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ROM-ES: Uncertainty quantification of reduced order model errors

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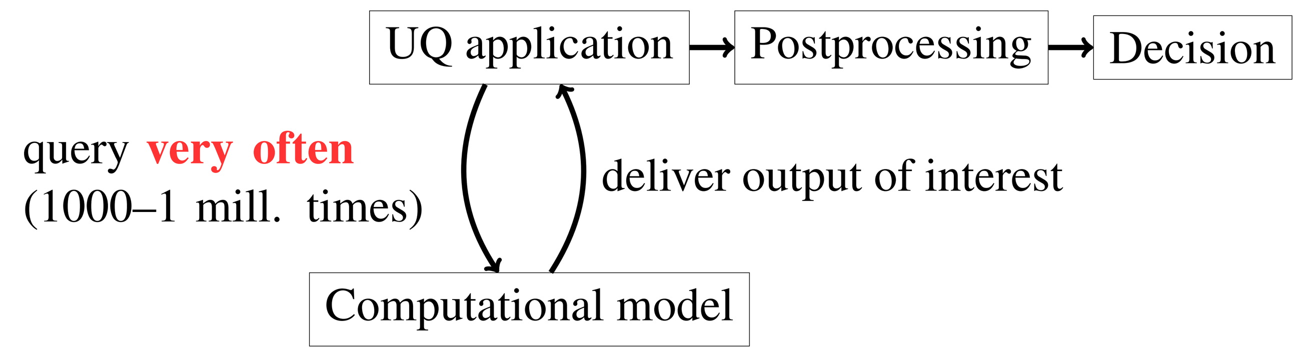
Problem description

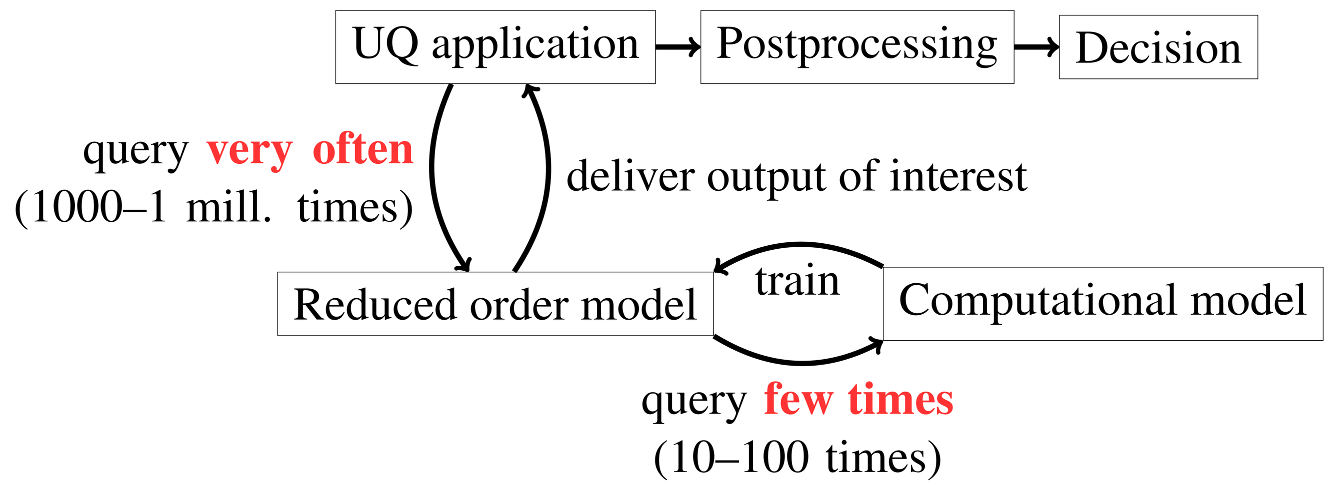
A huge challenge in model based decision making is the quantification of uncertainties. Once the most important sources of uncertainty are identified, the *ideal* process of decison making could look like this:

Ideal decision making



In this setting, the computational model has to be evaluated for lots of different parameters, and unless the problem is of very simple kind, the application will most likely excess the available compuational capacities very quickly. Therefore, the *slow* computational model is usually substituted by faster reduced order models (ROMs).

Decision making with reduced order models



Reduced order models ...

- introduce **ROM errors** into the application, which need to be **quantified**.
- can usually be categorized as either
  - **interpolation** (e.g. regression methods, kriging, ...) or
  - **projection** (e.g. POD, reduced basis methods, balanced truncation, ...).

Projection methods...

+ retain physical dynamics, and
+ usually ship with (rigorous) error bounds, that ...
  - often overestimate "true errors" significantly or
  - are very intrusive and slow.

Interpolation methods...

+ are faster to compute,
+ are nonintrusive,
- need more training data,
- do not have rigorous error bounds.

ROM-ES method combines advantages!

UQ of ROM errors

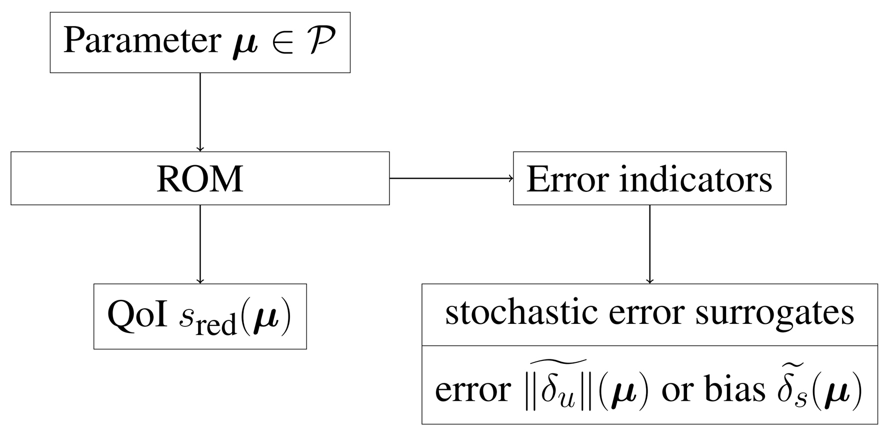
We want to quantify the two following uncertain values:

- The error $\|\delta_u\|$ is the **"true" error** between the state solutions of the full order model (FOM) and the ROM. **Note:** This is usually unknown, as the FOM solution is not computed.
- The difference $\delta_s = s_{\text{red}} - s$ is the **bias** for the quantity of interest (QoI) s.

In order to quantify these errors, we consider three approaches:

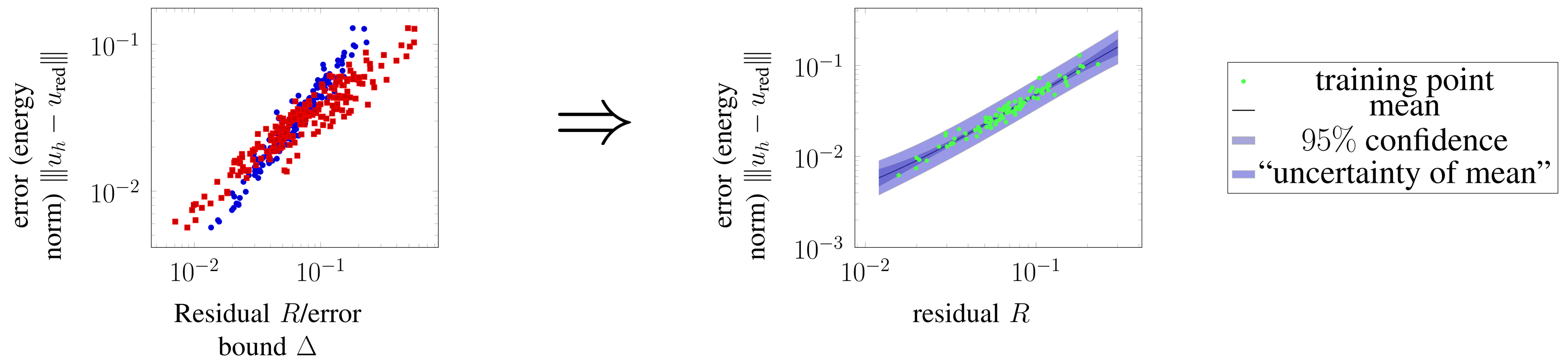
1. **Multifidelity analysis** substitutes the bias with a surrogate $\widetilde{\delta_s^{\text{MF}}}$ inferred from the mapping $\boldsymbol{\mu} \mapsto \delta_s(\boldsymbol{\mu})$.
2. **Error bounds** $\Delta_u \geq \|\delta_u\|$, $\Delta_s \geq \delta_s$ are intrusive, rigorous bounds of the reduction errors that ship with most projection ROMs.
3. The newly proposed **ROM-ES** (ROM error surrogates) combine both ideas, as they use stochastic surrogates for $\|\delta_u\|$ and δ_s, but trained with **cheap error indicators** as inputs.

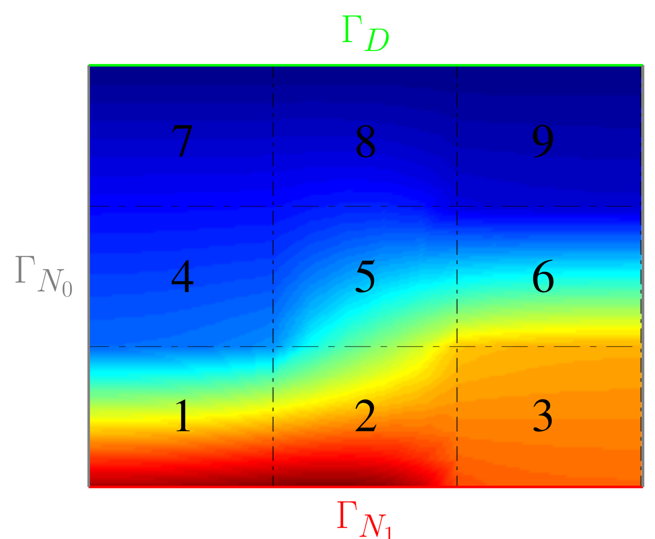
ROM-ES Schema



	ROMs based on projection	ROMs based on interpolation	multifidelity analysis	ROM-ES
non–intrusive	×	✓	✓	✓
bias correction	×	N/A	✓	✓
rigorous error bounds	✓	×	×	(✓)*
tight error bounds	(✓)†	×	×	✓

* rigorous for $x\%$ of evaluations
† good effectivity can only be obtained with very intrusive methods





Test problem (thermal block from RBmatlab [RBM] toolbox)**:**

- Parametrized heat equation: $\triangle c(x;\boldsymbol{\mu})u(x;\boldsymbol{\mu}) = 0 \quad \text{in } \Omega,$
- nine parameters: $\boldsymbol{\mu} \in \mathcal{P} := [0.1, 10]^9$.
- Output: $s(\boldsymbol{\mu}) = s(u(\boldsymbol{\mu})) := \int_{\Gamma_{N_1}} u(\boldsymbol{\mu})\,\mathrm{d}x$
- Reduced basis [cite] ROM with $N =$ 62 basis functions.
- compliant problem, i.e. $\delta_s = s - s_{\text{red}} = \|u - u_{\text{red}}\|^2_{\boldsymbol{\mu}} > 0.$
- **error indicator:** Residual $R(u)$
- tested surrogates: GP kernel [cite rasmussen] and RVM [cite Tipping] with inferred constant variance

References

- [DC13] M. Drohmann, K. T. Carlberg *Uncertainty quantification for+ surrogate models via error indicators with application to reduced-basis methods* to be submitted
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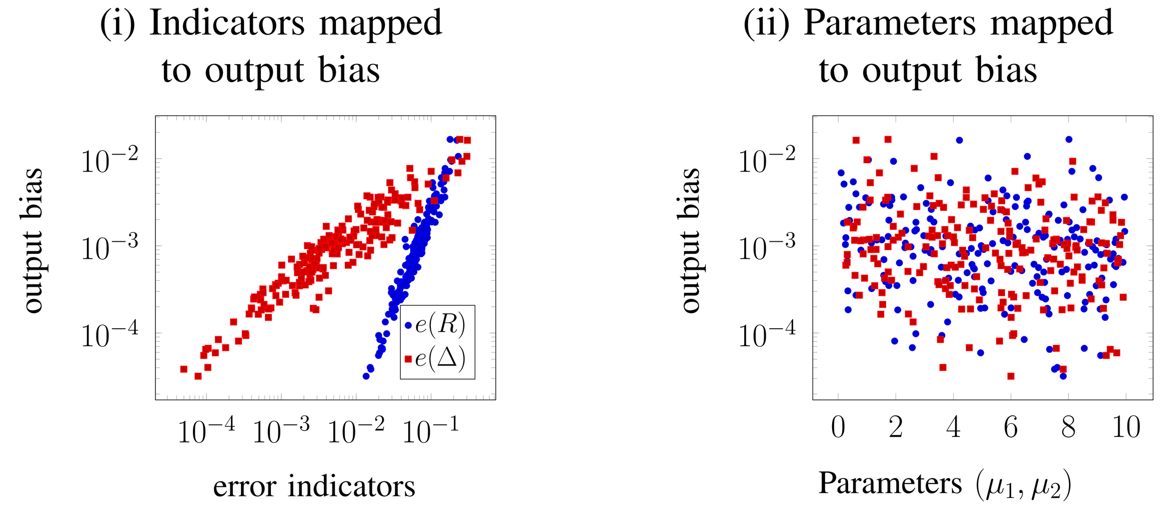
- [RBM] RBMatlab toolbox. http://www.morepas.org/software
- [Tip01] M. E. Tipping. *Sparse Bayesian learning and the Relevance Vector Machine.* Journal of Machine Learning Research, pp. 211–244 (1), **2001**
- [RW06] C. E. Rasmussen and C. K. I. Williams. *Gaussian Processes for Machine Learning* The MIT Press, **2006**

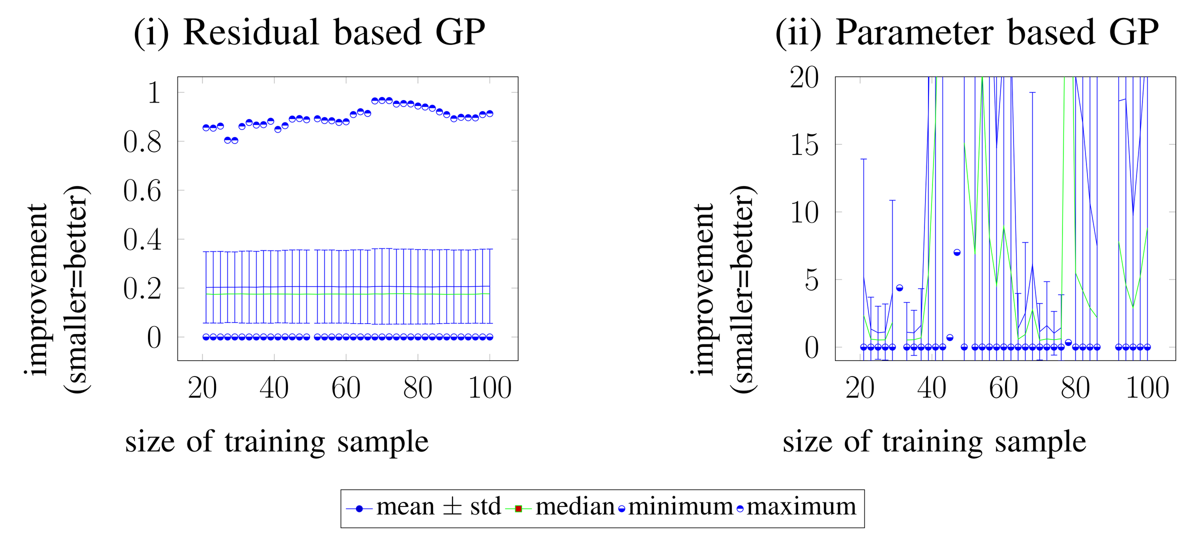
Results

- Mapping based on error indicators is far more structured compared to parameter mapping.

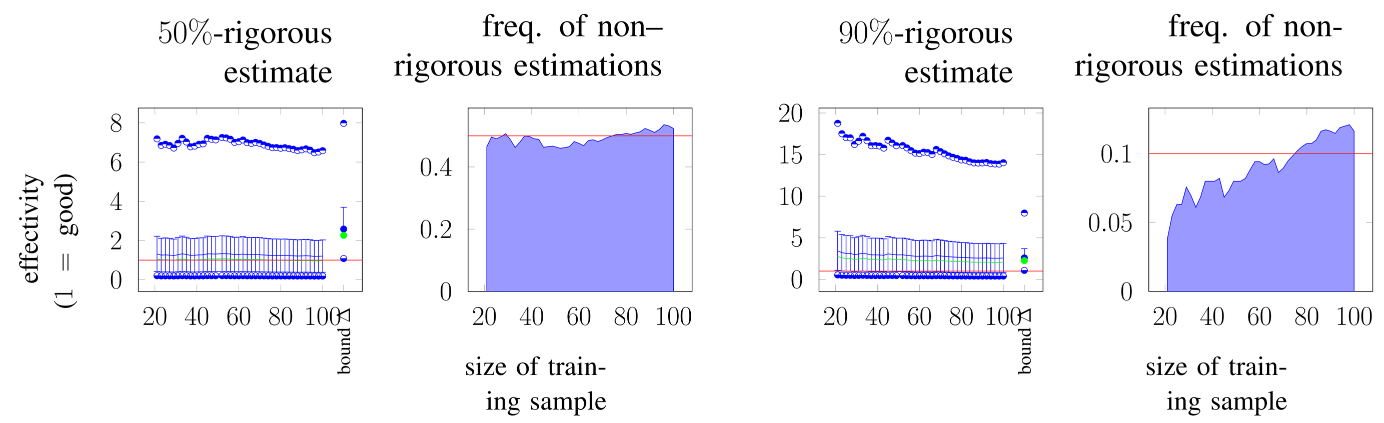


- Bias correction improves output by one order of magnitude, compared to worsening for multifidelity approach.

improvement $= E\left(\frac{s_{\text{red}} + \widetilde{\delta}_s}{s_{\text{red}}}\right)$



- Stochastic error estimates can compete with error bounds, but are far less intrusive. Probability of rigorous error estimates (overestimation) is controllable.



- The assumption of a Gaussian process could be validated
- "**Good convergence**": Only a few training samples are necessary to obtain reliable error surrogates.
- Especially for **non–linear** problems: Error surrogates can be computed non–intrusively.

Outlook:

- Integration into UQ application framework for performance evaluations
- Improvment of ROM generation with efficient ROM-ES error evaluations

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