Learning low-dimensional models via operator lifting and natural greedy algorithms

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Advances in Experimental Design, Optimization and Learning for Uncertain Complex Systems

Abstract

AEOLUS target problems in Advanced Materials & Manufacturing require multifaceted and integrated advances in applied mathematics for learning from data (e.g., inferring process models from sensor and imaging data). We present preliminary progress, supported by AEOLUS, on model reduction. The goal of model reduction is to reduce the dimensionality of a model, i.e,. replace the high-dimensional data by appropriate low-dimensional fast-to-evaluate models. This presentation summarizes our achievements from three perspectives, i.e., operator lifting for reduced model structure, domain decomposition for parametric dimensionality reduction, and natural greedy algorithms for efficient training.

Motivation

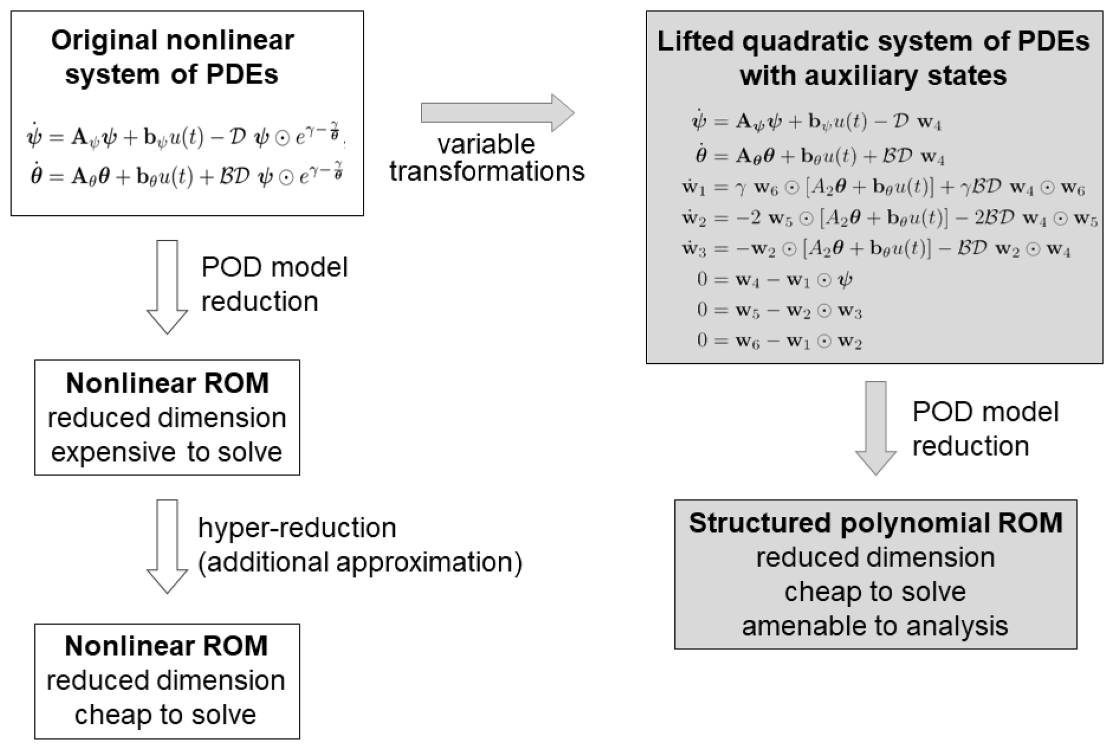
Key challenges must be addressed to make model reduction applicable, and applied, to a broader range of problems, including our applications in Advanced Materials & Manufacturing:

1. Reduction of nonlinear multiscale problems, where dynamics are not obviously amenable to approximation in a linear subspace.
2. Non-intrusive methods that have the flexibility of machine learning approaches, but retain the rigor, interpretability and physics-based predictive power of classical model reduction.
3. Reduction of the high dimensionality of input model parameters, especially in the case of having heterogeneous random fields.
4. Reduction of the intensive computational cost of building reduced bases using classic greedy algorithms.

Approach: operator lifting

We construct transforms at the PDE level to a structured form and then learn a structured low-dimensional discretized representation directly from data. Two key ingredients are:

- **Operator inference**: Derive a reduced model by learning the reduced operators directly from sampled state trajectory data via least squares optimization. This gives the flexibility of a black-box learning approach, but yields a formulation in which we can weakly enforce the governing physical equations in a reduced basis coordinate system.
- **Lifting**: Identify variable transformations and auxiliary state variables that transform a general nonlinear system of PDEs into a system of PDEs with polynomial form. This gives an equivalent representation of the nonlinear system with the explicit form needed for Operator Inference.



Approach: domain decomposition

Identify low-dimensional structures of parametric PDEs by decomposing both the input random field and the solution into sub-domains [1]. Two key ingredients are:

- **Domain decomposition**: Reduce the parametric dimension by re-parameterizing the input random field in sub-domains leading to faster eigenvalue decays; reduce the output dimension by generating reduced bases for local PDE solutions in sub-domains.
- **Operator approximation**: Exploit the dimension reduction to formulate and approximate a set of low-dimensional and local PDE operators, which leads to accurate and efficient operator approximation.

We consider the convection-dominated PDE

$$-\varepsilon\Delta u(x,\omega) + \boldsymbol{b}(x,\omega)\cdot\nabla u(x,\omega) = 0$$

with random velocity field $\boldsymbol{b}$, which leads to sharp transitions (shown in Figure 1)

The colored noise case:

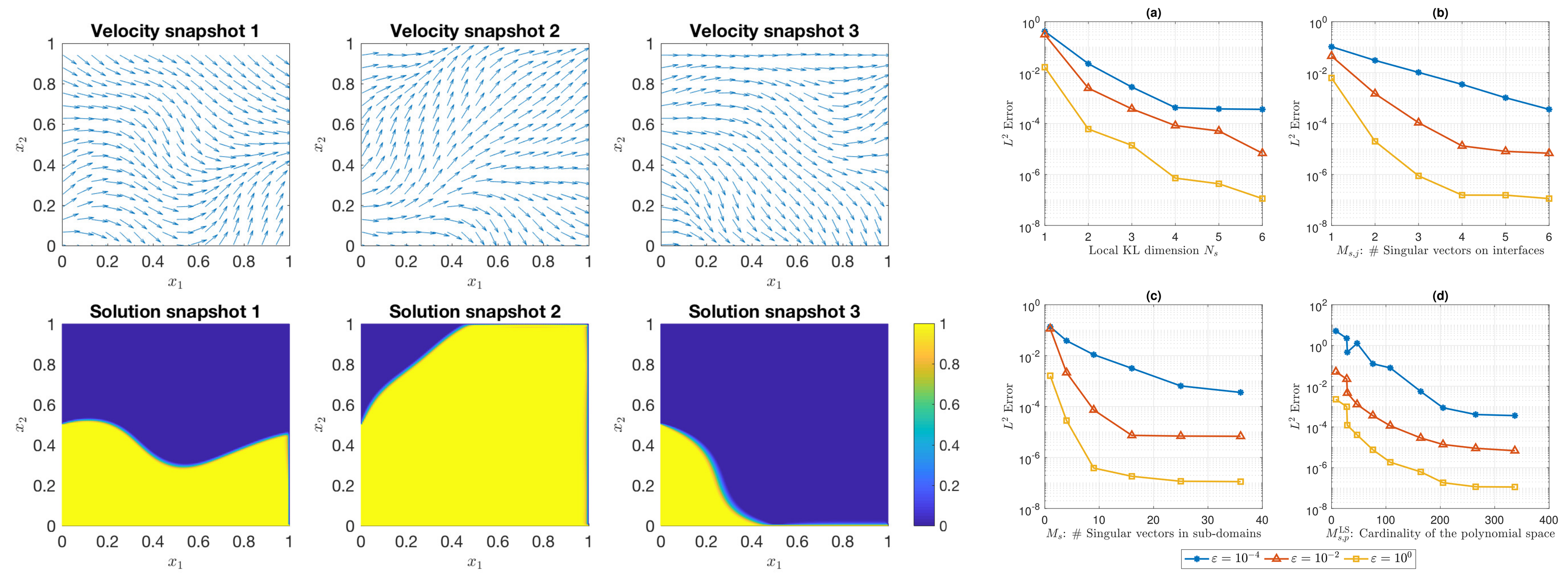


Figure 1:(Left) Three snapshots of the velocity field and the corresponding solution field of the PDE; (Right) Error decay with respect to four error sources: local KL dimension, dim of RB on interfaces, dim of RB in sub-domains, DoFs of operator approximation.

The white noise case:

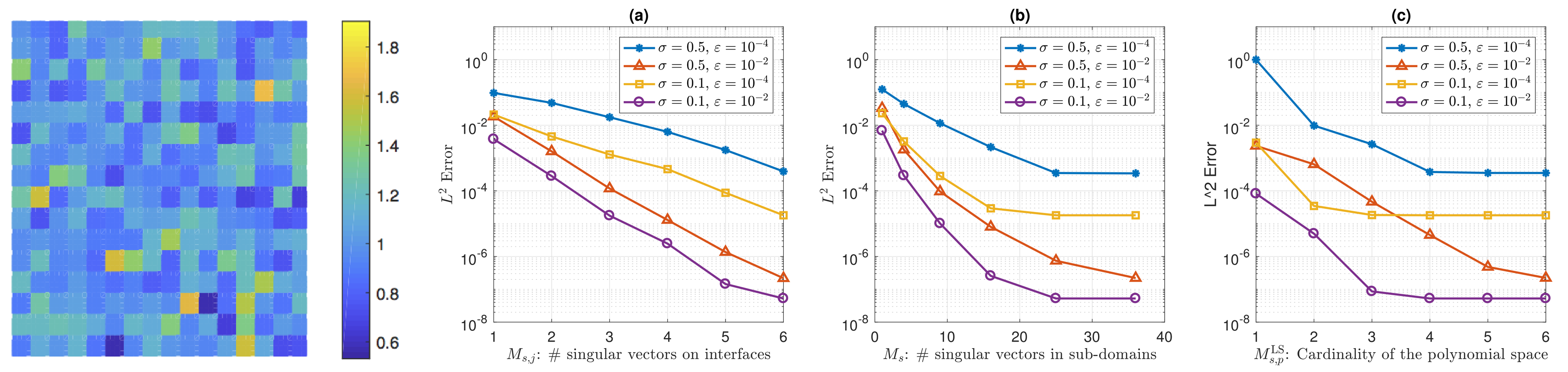


Figure 2:(Left) A snapshot of the velocity field involving 256 independent Gaussian random variables; (Right) Error decay with respect to three error sources:dim of RB on interfaces, dim of RB in sub-domains, DoFs of operator approximation.

Approach: natural greedy algorithm

We developed a new method for constructing reduced bases in a Banach space with arbitrary norm. Two key ingredients are:

- **Norm flexibility**: The choice of approximating norm is not restricted like in some other algorithms (e.g. the 2-norm for the Proper Orthogonal Decomposition or the ∞-norm for the Empirical Interpolation Method).
- **Computational simplicity**: The novel way of approximating in Banach spaces via specifically constructed linear projectors, which is performed by matrix arithmetic.

Let $(\mathcal{X}, \|\cdot\|)$ be a Banach space and let $\mathcal{F}\subset\mathcal{X}$ be a set that is required to be approximated. The Natural Greedy Algorithm iteratively constructs the sequence of vectors $g_1, g_2, \ldots$, which span the approximating subspaces $V_n = \operatorname{span}\{g_1,\ldots,g_n\}$:

- Step 1: For a set of already selected vectors $g_1,\ldots,g_n\in\mathcal{X}$ define operators
$$r_n(f) = f - F_{g_n}(f)\, g_n,$$
$$\mathcal{R}_n(f) = r_n\circ r_{n-1}\circ\ldots\circ r_1(f).$$
- Step 2: the next vector g_{n+1} is constructed by finding
$$f_{n+1} = \operatorname{argmax}_{f\in\mathcal{F}}\|\mathcal{R}_n(f)\| \text{ and taking } g_{n+1} = \frac{\mathcal{R}_n(f_{n+1})}{\|\mathcal{R}_n(f_{n+1})\|}.$$

As an illustration, we consider the following problem of approximating a parametric family of functions:

$$\mathcal{F}(x_1,x_2,\mu_1,\mu_2) = \sin(x_1\mu_1)\cos(x_2\mu_2)\exp(|x_1|\mu_1 + |x_2|\mu_2),$$
$$\mathcal{X} = L_1([0,1]\times[0,1]),\ \mathcal{D} = [\pi/3, 2\pi]\times[\pi/3, 2\pi]$$

and compare the performances of four methods:

- Standard Greedy Algorithm (GA)
- Natural Greedy Algorithm (NGA)
- Empirical Interpolation Method (EIM)
- Proper Orthogonal Decomposition (POD)

Performance metric: the inverse of the product of the maximal approximation error and the construction time for each of the reduced bases, i.e.,

$$\text{quality} = \frac{1}{\text{error}\times\text{cputime}}.$$

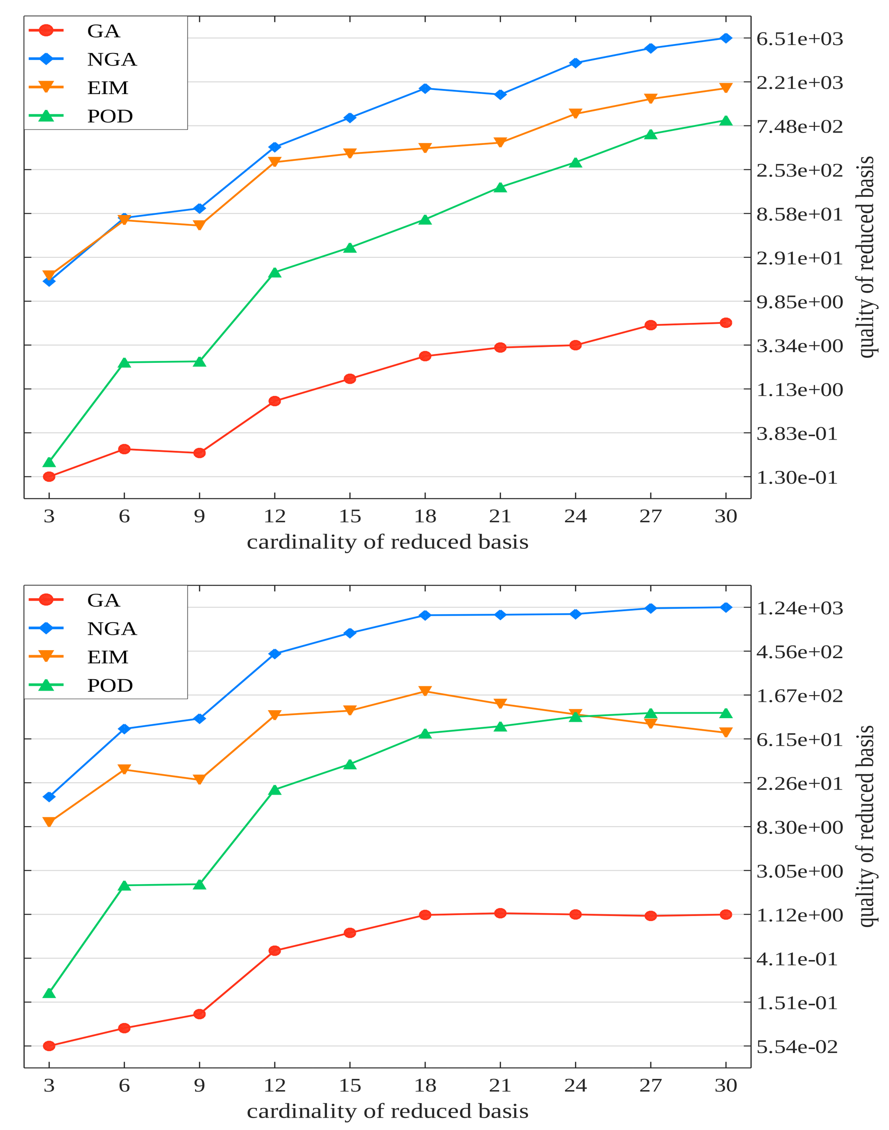


Figure 3:Performance of the reduced basis algorithms on the parametric family $\mathcal{F}(x,y,\lambda,\mu) = \sin(\lambda x)\cos(\mu y)\exp(\lambda|x| + \mu|y|)$, where $x,y\in[0,1]$ and $\lambda,\mu\in[\pi/3,2\pi]$. (Left) No noise; (Right) With additive noise.

References

[1] L. Mu and G. Zhang. A Domain-Decomposition Model Reduction Method for Linear Convection-Diffusion Equations with Random Coefficients. *SIAM Journal on Scientific Computing*, in revision, 2018, (arXiv:1802.04187).

[2] A. Dereventsov and C. Webster. The Natural Greedy Algorithm for reduced bases in Banach spaces. *Foundations of Computational Mathematics*, 2019.