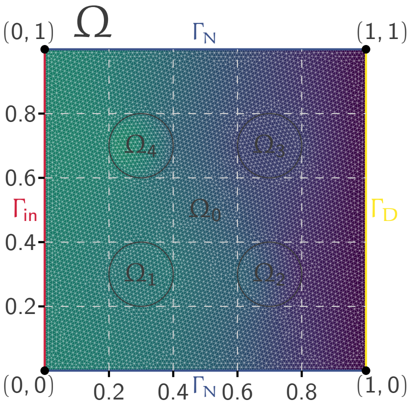


Optimal solution at time $t = 1$ for $\mu = (100, 0.1)$

- Discretized state system:

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

The cookie baking example
Problem setting



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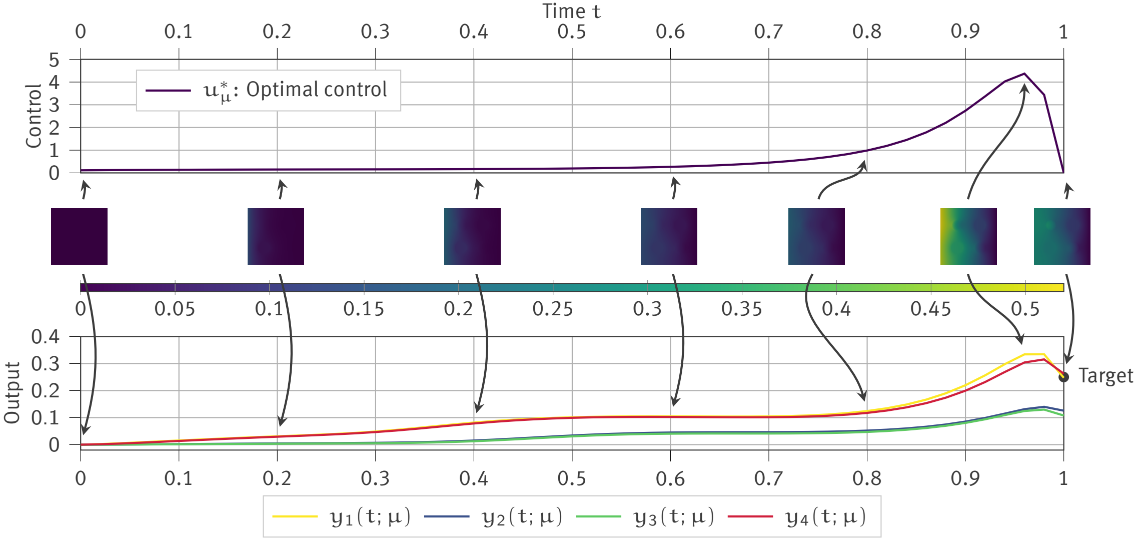
- Optimal control problem:

$$\min_{u\in G} \frac{1}{2}\left[\underbrace{\left\| C\left(x_\mu(T) - x_\mu^T\right)\right\|^2}_{\text{deviation of output}} + \underbrace{\int_0^T \langle u(t), R(t)u(t)\rangle \, dt}_{\text{control energy}}\right]$$

The cookie baking example

Optimal control and evolution of output for $\mu = (100, 0.1)$



Overview of the involved (reduced) models

Components applied in the hierarchy

- **Main goal:** Solve optimal control problem fast for many parameters!

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Different models available:

- Full order model
- Reduced basis reduced order model [K./Lazar/Molinari'24]
- Machine learning surrogate [Hesthaven/Ubbiali'18]

Details on the machine learning surrogate

- Builds on the reduced basis model

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- Uses the same underlying reduced space

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- Connection to reduced basis model allows to apply the same a posteriori error estimator

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Details on the machine learning surrogate

- Builds on the reduced basis model
- Uses the same underlying reduced space
- Approximates the map from parameter to reduced coefficients
- Connection to reduced basis model allows to apply the same a posteriori error estimator
- Different supervised machine learning methods are applicable, for instance neural networks, kernel methods, Gaussian process regression

Summary and comparison of the models

Full order model (FOM)

Pros:

- arbitrarily accurate solutions (serve as reference)

Cons:

- very slow when dealing with large systems

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Machine learning model (MLM)

Pros:

- faster than ROM
- reuses error estimator of the ROM

Cons:

- typically requires lots of training data and hyper-parameter tuning

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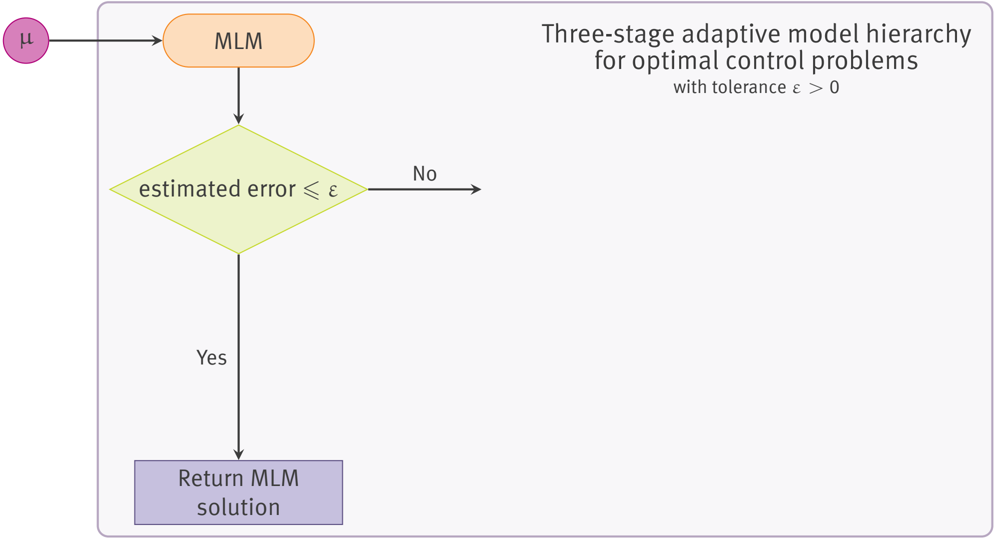
Three-stage model hierarchy for optimal control problems



Three-stage model hierarchy for optimal control problems

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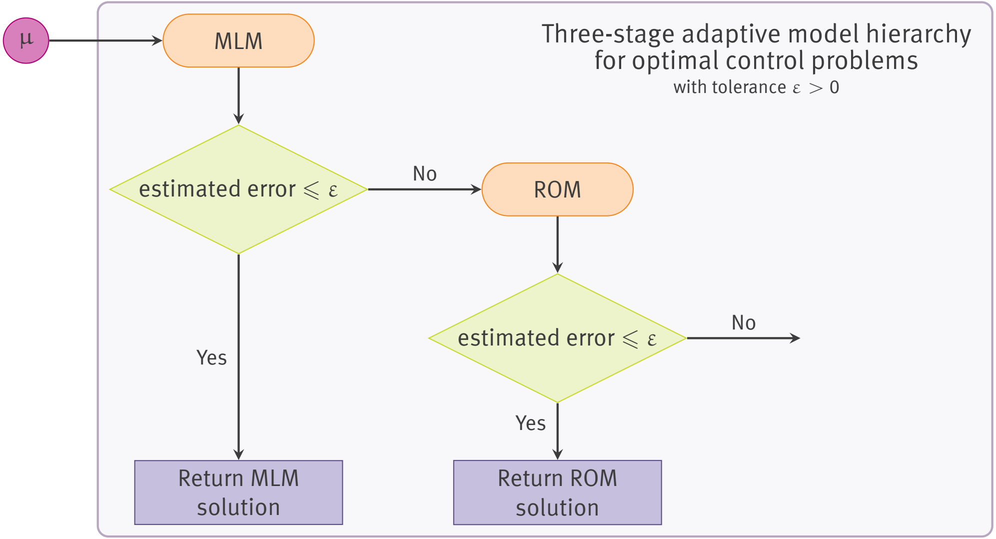

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Three-stage model hierarchy for optimal control problems

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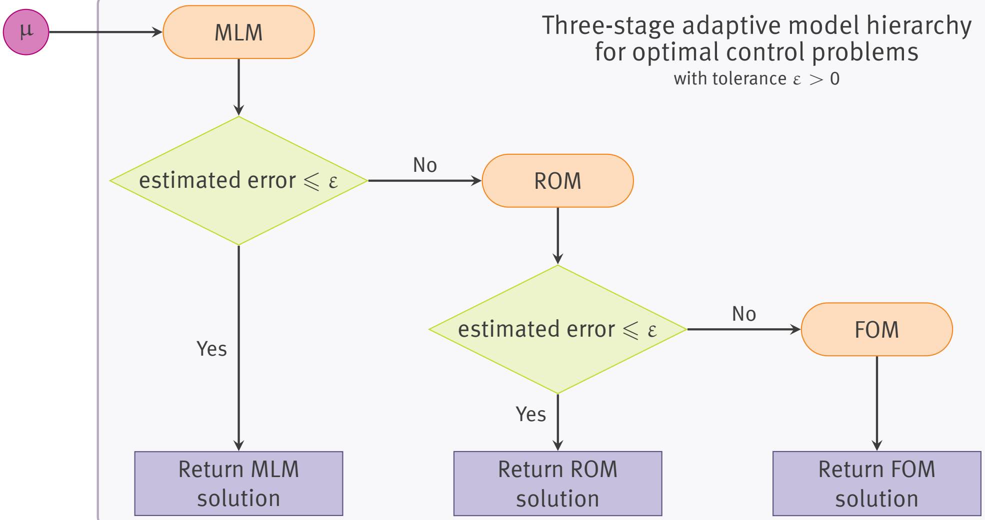


Three-stage adaptive model hierarchy for optimal control problems

with tolerance $\varepsilon > 0$

Numerical experiment

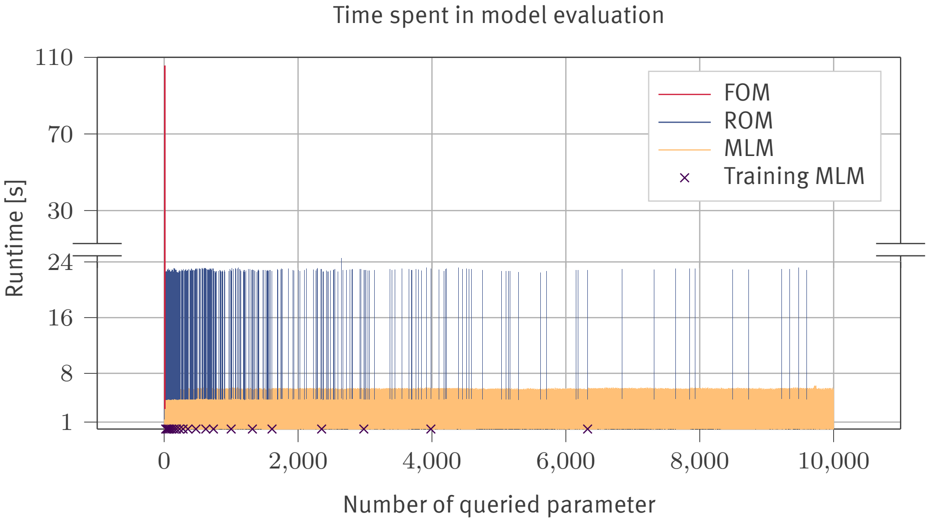
Numerical results: Applying the model hierarchy

The cookie baking example revisited

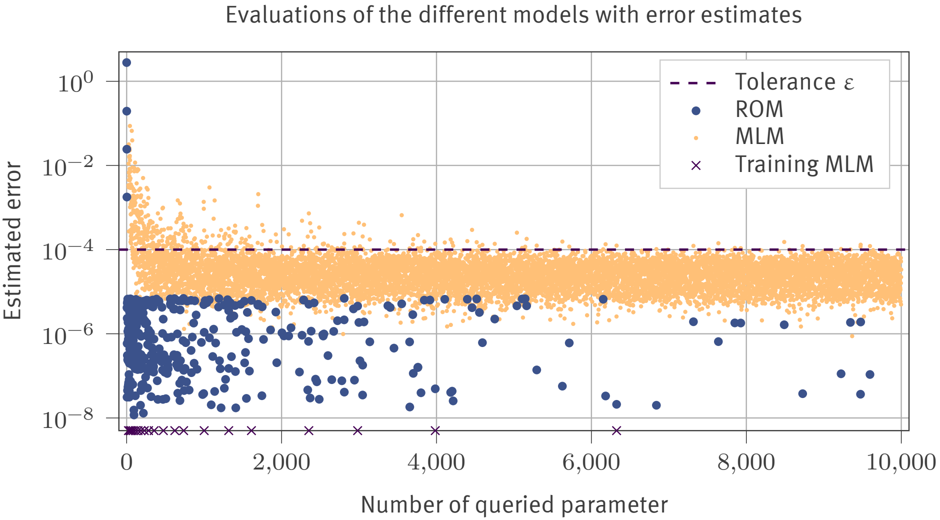
Model	Number of solves	Number of error estimates	Total time for error est. and solving [s]	Average time for error est. and solving per solve [s]
FOM	4	—	330.31	82.58
ROM	412	416	7,653.35	18.58
MLM	9,584	10,000	56,776.25	5.92

Numerical results: Applying the model hierarchy

The cookie baking example revisited



Numerical results: Applying the model hierarchy
The cookie baking example revisited



Outlook

- Extension of the reduced order models to other optimal control problems ($\rightarrow$ ongoing discussions with Cesare)

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- Application of different machine learning techniques

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- Application of different machine learning techniques
- Construction of adaptive model hierarchies in other contexts

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- Extension of the reduced order models to other optimal control problems
  ($\longrightarrow$ ongoing discussions with Cesare)
- Application of different machine learning techniques
- Construction of adaptive model hierarchies in other contexts
- Develop strategies for dealing with changing tolerances when querying the model hierarchy

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).

H. Kleikamp, M. Lazar, and C. Molinari.
Be greedy and learn: efficient and certified algorithms for parametrized optimal control problems, (2024).

H. Kleikamp.
Application of an adaptive model hierarchy to parametrized optimal control problems, (2024).

H. Kleikamp and L. Renelt.
Two-stage model reduction approaches for the efficient and certified solution of parametrized optimal control problems, (2024).

The source code for the papers is available open source:

- Greedy and learn: `https://doi.org/10.5281/zenodo.8188417`
- Three-stage hierarchy: `https://doi.org/10.5281/zenodo.10669855`
- Fully reduced models: `https://doi.org/10.5281/zenodo.13382950`
- Four-stage hierarchy: `https://doi.org/10.5281/zenodo.13652744`

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Thank you for your attention!

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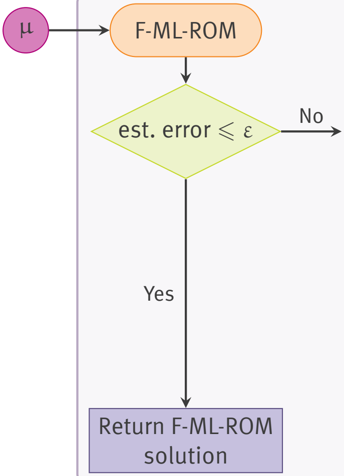
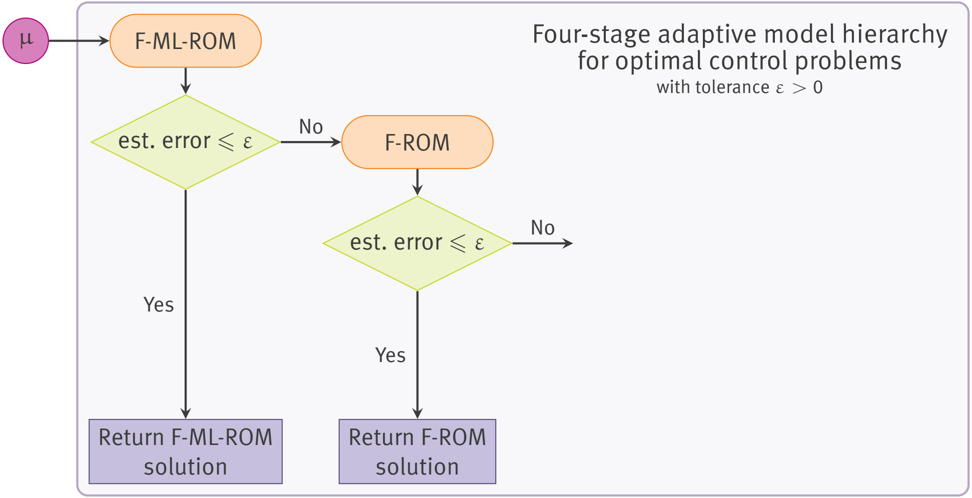
Four-stage model hierarchy for optimal control problems



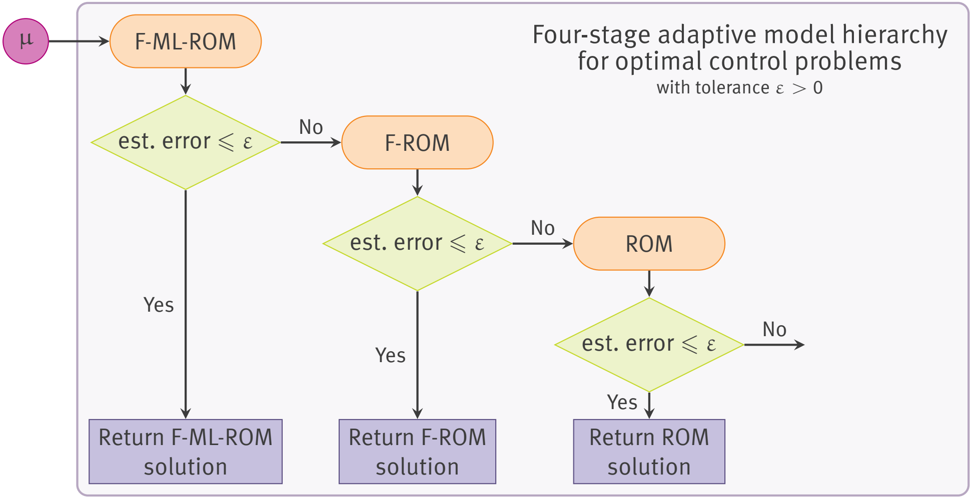
Four-stage adaptive model hierarchy for optimal control problems

with tolerance $\varepsilon > 0$

Four-stage model hierarchy for optimal control problems



Four-stage model hierarchy for optimal control problems



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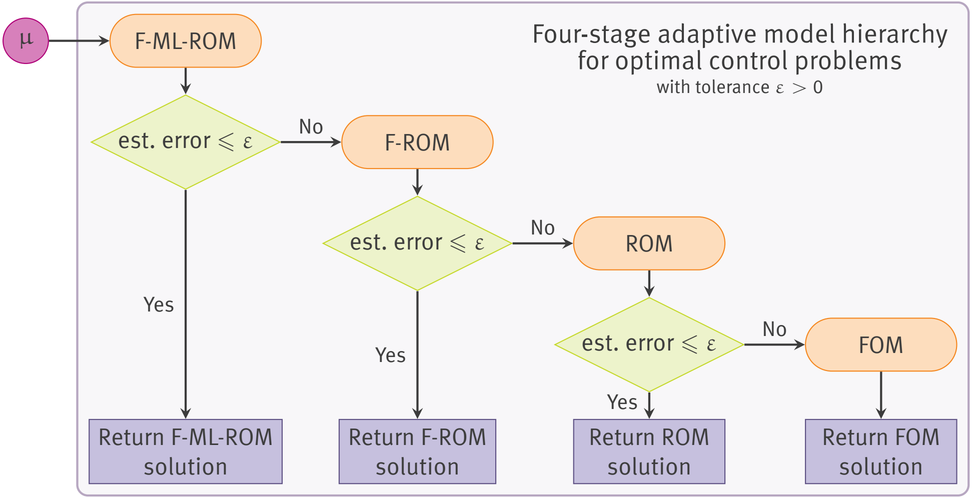

Numerical results: Applying the four-stage model hierarchy

The cookie baking example revisited

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
ROM	12	16	234.56	19.55
F-ROM	437	453	450.39	1.03
F-ML-ROM	9,547	10,000	5,136.95	0.54

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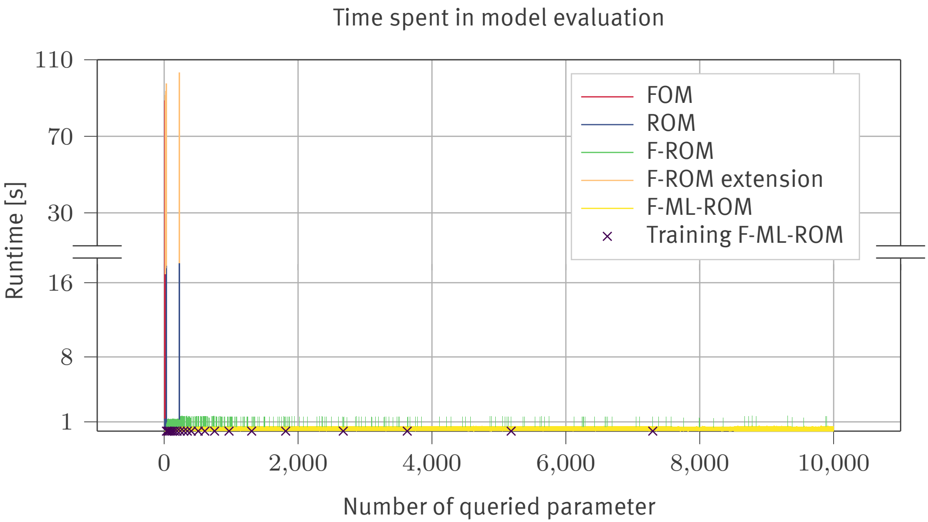
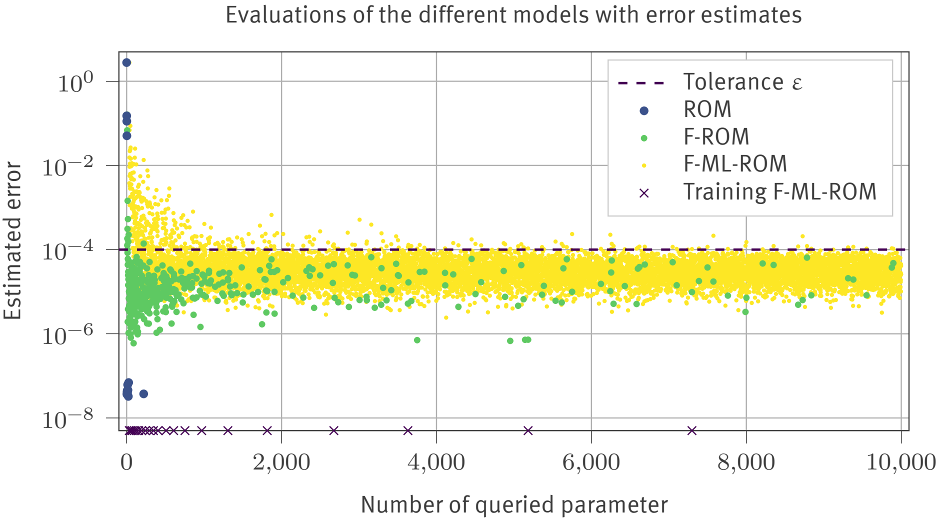
Numerical results: Applying the four-stage model hierarchy

The cookie baking example revisited



Numerical results: Applying the four-stage model hierarchy

The cookie baking example revisited



Parametrized optimal control problems
General setting

For a parameter $\mu \in \mathcal{P}$, solve

$$\min_{u \in G} \quad \frac{1}{2}\Bigg[\underbrace{\| C\left(x_\mu(T) - x_\mu^T\right) \|^2}_{\text{deviation of output}} + \underbrace{\int_0^T \langle u(t), R(t)u(t)\rangle \, dt}_{\text{control energy}}\Bigg],$$

$$\text{such that} \quad E\frac{d}{dt}x_\mu(t) = A(\mu)x_\mu(t) + B(\mu)u(t) \quad \text{for almost all } t \in [0,T],$$
$$x_\mu(0) = x_\mu^0 \in \mathbb{R}^n,$$

where

$$x_\mu \colon [0,T] \to \mathbb{R}^n, \qquad u \colon [0,T] \to \mathbb{R}^m, \qquad C \in \mathbb{R}^{l \times n}$$
$$E \in \mathbb{R}^{n \times n}, \qquad A(\mu) \in \mathbb{R}^{n \times n}, \qquad B(\mu) \in \mathbb{R}^{n \times m}.$$

The matrix $R(t) \in \mathbb{R}^{m \times m}$ is assumed to be positive-definite for almost all $t \in [0,T]$.

Optimality system

Theorem [K./Renelt'24]

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

$$\begin{aligned} E\frac{d}{dt}x_\mu(t) &= A(\mu;t)x_\mu(t) + B(\mu;t)u_\mu(t), \\ u_\mu(t) &= -R(t)^{-1}B(\mu;t)^\top \varphi_\mu(t), \\ -E^\top \frac{d}{dt}\varphi_\mu(t) &= A(\mu;t)^\top \varphi_\mu(t), \end{aligned}$$

for almost all $t \in [0, T]$ with initial respectively terminal conditions

$$x_\mu(0) = x_\mu^0, \qquad E^\top \varphi_\mu(T) = C^\top C\left(x_\mu(T) - x_\mu^T\right).$$

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Lemma [K./Renelt'24]

The optimal final time adjoint $\varphi_\mu^*(T) \in \mathbb{R}^n$ is given as the solution to the linear system

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

with

$$S(\mu) \coloneqq E^\top + C^\top C\Lambda(\mu) \in \mathbb{R}^{n\times n} \qquad \text{and} \qquad g(\mu) \coloneqq C^\top C\left(\Psi_\mu(T,0)x_\mu^0 - x_\mu^T\right) \in \mathbb{R}^n.$$

For $p \in \mathbb{R}^n$ we define

$$\Lambda(\mu)p \coloneqq -x_\mu(T)$$

as the solution of the optimality system for final time adjoint $\varphi_\mu(T) = p$ and $x_\mu(0) = 0$.

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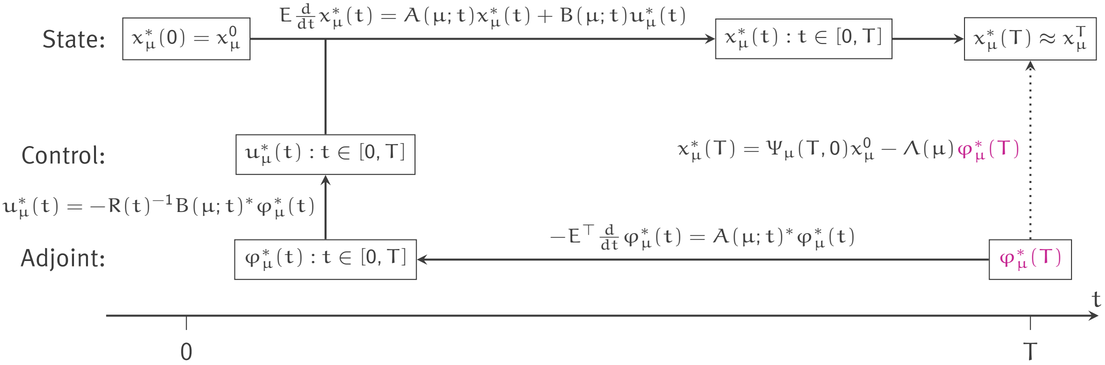
Visualization of the primal, adjoint and control equations



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Reduced order modeling

Fully reduced model
Overview of the main components

- **Main goal:** Approximate optimal final time adjoints fast!

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1. Reduced order model for optimal final time adjoints [K./Lazar/Molinari'24]
   $\rightarrow$ still involves high-dimensional computations

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   $\longrightarrow$ still involves high-dimensional computations
2. Reduced order model for dynamical systems [Haasdonk/Ohlberger'11]
   $\longrightarrow$ approximation of primal and adjoint system

Fully reduced model

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   $\rightarrow$ still involves high-dimensional computations
2. Reduced order model for dynamical systems [Haasdonk/Ohlberger'11]
   $\rightarrow$ approximation of primal and adjoint system
3. Combination of 1. and 2. to a fully reduced model [Fabrini/Iapichino/Volkwein'18],[K./Renelt'24]
   $\rightarrow$ completely independent of the high-dimensional state space

Motivation for approximation by a low-dimensional subspace

Lemma [K./Renelt'24]

For all $\mu \in \mathcal{P}$ we have

$$\varphi_\mu^*(T) = E^{-\top} C^\top C \left(\Psi_\mu(T, 0) x_\mu^0 - x_\mu^T - \Lambda(\mu) \varphi_\mu^*(T) \right) \in \operatorname{Im}(E^{-\top} C^\top C).$$

There holds in particular

$$\boxed{\dim \left(\operatorname{span} \left(\varphi_\mu^*(T) : \mu \in \mathcal{P} \right) \right) \leqslant \operatorname{rank}(C) \leqslant l} \qquad (\text{output dimension: } C \in \mathbb{R}^{l \times n}).$$

Part 1: Reduced model for final time adjoints (ROM)
Computation of the reduced solution

Given a linear N-dimensional subspace $X^N \subset \mathbb{R}^n$, approximate the optimal final time adjoint by

$$\tilde{\varphi}_\mu^N \coloneqq \operatorname*{arg\,min}_{p \in X^N} \| g(\mu) - S(\mu)p \|^2,$$

i.e. $\tilde{\varphi}_\mu^N$ is the least squares solution of the linear system.

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i.e. $\tilde{\varphi}_\mu^N$ is the least squares solution of the linear system.

Hence, we can compute $\tilde{\varphi}_\mu^N$ as the solution of

$$S(\mu)\tilde{\varphi}_\mu^N = P_{\mathcal{Y}_\mu^N}\big(g(\mu)\big),$$

where $\mathcal{Y}_\mu^N \subset \mathbb{R}^n$ is defined as

$$\mathcal{Y}_\mu^N \coloneqq S(\mu)X^N.$$

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A posteriori error estimator

For a parameter $\mu \in \mathcal{P}$ and an approximate final time adjoint $p \in \mathbb{R}^n$, define the error estimator as

$$\boxed{\eta_\mu(p) \coloneqq C_{op} \, \| \, g(\mu) - S(\mu)p \, \| \, ,}$$

where C_{op} is a constant such that

$$C_{op} \geqslant \left\| \, S(\mu)^{-1} \, \right\| .$$

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where C_{op} is a constant such that

$$C_{\mathrm{op}} \geqslant \left\| S(\mu)^{-1} \right\|.$$

Then we have

$$\boxed{\left\| \varphi_\mu^*(T) - p \right\| \leqslant \eta_\mu(p).}$$

Part 2: Reduced model for system dynamics

Definition of the reduced systems

Given matrices $V_{pr} \in \mathbb{R}^{n \times k_{pr}}$, $W_{pr} \in \mathbb{R}^{n \times k_{pr}}$, $V_{ad} \in \mathbb{R}^{n \times k_{ad}}$ and $W_{ad} \in \mathbb{R}^{n \times k_{ad}}$, we define the projected optimality system as

$$\begin{aligned} \hat{E}_{pr} \frac{d}{dt} \hat{x}_\mu(t) &= \hat{A}_{pr}(\mu; t) \hat{x}_\mu(t) + \hat{B}_{pr}(\mu; t) u(t), \\ \hat{u}_\mu(t) &= -R(t)^{-1} \hat{B}_{ad}(\mu; t)^\top \hat{\varphi}_\mu(t), \\ -\hat{E}_{ad} \frac{d}{dt} \hat{\varphi}_\mu(t) &= \hat{A}_{ad}(\mu; t)^\top \hat{\varphi}_\mu(t), \end{aligned}$$

with projected initial and terminal conditions

$$\hat{x}_\mu(0) = \hat{\bar{x}} = V_{pr}^\top \bar{x}, \qquad \hat{\varphi}_\mu(T) = \hat{\bar{\varphi}} = V_{ad}^\top \bar{\varphi},$$

where the projected system matrices are defined as

$$\begin{aligned} \hat{E}_{pr} &= W_{pr}^\top E V_{pr} \in \mathbb{R}^{k_{pr} \times k_{pr}}, & \hat{E}_{ad} &= W_{ad}^\top E V_{ad} \in \mathbb{R}^{k_{ad} \times k_{ad}}, \\ \hat{A}_{pr}(\mu; t) &= W_{pr}^\top A(\mu; t) V_{pr} \in \mathbb{R}^{k_{pr} \times k_{pr}}, & \hat{B}_{pr}(\mu; t) &= W_{pr}^\top B(\mu; t) \in \mathbb{R}^{k_{pr} \times m}, \\ \hat{A}_{ad}(\mu; t) &= W_{ad}^\top A(\mu; t) V_{ad} \in \mathbb{R}^{k_{ad} \times k_{ad}}, & \hat{B}_{ad}(\mu; t)^\top &= B(\mu; t)^\top V_{ad} \in \mathbb{R}^{m \times k_{ad}}. \end{aligned}$$

Part 2: Reduced model for system dynamics
Offline-online decomposition

- Parameter-separability:

$$A(\mu;t) = \sum_{q=1}^{Q_A} \theta_A^q(\mu;t)A_q \qquad \text{and} \qquad B(\mu;t) = \sum_{q=1}^{Q_B} \theta_B^q(\mu;t)B_q,$$

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- Online phase:

$$\hat{A}_{\text{pr}}(\mu;t) = \sum_{q=1}^{Q_A} \theta_A^q(\mu;t)\hat{A}_{\text{pr}}^q \qquad \text{and} \qquad \hat{B}_{\text{pr}}(\mu;t) = \sum_{q=1}^{Q_B} \theta_B^q(\mu;t)\hat{B}_{\text{pr}}^q.$$

Define the residual for the primal equation as

$$R_{\mu}^{\text{pr}}\left[\hat{x}, u\right](t) \coloneqq A(\mu; t)\hat{x}(t) + B(\mu; t)u(t) - E\frac{d}{dt}\hat{x}(t).$$

Part 2: Reduced model for system dynamics
Residual-based a posteriori estimation

Define the residual for the primal equation as

$$R_\mu^{\mathrm{pr}}[\hat{x}, u](t) := A(\mu; t)\hat{x}(t) + B(\mu; t)u(t) - E\frac{d}{dt}\hat{x}(t).$$

Then we can estimate the error for the reduced primal solution as

$$\boxed{\| x_\mu(t) - \hat{x}_\mu(t) \| \leqslant \Delta_\mu^{\mathrm{pr}}[u](t).}$$

The error estimator $\Delta_\mu^{\mathrm{pr}}[u]$ is given as

$$\Delta_\mu^{\mathrm{pr}}[u](t) := C_1(\mu) \| x_\mu^0 - V_{\mathrm{pr}}V_{\mathrm{pr}}^\top x_\mu^0 \| + C_1(\mu)\int_0^t \| E^{-1}R_\mu^{\mathrm{pr}}[\hat{x}_\mu, u](s) \| \, ds$$

for a suitable constant $C_1(\mu)$.

Computation of the fully reduced solution

The fully reduced solution $\hat{\varphi}_{\mu}^{N,\mathrm{red}} \in X^N$ is defined as

$$\boxed{\hat{\varphi}_{\mu}^{N,\mathrm{red}} \coloneqq \operatorname*{arg\,min}_{p \in X^N} \left\| \hat{g}(\mu) - \hat{S}(\mu)p \right\|_X^2,}$$

where

$$\hat{S}(\mu) \coloneqq E^\top + C^\top C \hat{\Lambda}(\mu) V_{\mathrm{ad}} V_{\mathrm{ad}}^\top \in \mathbb{R}^{n \times n}$$

and

$$\hat{g}(\mu) \coloneqq C^\top C \left(\hat{\Psi}_{\mu}^{\mathrm{pr}}(T,0) V_{\mathrm{pr}} V_{\mathrm{pr}}^\top x_{\mu}^0 - x_{\mu}^T \right) \in \mathbb{R}^n.$$

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Part 3: Fully reduced model (F-ROM)
Computation of the fully reduced solution

The fully reduced solution $\hat{\varphi}_\mu^{N,\text{red}} \in X^N$ is defined as

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This least squares problem can be solved as before by orthogonal projection in $\mathbb{R}^n$, i.e.

$$\hat{S}(\mu) \hat{\varphi}_\mu^{N,\text{red}} = P_{\hat{S}(\mu) X^N} \hat{g}(\mu).$$

For an approximate final time adjoint φ^N we define the error estimator

$$\boxed{\eta_\mu^{\text{red}}(\varphi^N) := C_{\text{op}}\left(\|C^\top C\|\,\Delta_\mu^{\text{pr}}[0](T) + \hat{\eta}_\mu(\varphi^N) + \|C^\top C\|\,\Delta_\mu^{\Lambda}[\varphi^N]\right),}$$

where the reduced error estimator is given as

$$\hat{\eta}_\mu(\varphi^N) := \left\| \hat{g}(\mu) - \hat{S}(\mu)\varphi^N \right\|$$

and the Gramian error estimator is given as

$$\Delta_\mu^{\Lambda}[\varphi^N] := C_1(\mu)C_2(\mu)\int_0^T \Delta_\mu^{\text{ad}}[\varphi^N](s)\,ds + C_1(\mu)\int_0^T \left\| E^{-1}R_\mu^{\text{pr}}[\hat{x}_\mu,\hat{u}_\mu](s)\right\| ds.$$

Part 3: Fully reduced model (F-ROM)

Practical remarks

- Fully reduced model can be decomposed offline-online such that online phase is completely independent of n.

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- Fully reduced model can be decomposed offline-online such that online phase is completely independent of n.

- A posteriori error estimator can be evaluated in a complexity independent of n as well.

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Part 3: Fully reduced model (F-ROM)
Practical remarks

- Fully reduced model can be decomposed offline-online such that online phase is completely independent of n.
- A posteriori error estimator can be evaluated in a complexity independent of n as well.
- Several approaches for the construction of X^N and $V_{\text{pr}}, V_{\text{ad}}, W_{\text{pr}}, W_{\text{ad}}$ are possible, see [K./Renelt'24] for details.

Part 3: Fully reduced model (F-ROM)
Practical remarks

- Fully reduced model can be decomposed offline-online such that online phase is completely independent of n.
- A posteriori error estimator can be evaluated in a complexity independent of n as well.
- Several approaches for the construction of X^N and $V_{\text{pr}}, V_{\text{ad}}, W_{\text{pr}}, W_{\text{ad}}$ are possible, see [K./Renelt'24] for details.
- Here, we construct reduced spaces adaptively within a model hierarchy, see below.

Machine learning surrogate (F-ML-ROM)

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

- Observation: Given a basis $\varphi_1, \dots, \varphi_N \in X^N$, the reduced coefficients $\hat{\alpha}_\mu^{N,\text{red}} \in \mathbb{R}^N$ determine $\hat{\varphi}_\mu^{N,\text{red}} \in X^N$ as

$$\hat{\varphi}_\mu^{N,\text{red}} = \sum_{i=1}^{N} \left[\hat{\alpha}_\mu^{N,\text{red}}\right]_i \cdot \varphi_i.$$

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$$\hat{\varphi}_\mu^{N,\mathrm{red}} = \sum_{i=1}^{N} \left[\hat{\alpha}_\mu^{N,\mathrm{red}}\right]_i \cdot \varphi_i.$$

- Idea: Learn the map from parameter to reduced coefficients, i.e. approximate

$$\pi_N \colon \mathcal{P} \ni \mu \mapsto \hat{\alpha}_\mu^{N,\mathrm{red}} \in \mathbb{R}^N$$

by a machine learning surrogate $\hat{\pi} \colon \mathcal{P} \to \mathbb{R}^N$.

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- Compute machine learning reduced solution as

$$\hat{\varphi}_\mu^{N,\text{red,ml}} = \sum_{i=1}^{N} [\hat{\pi}(\mu)]_i \cdot \varphi_i.$$

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$$\hat{\varphi}_\mu^{N,\text{red,ml}} = \sum_{i=1}^{N} [\hat{\pi}(\mu)]_i \cdot \varphi_i.$$

- Solve reduced dynamical systems from the F-ROM to compute the approximate control using $\hat{\varphi}_\mu^{N,\text{red,ml}}$ as final time adjoint.

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