A biased introduction to projection-based model reduction

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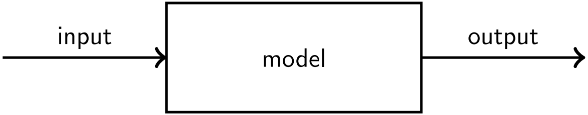
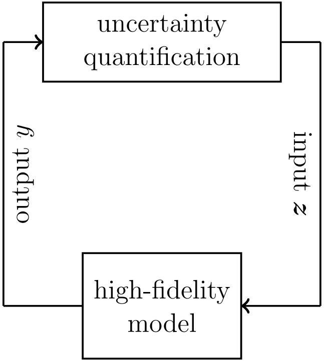
Intro: Models and outer-loop applications

Model

- Model describes response of system to inputs, parameters
- Many models described as differential equations
- Evaluating a model requires numerical simulations



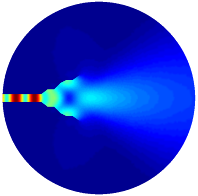


Outer loop applications [P., Willcox, Gunzburger, SIAM Review, 2018]

- Form outer loops around a model
- In each iteration an input μ is received and the corresponding model output y is computed
- An overall outer loop result is obtained at the termination of the outer loop

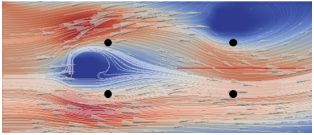
Challenge: Single model solve expensive; repeated solves in outer loop prohibitive

Intro: Outer-loop applications



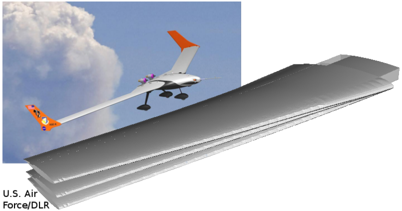
optimization

control



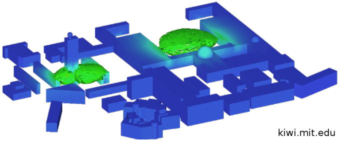
inference

model calibration



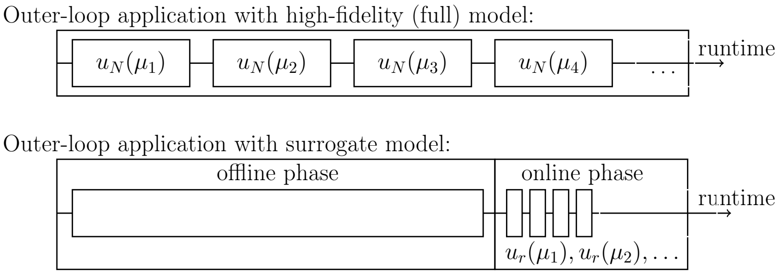
multi-discipline coupling

visualization



uncertainty quantification

Intro: Offline/online decomposition



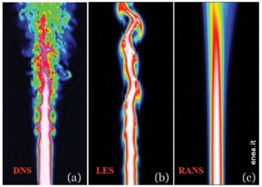
Offline (training) phase

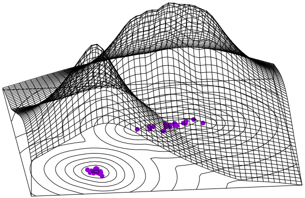
- Generate snapshots (data) using the expensive, high-fidelity model
- Extract patterns from data and derive cheap surrogate model

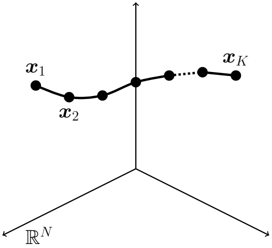
Online (evaluation) phase

- Evaluate surrogate model instead of high-fidelity model (or both $\rightarrow$ multi-fidelity)
- Rapid prediction, control, optimization, uncertainty quantification

Intro: Three types of surrogate models







simplified surrogates

- Simplifying physics
- Coarser discretizations
- Linearized models
- Early stopping of iterative solvers

data-fit surrogates

- Fitting model to data of input-output map given by high-fidelity model
- Response surfaces
- SVMs, Gaussian processes
- Neural networks

reduced models

- Extract important dynamics of full-model states from *data*
- Approximate high-dimensional states in subspaces
- Restrict solving governing equations to subspaces

[P., Willcox, Gunzburger, SIAM Review, 2018]

Outline

1. Introduction to projection-based model reduction
   - Solution manifold, smoothness, low-rank structure
   - Basis generation
   - Online efficiency
2. Model reduction for time-dependent problems
3. Model reduction for nonlinear problems
4. Multi-fidelity methods for certifying outer-loop results

Outline

1. **Introduction to projection-based model reduction**
   - Solution manifold, smoothness, low-rank structure
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3. Model reduction for nonlinear problems
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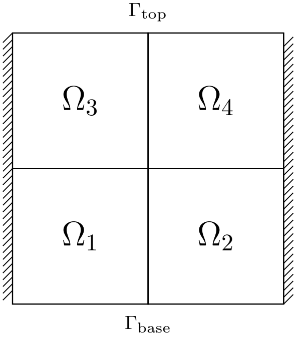
MOR: Model problem

Steady heat conduction (thermal block) [Rozza et al., 2007]

$$\nabla \cdot (c(\boldsymbol{x};\boldsymbol{\mu})\nabla u(\boldsymbol{x};\boldsymbol{\mu})) = g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega,$$
$$u(\boldsymbol{x};\boldsymbol{\mu}) = 0, \qquad \boldsymbol{x} \in \Gamma_{\text{top}}$$
$$\nabla u(\boldsymbol{x};\boldsymbol{\mu}) \cdot n = 0, \qquad \boldsymbol{x} \in \Gamma_{\text{side}}$$
$$\nabla u(\boldsymbol{x};\boldsymbol{\mu}) \cdot n = 1, \qquad \boldsymbol{x} \in \Gamma_{\text{base}}$$

Conductivity coefficient $\boldsymbol{\mu} = [\mu_1, \dots, \mu_d]^T \in \mathcal{D} \subset \mathbb{R}^d$

$$c(\boldsymbol{x};\boldsymbol{\mu}) = \mu_i 1_{\Omega_i}(\boldsymbol{x})$$



Consider Hilbert space $\mathcal{V}$ and weak form of problem from above

$$a(u(\boldsymbol{\mu}), w; \boldsymbol{\mu}) = g(w; \boldsymbol{\mu}), \qquad \forall w \in \mathcal{V}$$

- Solution field $u(\boldsymbol{\mu}) : \Omega \to \mathbb{R}$, bilinear form $a : \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ and linear form $g : \mathcal{V} \to \mathbb{R}$
- Assume well posedness (here a coercive and a, g continuous for all $\boldsymbol{\mu} \in \mathcal{D}$)

MOR: Discretized ("full") model problem

Exact solution $u(\boldsymbol{\mu})$ unavailable and therefore need to resort to numerical approximation

Approximation space $\mathcal{V}_N \subset \mathcal{V}$ of dimension $N \in \mathbb{N}$

- Example: finite element method with triangulation and piecewise linear basis functions
- Basis of space $\{\varphi_i\}_{i=1}^N$

For each $\boldsymbol{\mu} \in \mathcal{D}$, obtain the discrete problem via Galerkin projection (e.g., [Hesthaven et al., 2016])

$$a(u_N(\boldsymbol{\mu}), w_N; \boldsymbol{\mu}) = g(w_N; \boldsymbol{\mu}), \qquad \forall w_N \in \mathcal{V}_N$$

and in algebraic form

$$\boldsymbol{A}(\mu)\boldsymbol{u}_N(\mu) = \boldsymbol{g}(\boldsymbol{\mu}), \qquad \boldsymbol{u}_N(\boldsymbol{\mu}) \in \mathbb{R}^N \tag{1}$$

with matrix $\boldsymbol{A}(\mu) \in \mathbb{R}^{N \times N}$ and vector $\boldsymbol{g}(\boldsymbol{\mu}) \in \mathbb{R}^N$

Computing $u_N(\boldsymbol{\mu})$ means solving linear system of equations (1)
$\rightarrow$ computational costs depend directly on dimension N

MOR: Solution manifold

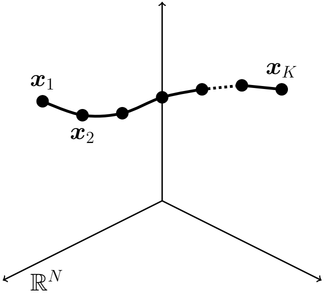
Manifold of "exact" solutions

$$\mathcal{M} = \{u(\boldsymbol{\mu}) \,|\, \boldsymbol{\mu} \in \mathcal{D}\} \subset \mathcal{V}$$

Standard numerical analysis (e.g., FEM) spaces $\mathcal{V}_N$

$$\mathcal{M}_N = \{u_N(\boldsymbol{\mu}) \,|\, \boldsymbol{\mu} \in \mathcal{D}\} \subset \mathcal{V}_N \subset \mathcal{V}$$

- Typically $\|u(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_{\mathcal{V}}$ can be made arbitrarily small by increasing dimension N of space $\mathcal{V}_N$...
- ... but might need large N to achieve acceptable accuracy



Model reduction exploits that solution manifold $\mathcal{M}_N$ is often smooth

- There exist spaces $\mathcal{V}_r$ with dimension $r \ll N$ that approximate $\mathcal{M}_N$ well
- Can we find such a *reduced space* $\mathcal{V}_r$?

MOR: Computing a basis of a reduced space

Best approximation error given by the Kolmogorov r-width [Pinkus, 1985],[Maday et al., 2002],[Binev et al., 2011]

$$d_r(\mathcal{M}_N) = \inf_{\substack{\mathcal{V}_r \subset \mathcal{V}_N \\ \dim(\mathcal{V}_r) = r}} \sup_{u_N(\boldsymbol{\mu}) \in \mathcal{M}_N} \inf_{u_r(\boldsymbol{\mu}) \in \mathcal{V}_r} \|u_N(\boldsymbol{\mu}) - u_r(\boldsymbol{\mu})\|_{\mathcal{V}}$$

- Computationally not tractable in general
- Note that if $d_r(\mathcal{M}_N)$ decays slowly with dimension r, then model reduction fails ($\rightarrow$ later)

Minimizing a discrete version of the Kolmogorov r-width (e.g., [Benner et al., 2015], [Hesthaven et al., 2016])

- Select a finite subset $\mathcal{D}_T = \{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_M\} \subset \mathcal{D}$ of M parameters
- Consider M snapshots $u_N(\boldsymbol{\mu}_1), \dots, u_N(\boldsymbol{\mu}_M)$
- Find orthonormal $v_1, \dots, v_r \in \mathcal{V}_N$ that minimize

$$\frac{1}{M} \sum_{i=1}^{M} \inf_{u_r \in \mathrm{span}\{v_1, \dots, v_r\}} \|u_N(\boldsymbol{\mu}_i) - u_r\|_{\mathcal{V}}$$

- Define reduced space $\mathcal{V}_r$ as span of $v_1, \dots, v_r$

MOR: Computing a basis of a reduced space (cont'd)

Optimal $v_1, \dots, v_r$ are the eigenvectors with largest eigenvalues $\lambda_1 \geq \cdots \geq \lambda_r$ of operator

$$C(v) = \frac{1}{M} \sum_{i=1}^{M} \langle v, u_N(\boldsymbol{\mu}_i) \rangle_{\mathcal{V}} \; u_N(\boldsymbol{\mu}_i)$$

- Optimality property
$$\frac{1}{M} \sum_{i=1}^{M} \| u_N(\boldsymbol{\mu}_i) - \mathcal{P}_r[u_N(\boldsymbol{\mu}_i)] \|_{\mathcal{V}}^2 = \sum_{i=r+1}^{M} \lambda_i$$
with projection $\mathcal{P}_r[u]$ of $u \in \mathcal{V}_N$ onto $\mathcal{V}_r$ with respect to $\langle \cdot, \cdot \rangle_{\mathcal{V}}$
- Optimality holds only for parameters in training set $\boldsymbol{\mu} \in \mathcal{D}_T$; not for $\boldsymbol{\mu} \in \mathcal{D}$

Basis $v_1, \dots, v_r$ has many names (e.g., [Benner et al., 2015], [Hesthaven et al., 2016])

- Called proper orthogonal decomposition (POD) basis in model reduction
- Same basis is obtained with principal component analysis (PCA), Karhunen-Loève, singular value decomposition (SVD), etc.

MOR: Linear algebra view on learning a POD space

Two steps to compute POD basis in practice

1. Assemble snapshot matrix

$$\boldsymbol{S} = \begin{bmatrix} | & & | \\ \boldsymbol{u}_N(\boldsymbol{\mu}_1) & \dots & \boldsymbol{u}_N(\boldsymbol{\mu}_M) \\ | & & | \end{bmatrix} \in \mathbb{R}^{N \times M}$$

2. Compute singular value decomposition with the first r left-singular vectors

$$\boldsymbol{V}_r = \begin{bmatrix} | & & | \\ \boldsymbol{v}_1 & \dots & \boldsymbol{v}_r \\ | & & | \end{bmatrix} \in \mathbb{R}^{N \times r}$$

(Note: Replaced $\langle \cdot, \cdot \rangle_{\mathcal{V}}$ with ℓ^2 inner product for computational convenience.)

Computational costs

1. Computing M high-fidelity solutions to assemble snapshot matrix
2. Singular value decomposition with complexity $\mathcal{O}(MN^2)$ (or $\mathcal{O}(NM^2)$)

$\rightarrow$ high costs but (extremely) efficiently implemented in standard numerical linear algebra packages

MOR: Basis generation methods and references [Benner et al., 2015]

Proper orthogonal decomposition (POD) [Lumley, 1967], [Sirovich, 1981]

- Use snapshot data to generate empirical eigenfunctions
- Easy to implement with standard numerical linear algebra packages

Interpolatory methods [Gallivan, Grimme, van Dooren, 1994], [Feldmann, Freund, 1995], [Gugercin et al., 2008]

- Rational interpolation

Balanced truncation [Moore, 1981], [Li, White, 2002], [Benner et al., 2008, 2013]

- Guaranteed stability and error bound for linear time-invariant systems
- Close connection between POD and balanced truncation [Willcox, Peraire, 2002]

Reduced basis methods [Patera, Rozza, 2007], [Maday et al., 2002], [Veroy et al., 2001,2003, 2005], [Grepl, 2005]

- Efficient greedy methods for constructing basis
- Strong focus on error estimation for selected PDEs

Eigensystem realization algorithm (ERA) [Juang, Pappa, 1985], **Dynamic mode decomposition (DMD)** [Schmid, 2010], **Loewner model reduction** [Mayo, Antoulas, 2007]

- Constructing reduced models purely from data (data-driven, non-intrusive)

MOR: Reduced model

Given a reduced space $\mathcal{V}_r$, reduced model solution $u_r(\boldsymbol{\mu})$ obtained via Galerkin projection

$$a(u_r(\boldsymbol{\mu}), w; \boldsymbol{\mu}) = g(w; \boldsymbol{\mu}), \qquad \forall w \in \mathcal{V}_r$$

Error of reduced solution

$$\|u(\boldsymbol{\mu}) - u_r(\boldsymbol{\mu})\|_{\mathcal{V}} \leq \underbrace{\|u(\boldsymbol{\mu}) - u_N(\boldsymbol{\mu})\|_{\mathcal{V}}}_{e_1} + \underbrace{\|u_N(\boldsymbol{\mu}) - u_r(\boldsymbol{\mu})\|_{\mathcal{V}}}_{e_2}$$

- Select high-dimensional (fine mesh) space $\mathcal{V}_N$ to keep e_1 small
- Train a reduced space $\mathcal{V}_r$ to keep e_2 small

Connection best-approximation in reduced space $\mathcal{V}_r$ to error of reduced solution (stability)

$$\|u(\boldsymbol{\mu}) - u_r(\boldsymbol{\mu})\|_{\mathcal{V}} \leq \left(1 + \frac{\gamma(\boldsymbol{\mu})}{\alpha(\boldsymbol{\mu})}\right) \inf_{u \in \mathcal{V}_r} \|u(\boldsymbol{\mu}) - u\|_{\mathcal{V}}$$

with coercivity and continuity constant $\alpha(\boldsymbol{\mu})$ and $\gamma(\boldsymbol{\mu})$, respectively (restrictive setting)

[Rozza et al., 2007], [Hesthaven et al., 2016]

MOR: Linear algebra view on reduced model

Reduced solution $\boldsymbol{u}_r(\boldsymbol{\mu}) \in \mathbb{R}^r$ solves

$$\boldsymbol{A}_r(\boldsymbol{\mu})\boldsymbol{u}_r(\boldsymbol{\mu}) = \boldsymbol{g}_r(\boldsymbol{\mu})\,,$$

with matrix $\boldsymbol{A}_r(\boldsymbol{\mu}) = \boldsymbol{V}_r^T\boldsymbol{A}(\boldsymbol{\mu})\boldsymbol{V}_r \in \mathbb{R}^{r\times r}$ and vector $\boldsymbol{g}_r(\boldsymbol{\mu}) = \boldsymbol{V}_r^T\boldsymbol{g}(\boldsymbol{\mu}) \in \mathbb{R}^r$

Realizing offline/online splitting via affine parameter dependence

- Affine parameter dependence means (our model problem has affine parameter dependence)

$$a(u,w;\boldsymbol{\mu}) = \sum_{i=1}^{Q_a}\Theta_i^{(a)}(\boldsymbol{\mu})a_i(u,w)\,,\quad g(w;\boldsymbol{\mu}) = \sum_{j=1}^{Q_g}\Theta_j^{(f)}(\boldsymbol{\mu})g_j(w)\,,\qquad \Theta_i^{(a)},\Theta_j^{(g)}:\mathcal{D}\to\mathbb{R}$$

- Pre-compute offline (parameter independent)

$$\boldsymbol{A}_r^{(i)} = \boldsymbol{V}_r^T\boldsymbol{A}^{(i)}\boldsymbol{V}_r\,,\qquad \boldsymbol{g}_r^{(j)} = \boldsymbol{V}_r^T\boldsymbol{g}^{(j)}\,,\qquad i=1,\dots,Q_a,\quad j=1,\dots,Q_g$$

- Assemble online (fast)

$$\boldsymbol{A}_r(\boldsymbol{\mu}) = \sum_{i=1}^{Q_a}\Theta_i^{(a)}(\boldsymbol{\mu})\boldsymbol{A}_r^{(i)}\,,\qquad \boldsymbol{g}_r(\boldsymbol{\mu}) = \sum_{j=1}^{Q_g}\Theta_j^{(g)}(\boldsymbol{\mu})\boldsymbol{g}_r^{(j)}$$

MOR: Offline/online computations

Offline (training):

1. Select training set

$$\mathcal{D}_T = \{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_M\}$$

2. Compute snapshots via full-model solves

$$\mathcal{S} = \{\boldsymbol{u}_N(\boldsymbol{\mu}_1), \ldots, \boldsymbol{u}_N(\boldsymbol{\mu}_M)\} \subset \mathbb{R}^N$$

3. Construct reduced basis (e.g., POD)

$$\boldsymbol{V} = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_r] \in \mathbb{R}^{N \times r}$$

4. Project operators

$$\boldsymbol{A}_r^{(i)} = \boldsymbol{V}_r^T \boldsymbol{A}^{(i)} \boldsymbol{V}_r\,, \qquad \boldsymbol{g}_r^{(j)} = \boldsymbol{V}_r^T \boldsymbol{g}^{(j)}$$

Online (evaluation):

1. Receive $\boldsymbol{\mu} \in \mathcal{D} \setminus \mathcal{D}_T$ not in training set

2. Assemble reduced operators

$$\boldsymbol{A}_r(\boldsymbol{\mu}) = \sum_{i=1}^{Q_a} \Theta_i^{(a)}(\boldsymbol{\mu}) \boldsymbol{A}_r^{(i)}\,,$$

$$\boldsymbol{g}_r(\boldsymbol{\mu}) = \sum_{j=1}^{Q_g} \Theta_i^{(g)}(\boldsymbol{\mu}) \boldsymbol{g}_r^{(j)}$$

3. Solve $r \times r$ system to compute $\boldsymbol{u}_r(\boldsymbol{\mu})$

$$\boldsymbol{A}_r(\boldsymbol{\mu}) \boldsymbol{u}_r(\boldsymbol{\mu}) = \boldsymbol{g}_r(\boldsymbol{\mu})$$

MOR: Computational costs

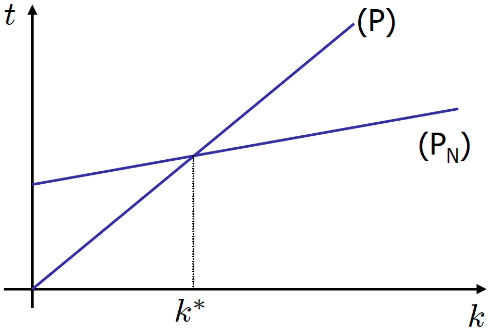
Offline complexity $\mathcal{O}(MN^2 + Q_a rN^2 + Q_g rN)$

- M snapshots and POD basis $\mathcal{O}(MN + MN^2)$
- Computing $\boldsymbol{A}_r^{(1)}, \ldots, \boldsymbol{A}_r^{(Q_a)}$ matrices $\mathcal{O}(Q_a rN^2)$
- Computing $\boldsymbol{g}_r^{(1)}, \ldots, \boldsymbol{g}_r^{(Q_f)}$ matrices $\mathcal{O}(Q_g rN)$

Online complexity $\mathcal{O}(Q_a r^2 + Q_g r + r^3)$

- Assemble reduced operators: $\mathcal{O}(Q_a r^2 + Q_g r)$
- Solving for dense reduced system: $\mathcal{O}(r^3)$

$\rightarrow$ independent of N



full model (P) vs. reduced model (P_N)

[Haasdonk, 2017]

Runtime for k simulations

- Full model alone: $t = k \times t_{\text{full}}$
- Reduced model: $t = t_{\text{offline}} + k \times t_{\text{online}}$
- Model reduction pays off only for $k > k^*$ with $k^* = \frac{t_{\text{offline}}}{t_{\text{full}} - t_{\text{online}}}$

MOR: Error bounds and error estimation

Large part of model reduction community working on *a posteriori* error estimation

$$\|u_N(\boldsymbol{\mu}) - u_r(\boldsymbol{\mu})\| \leq \eta(\boldsymbol{\mu}), \qquad \boldsymbol{\mu} \in \mathcal{D}$$

- Computable, upper bound of (generalization) error over $\mathcal{D}$ (*not* only training set $\mathcal{D}_T$)
- Strong theoretical foundations for linear state dependence [Patera, Rozza, 2007], [Maday et al., 2002], [Veroy et al., 2001,2003, 2005], [Grepl, 2005]
- Heuristics via error indicators available through, e.g., residual
- Not many rigorous statements beyond linear state dependence

Other error bounds

- Error bounds for linear time-invariant systems of ODEs [Moore, 1981]
- A priori analysis of reduced models for elliptic problems with greedy basis construction [Maday et al., 2002], [Binev et al., 2011]

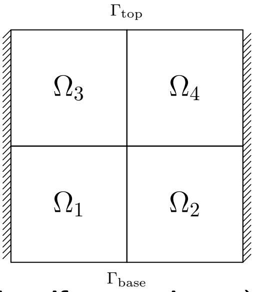
MOR: Thermal block

Steady heat conduction (thermal block) [Rozza et al., 2007]

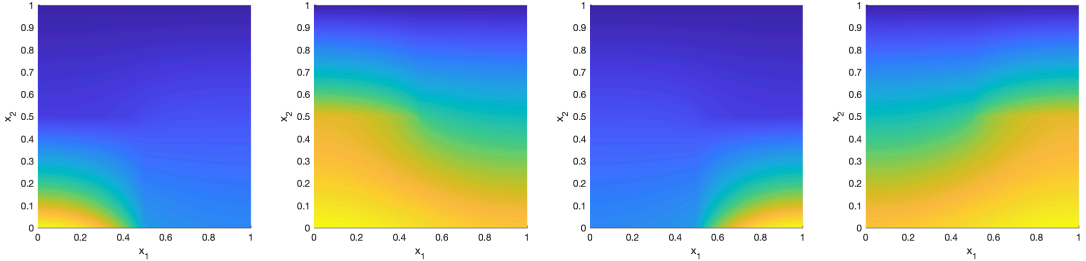
$$\nabla \cdot (c(\boldsymbol{x};\boldsymbol{\mu})\nabla u(\boldsymbol{x};\boldsymbol{\mu})) = g(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega,$$

Conductivity coefficient with parameter $\boldsymbol{\mu} \in \mathcal{D} \subset \mathbb{R}^d$

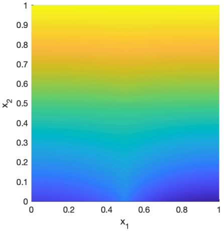
$$c(\boldsymbol{x};\boldsymbol{\mu}) = \mu_i 1_{\Omega_i}(\boldsymbol{x})$$



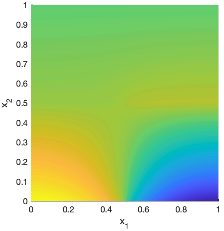
Examples of solutions $u_N(\mu)$ (we take $M = 1000$ snapshots with uniform random μ)



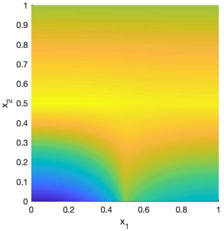
MOR: Thermal block: First 8 POD basis functions



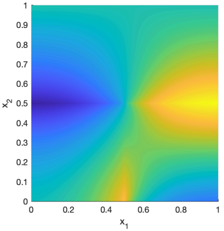
$\boldsymbol{v}_1$



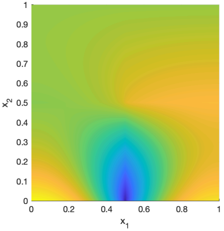
$\boldsymbol{v}_2$



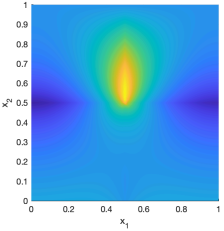
$\boldsymbol{v}_3$



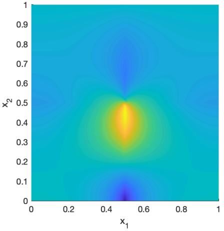
$\boldsymbol{v}_4$



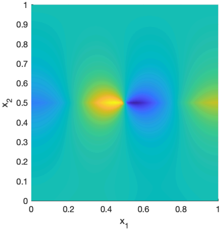
$\boldsymbol{v}_5$



$\boldsymbol{v}_6$

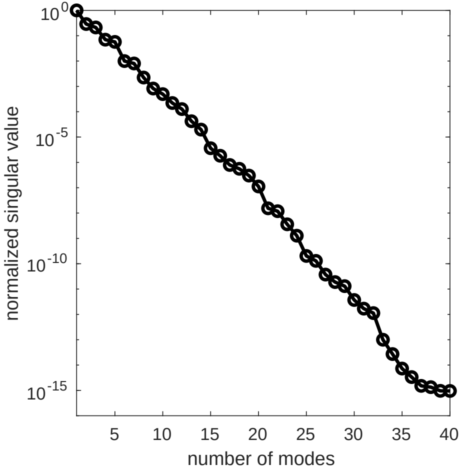


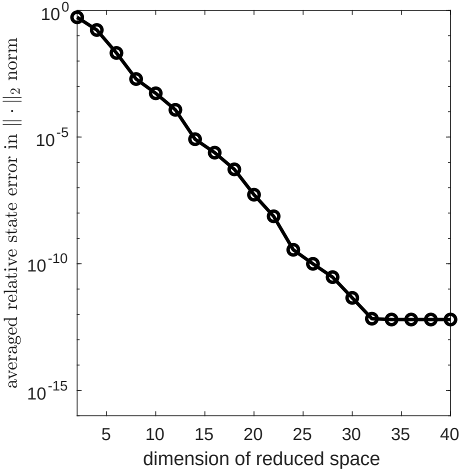
$\boldsymbol{v}_7$



$\boldsymbol{v}_8$

MOR: Thermal block: Singular values and error



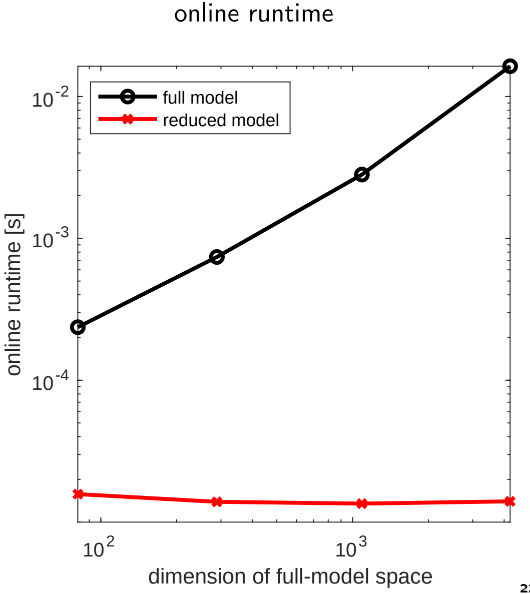


- Singular values decay fast; empirically shows that low-dimensional spaces are sufficient here
- State error over test set $\mathcal{D}_{\text{test}}$ decays with a similar rate as the singular values in this example

MOR: Thermal block: Computational costs

Online runtime of full and reduced model

- Online runtime to compute one solution
- Increasing dimension N of full model, increases full-model runtime
- Runtime of solving reduced model is independent of N, if reduced dimension $r = 20$ fixed



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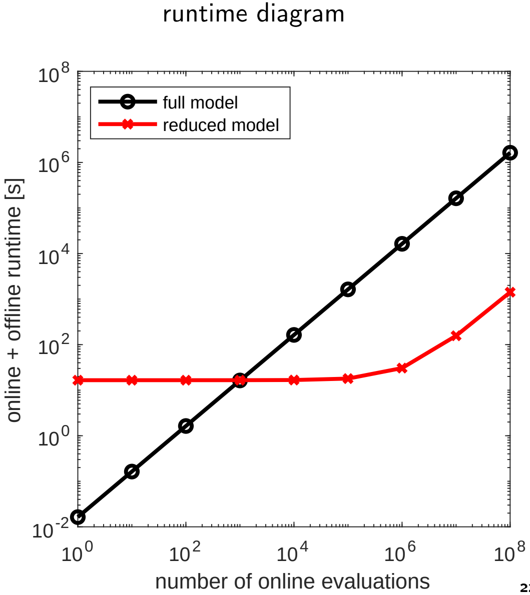
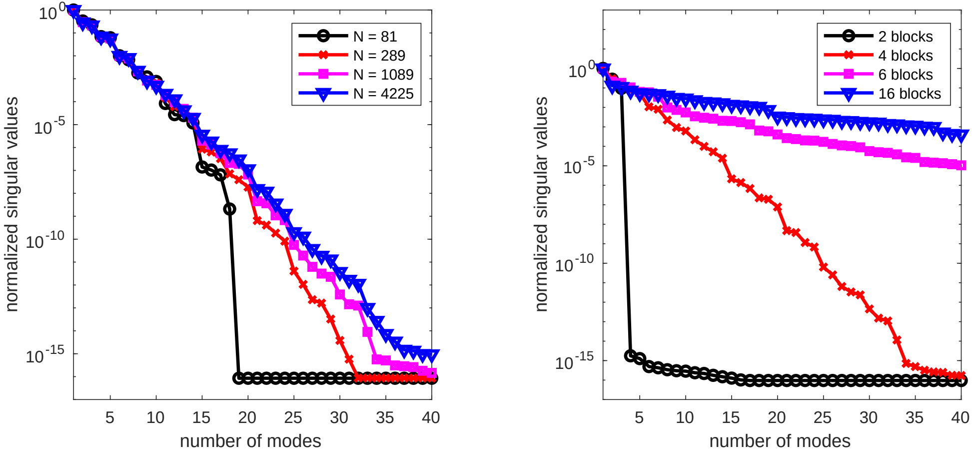
Runtime diagram

- Break even is at 10^3 online evaluations
- Costs of reduced model dominated by offline costs until about 10^5 online evaluations



MOR: Thermal block: Making the problem harder



- Singular values saturate quickly for increasing full-model dimension N
- In contrast, increasing number of blocks (parameters) leads to slower decay of singular values

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3. Model reduction for nonlinear problems

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Time: Systems of ordinary differential equations

System of ordinary differential equations (e.g., after discretization in space)

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t;\boldsymbol{\mu}) = \boldsymbol{f}(\boldsymbol{u}(t;\boldsymbol{\mu}), \boldsymbol{g}(t); \boldsymbol{\mu})$$

- State $\boldsymbol{u}(t;\boldsymbol{\mu}) \in \mathbb{R}^N$ and parameter $\boldsymbol{\mu} \in \mathcal{D}$
- Input $\boldsymbol{g}(t) \in \mathbb{R}^p$
- Right-hand side function $\boldsymbol{f} : \mathbb{R}^N \times \mathbb{R}^p \times \mathcal{D} \to \mathbb{R}^N$
- Time discretized into K time steps $0 = t_0 < t_1 < \cdots < t_K = T$

Special case: Linear time-invariant systems

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t;\boldsymbol{\mu}) = \boldsymbol{A}(\boldsymbol{\mu})\boldsymbol{u}(t;\boldsymbol{\mu}) + \boldsymbol{B}(\boldsymbol{\mu})\boldsymbol{g}(t)\,,$$

- Matrices $\boldsymbol{A}(\boldsymbol{\mu}) \in \mathbb{R}^{N\times N}$ and $\boldsymbol{B}(\boldsymbol{\mu}) \in \mathbb{R}^{N\times p}$

Time: Reduced model via POD

Can apply same procedure as for steady-state problem to system of ODEs

1. Snapshot collection over parameters and time

$$\boldsymbol{S} = \begin{bmatrix} | & & | & & | & & | \\ \boldsymbol{u}_N(t_1;\boldsymbol{\mu}_1) & \dots & \boldsymbol{u}_N(t_K;\boldsymbol{\mu}_1) & \dots & \boldsymbol{u}_N(t_1;\boldsymbol{\mu}_M) & \dots & \boldsymbol{u}_N(t_K;\boldsymbol{\mu}_M) \\ | & & | & & | & & | \end{bmatrix} \in \mathbb{R}^{N \times KM}$$

2. POD basis $\boldsymbol{V}_r \in \mathbb{R}^{N \times r}$ via, e.g., (randomized) SVD of $\boldsymbol{S}$
3. Projection

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}_r(t;\boldsymbol{\mu}) = \boldsymbol{A}_r(\boldsymbol{\mu})\boldsymbol{u}_r(t;\boldsymbol{\mu}) + \boldsymbol{B}_r(\boldsymbol{\mu})\boldsymbol{g}(t)$$

Limitations

- No reduction in time (same number of time steps in full and reduced model)
- Asymptotic stability (passivity, etc.) of full model not necessarily preserved
- In general, structure such as Hamiltonian, Lagrangian, second-order not preserved [Beattie et al., 2011], [Gugercin et al., 2012], [Chaturantabut et al., 2016], [Peng et al., 2016], [Afkham, Hesthaven, 2017]

Time: Frequency domain view on LTI systems

LTI systems with outputs (no parameter for simplicity)

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{u}(t) = \boldsymbol{A}\boldsymbol{u}(t) + \boldsymbol{B}g(t)\,,$$
$$y(t) = \boldsymbol{C}\boldsymbol{u}(t)$$

- Single input $g(t) \in \mathbb{R}$ and single output $y(t) \in \mathbb{R}$ but high-dimensional state $\boldsymbol{u}(t) \in \mathbb{R}^N$
- Often care about approximating input-output map $g(t) \mapsto y(t)$

Input-output map is specified by transfer function (e.g., [Antoulas, 2005], [Antoulas et al., 2020])

$$H(s) = \boldsymbol{C}^T(s\boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{B}\,, \qquad s \in \mathbb{C}$$

- Approximation H_r of H with error in $\mathcal{H}_\infty$

$$\|H - H_r\|_{\mathcal{H}_\infty} = \sup_{|s|=1} |H(s) - H_r(s)|$$

- If H_r approximates H well in $\|\cdot\|_{\mathcal{H}_\infty}$, then $y_r(t)$ approximates $y(t)$ well (e.g., [Benner et al., 2015])

$$\|y - y_r\|_{L_2} \leq \|H - H_r\|_{\mathcal{H}_\infty}\|g\|_{L_2}$$

Time: Interpolating transfer functions

Select $2r$ interpolation points

$$s_1, \dots, s_{2r} \in \mathbb{C}$$

Construct bases as (e.g., [Antoulas, 2005], [Benner et al., 2015], [Antoulas et al., 2020])

$$\boldsymbol{V}_r = \left[(s_1\boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{B} \quad \dots \quad (s_r\boldsymbol{I} - \boldsymbol{A})^{-1}\boldsymbol{B}\right] \in \mathbb{R}^{N\times r}$$
$$\boldsymbol{W}_r = \left[(s_{r+1}\boldsymbol{I} - \boldsymbol{A}^T)^{-1}\boldsymbol{C} \quad \dots \quad (s_{2r}\boldsymbol{I} - \boldsymbol{A}^T)^{-1}\boldsymbol{C}\right] \in \mathbb{R}^{N\times r}$$

Projection via Petrov-Galerkin to obtain reduced operators

$$\boldsymbol{E}_r = \boldsymbol{W}_r^T\boldsymbol{V}_r\,, \qquad \boldsymbol{A}_r = \boldsymbol{W}^T\boldsymbol{A}\boldsymbol{V}_r\,, \qquad \boldsymbol{B}_r = \boldsymbol{W}_r^T\boldsymbol{B}\,, \qquad \boldsymbol{C}_r = \boldsymbol{C}\boldsymbol{V}_r$$

Corresponding reduced model has transfer function H_r that interpolates H at $s_1, \dots, s_{2r}$

$$H(s_i) = H_r(s_i)\,, \qquad i = 1, \dots, 2r$$

Requires $2r$ "full-model solves," which is typically less than what is required with POD

Time: Interpolating transfer functions (cont'd)

Choice of interpolation points

- Optimal (first-order) selection of points
- Iterative Rational Krylov Algorithm (IRKA)

***Learning* reduced models from data**

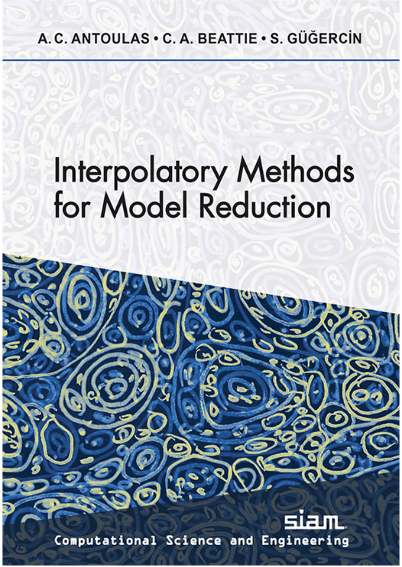
- Matrices $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ not necessarily needed
- Loewner constructs reduced model from data alone

$$\{(s_1, H(s_1)), \ldots, (s_{2r}, H(s_{2r}))\} \subset \mathbb{C}^2$$

- Extends scope to problems with data only

Various extensions

- Matching moments of transfer function
- Multi-input-multi-output (MIMO) systems
- Parametrized systems, ...



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Nonlinear: From linear to nonlinear

Needed linearity in state and affine parameter dependence for efficient online phase

- Compute in offline phase with cost complexity scaling with N

$$\boldsymbol{A}_r^{(i)} = \boldsymbol{V}_r^T \boldsymbol{A}^{(i)} \boldsymbol{V}_r$$

- Cost complexity of online assembly independent of N (provided cost of $\Theta_i^{(a)}$ independent of N)

$$\boldsymbol{A}_r(\boldsymbol{\mu}) = \sum_{i=1}^{Q_a} \Theta_i^{(a)}(\boldsymbol{\mu}) \boldsymbol{A}_r^{(i)}$$

System with nonlinear term (e.g., reaction term)

$$\boldsymbol{A}\boldsymbol{u}_N(\boldsymbol{\mu}) + \boldsymbol{f}(\boldsymbol{u}_N(\boldsymbol{\mu}); \boldsymbol{\mu}) = \boldsymbol{g}$$

- Lifting bottleneck when evaluating reduced nonlinear term $\boldsymbol{f}_r : \mathbb{R}^r \times \mathcal{D} \to \mathbb{R}^r$ [Barrault et al., 2004]

$$\boldsymbol{f}_r(\boldsymbol{u}_r(\boldsymbol{\mu}); \boldsymbol{\mu}) = \underbrace{\boldsymbol{V}_r^T}_{r \times N} \boldsymbol{f}(\underbrace{\boldsymbol{V}_r}_{N \times r} \boldsymbol{u}_r(\boldsymbol{\mu}); \boldsymbol{\mu})$$

- Cost complexity of evaluating reduced $\boldsymbol{f}_r$ online is the same as evaluating $\boldsymbol{f}$ of full model
- Breaks online efficiency → no or little speedups

Nonlinear: Interpolation in subspace

Approximate map $\boldsymbol{u}_r \mapsto \boldsymbol{f}(\boldsymbol{V}_r \boldsymbol{u}_r)$ in subspace given by

$$\boldsymbol{Q} = [\boldsymbol{q}_1, \dots, \boldsymbol{q}_m] \in \mathbb{R}^{N \times m}$$

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$$\boldsymbol{Q} = [\boldsymbol{q}_1, \dots, \boldsymbol{q}_m] \in \mathbb{R}^{N \times m}$$

Find coefficients $\boldsymbol{c}(\boldsymbol{u}_r) \in \mathbb{R}^m$ such that

$$\boldsymbol{f}(\boldsymbol{V}_r\boldsymbol{u}_r) \approx \boldsymbol{Q}\boldsymbol{c}(\boldsymbol{u}_r)$$

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Enforce interpolation conditions by selecting m components $p_1, \dots, p_m$ of $\boldsymbol{f}$ such that

$$\boldsymbol{P}^T\boldsymbol{Q}\boldsymbol{c}(\boldsymbol{u}_r) = \boldsymbol{P}^T\boldsymbol{f}(\boldsymbol{V}_r\boldsymbol{u}_r)$$

where $\boldsymbol{P}^T$ extracts the m rows with indices $p_1, \dots, p_m$

$$\boldsymbol{P} = [\boldsymbol{e}_{p_1}, \dots, \boldsymbol{e}_{p_m}] \in \mathbb{R}^{N\times m}$$

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$$\boldsymbol{P} = [\boldsymbol{e}_{p_1}, \dots, \boldsymbol{e}_{p_m}] \in \mathbb{R}^{N\times m}$$

Solve for $\boldsymbol{c}(\boldsymbol{u}_r)$ via system of linear equations

$$\boldsymbol{c}(\boldsymbol{u}_r) = (\boldsymbol{P}^T\boldsymbol{Q})^{-1}\boldsymbol{P}^T\boldsymbol{f}(\boldsymbol{V}_r\boldsymbol{u}_r)$$

$\rightsquigarrow$ requires evaluating $\boldsymbol{f}$ at only $m \ll N$ components

[Barrault et al., 2004], [Everson, Sirovich, 1995], [Astrid et al., 2004, 2008], [Chaturantabut, Sorensen, 2010], [Drmač, Gugercin, 2016]

Nonlinear: Empirical interpolation in model reduction

Step 1.: Compute POD basis $\boldsymbol{Q} \in \mathbb{R}^{N \times m}$ of nonlinear snapshots

$$\{\boldsymbol{f}(\boldsymbol{u}(\boldsymbol{\mu}_1)), \dots, \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{\mu}_M))\} \subset \mathbb{R}^{N \times M}$$

Step 2.: Select interpolation points $\boldsymbol{P} \in \{0, 1\}^{N \times m}$ at which components to evaluate $\boldsymbol{f}$ online

Step 3.: Approximate $\boldsymbol{f}$ online as

$$\underbrace{\boldsymbol{V}_r^T \boldsymbol{A} \boldsymbol{V}_r}_{r \times r} \boldsymbol{u}_r(\boldsymbol{\mu}) + \underbrace{\boldsymbol{V}_r^T \boldsymbol{Q}(\boldsymbol{P}^T \boldsymbol{Q})^{-1}}_{r \times m} \underbrace{\boldsymbol{P}^T \boldsymbol{f}(\boldsymbol{V}_r \boldsymbol{u}_r(\boldsymbol{\mu}))}_{m \times 1} = \boldsymbol{V}^T \boldsymbol{g}$$

- Requires evaluating $\boldsymbol{f}$ at $m \ll N$ components online
- Empirical interpolation avoids lifting bottleneck

Nonlinear: Selecting interpolation points

Error of EIM approximation

$$\|\boldsymbol{f}(\boldsymbol{u}) - \boldsymbol{Q}(\boldsymbol{P}^T\boldsymbol{Q})^{-1}\boldsymbol{P}^T\boldsymbol{f}(\boldsymbol{u})\|_2 \leq \underbrace{\|(\boldsymbol{P}^T\boldsymbol{Q})^{-1}\|_2}_{\text{points}}\underbrace{\|\boldsymbol{f}(\boldsymbol{u}) - \boldsymbol{Q}\boldsymbol{Q}^T\boldsymbol{f}(\boldsymbol{u})\|_2}_{\text{space}}$$

- Choice of interpolation points $\boldsymbol{P}$ enter in $\|(\boldsymbol{P}^T\boldsymbol{Q})^{-1}\|_2$ only
- Term $\|(\boldsymbol{P}^T\boldsymbol{Q})^{-1}\|_2$ is a Lebesgue constant and grows with dimension m of EIM space

Select interpolation points with greedy algorithm [Barrault et al., 2004], [Chaturantabut, Sorensen, 2010]

```
function p = deim(Q, m)
[~, n] = size(Q);
r = Q(:, 1); [~, p] = max(abs(r));
for i=2:m
    a = Q(p, 1:i-1)\Q(p, i);
    r = Q(:, i) - Q(:, 1:i-1)*a;
    [~, I] = max(abs(r));
    p(i) = I(1);
end
```

Nonlinear: Empirical interpolation (cont'd)

Nonlinear model reduction via discrete **empirical interpolation**
S Chaturantabut, DC Sorensen - SIAM Journal on Scientific Computing, 2010 - SIAM
… method called discrete **empirical interpolation** is proposed and … The original **empirical interpolation** method (EIM) is a … We propose a discrete **empirical interpolation** method (DEIM), a …
Save Cite Cited by 1884 Related articles All 14 versions

An '**empirical interpolation**'method: application to efficient reduced-basis discretization of partial differential equations
M Barrault, Y Maday, NC Nguyen, AT Patera - Comptes Rendus …, 2004 - Elsevier
… equations is certainly a natural candidate for the application of this '**empirical interpolation**' method; we would like to thank this group for many stimulating and beneficial exchanges. …
Save Cite Cited by 1806 Related articles All 13 versions

Model reduction with EIM works well in practice

- Considered a "breakthrough" in model reduction
- Leap towards efficient reduction of nonlinear problems

Issues with EIM

- Stability with poorly chosen points → oversample (gappy POD) [Astrid et al., 2004, 2008], [Carlberg et al., 2011], [Zimmermann, Willcox, 2016], [P., Drmac, Gugercin, 2020]
- Can need tremendous amounts of points if no low-rank structure → adaptivity [P., Willcox, 2015]
- Have to "go back" to full model during online phase → implementation more difficult

Alternatives to EIM for efficient model reduction of nonlinear problems

- Structured nonlinear problems (bilinear, quadratic-bilinear) [Benner, Breiten, 2015], [Benner, Goyal, Gugercin, 2018], [Antoulas et al., 2020]
- Lifting of generally nonlinear problems into quadratic-bilinear problems [Gu, 2011], [Kramer, Willcox, 2019], [Swischuk, Kramer, Huang, Willcox, 2019], [Qian, Kramer, P., Willcox, 2019]

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Using surrogate models alone often means loss of guarantees

Replace model g with a surrogate model

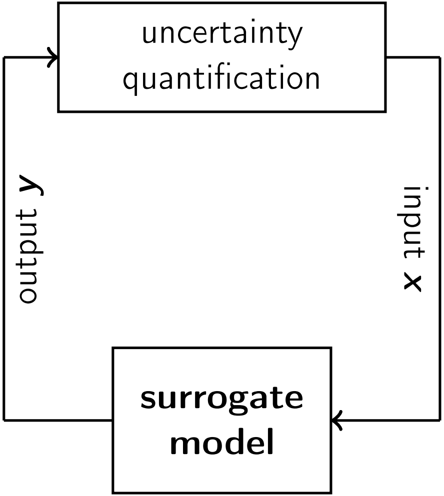
- Costs of outer loop reduced
- Often orders of magnitude speedups

Estimate depends on surrogate accuracy

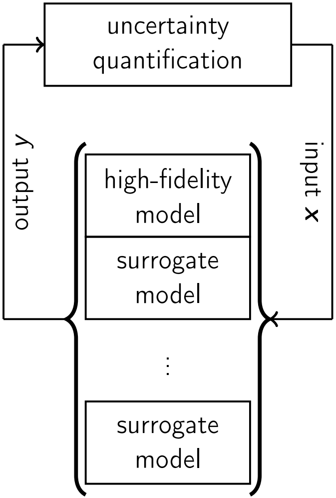
- Control with error bounds/estimators
- Rebuild if accuracy too low
- No guarantees without bounds/estimators

Surrogates alone often mean loss of guarantees

- Propagation of surrogate error on estimate
- Surrogates without error control
- Costs of rebuilding a surrogate model



Multi-fidelity methods to certify outer-loop results



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Survey of Multifidelity Methods in Uncertainty Propagation, Inference, and Optimization*

Benjamin Peherstorfer†
Karen Willcox‡
Max Gunzburger§

Abstract. In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, while lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Outer-loop applications, such as optimization, inference, and uncertainty quantification, require multiple model evaluations at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. This work surveys multifidelity methods that accelerate the solution of outer-loop applications by combining high-fidelity and low-fidelity model evaluations, where the low-fidelity evaluations arise from an explicit low-fidelity model (e.g., a simplified physics approximation, a reduced model, a data-fit surrogate) that approximates the same output quantity as the high-fidelity model. The overall premise of these multifidelity methods is that low-fidelity models are leveraged for speedup while the high-fidelity model is kept in the loop to establish accuracy and/or convergence guarantees. We categorize multifidelity methods according to three classes of strategies: adaptation, fusion, and filtering. The paper reviews multifidelity methods in the outer-loop contexts of uncertainty propagation, inference, and optimization.

Key words. multifidelity, surrogate models, model reduction, multifidelity uncertainty quantification, multifidelity uncertainty propagation, multifidelity statistical inference, multifidelity optimization

AMS subject classifications. 65-02, 62-02, 49-02

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Monte Carlo estimation

Take realizations of input random variable

$$X_1, \dots, X_n \sim X$$

Compute model outputs via numerical simulations

$$g(X_1), \dots, g(X_n)$$

Monte Carlo estimator

$$\overline{y}_n = \frac{1}{n} \sum_{i=1}^{n} g(X_i)$$

Estimator is unbiased $\mathbb{E}[g(X)] = \mathbb{E}[\overline{y}_n]$ with

$$e(\overline{y}_n) = \frac{1}{n} \mathrm{Var}[g(X)]$$

[Figure: PeakPX]

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Why Monte Carlo?

- Models treated as black box

[Figure: PeakPX]

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[Figure: PeakPX]

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Why Monte Carlo?

- Models treated as black box
- Dimension independent
- Easily parallelizable

[Figure: PeakPX]

Monte Carlo estimators with surrogate models

$$\bar{y}_{m_i}^{(i)} = \frac{1}{m_i} \sum_{i=1}^{m_i} g^{(i)}(X_i)\,, \quad i = 1, \dots, k$$

Multifidelity Monte Carlo (MFMC) estimator

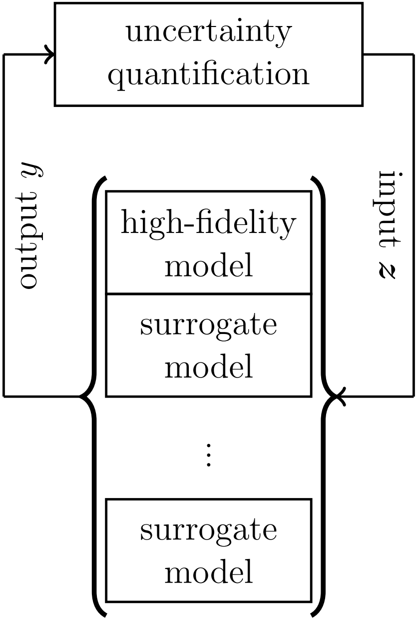
$$\hat{s} = \underbrace{\bar{y}_{m_1}}_{\text{from HFM}} + \sum_{i=1}^{k} \alpha_i \underbrace{\left(\bar{y}_{m_i}^{(i)} - \bar{y}_{m_{i-1}}^{(i)}\right)}_{\text{from surrogate models}}$$

- Control variates help reducing variance of estimator
- Speedup depends on model costs and correlation

$$\rho_i = \frac{\mathrm{Cov}[g(X), g^{(i)}(X)]}{\mathrm{Var}[g(X)]\,\mathrm{Var}[g^{(i)}(X)]}$$

- Estimator remains unbiased

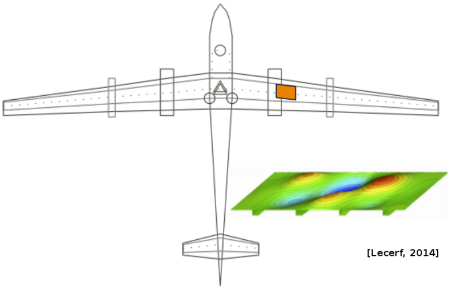
$$\mathbb{E}[\hat{s}] = \mathbb{E}[g(X)]$$



MFMC: Numerical example

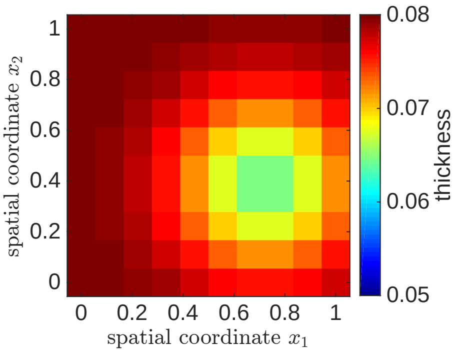
Locally damaged plate in bending

- Inputs: nominal thickness, load, damage
- Output: maximum deflection of plate
- **Only distribution of inputs known**
- Estimate **expected** deflection



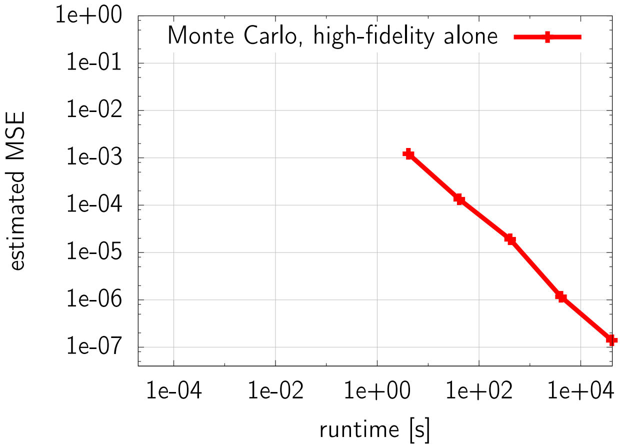
Six models

- High-fidelity model: FEM, 300 DoFs
- Reduced model: POD, 10 DoFs
- Reduced model: POD, 5 DoFs
- Reduced model: POD, 2 DoFs
- Data-fit model: linear interp., 256 pts
- Support vector machine: 256 pts



Var, corr, and costs est. from 100 samples

MFMC: Speedups in uncertainty propagation



- Monte Carlo needs 12h runtime for estimate with error below 10^{-7}
- Multifidelity provides estimator with error below 10^{-7} after 9 seconds

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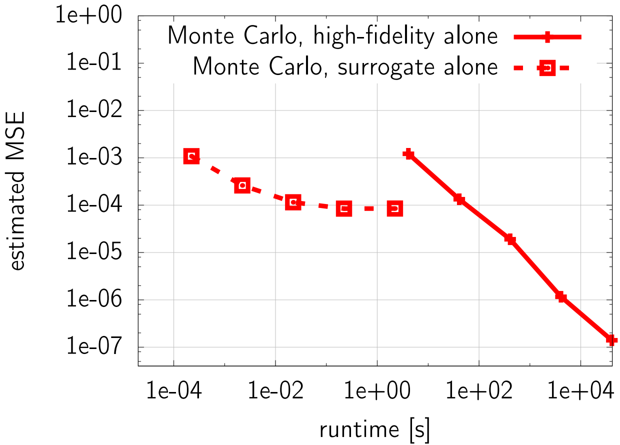

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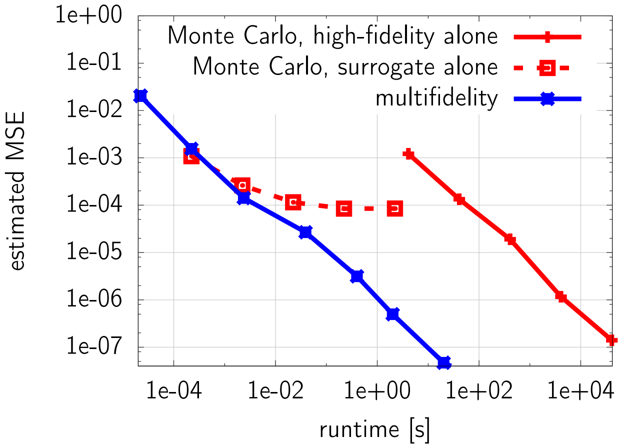

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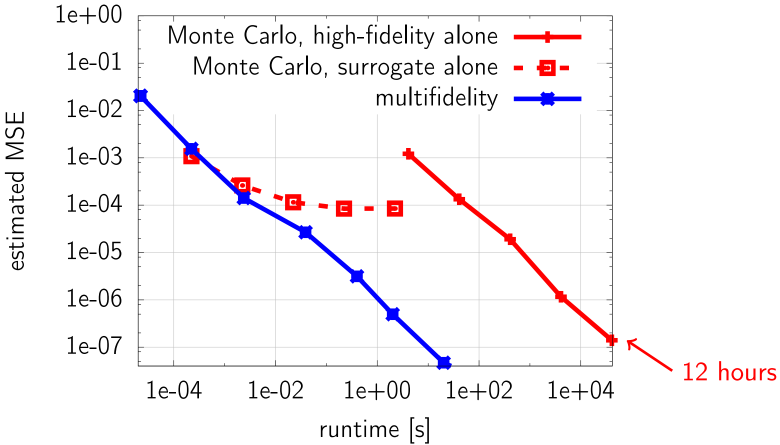

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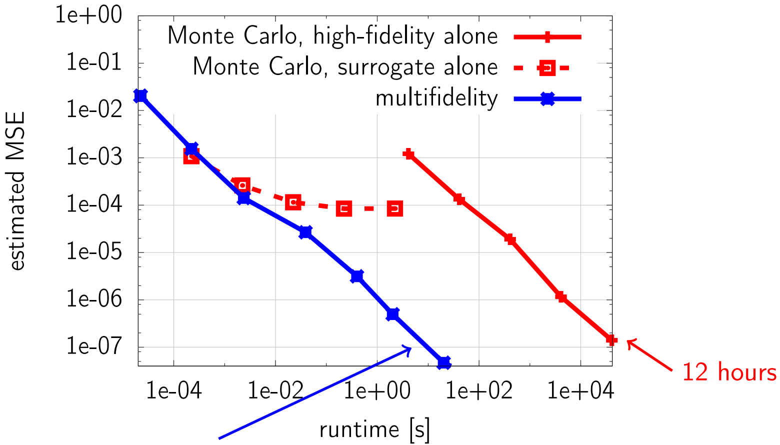

9 seconds: enables design, control, sensitivity analysis *under uncertainty*

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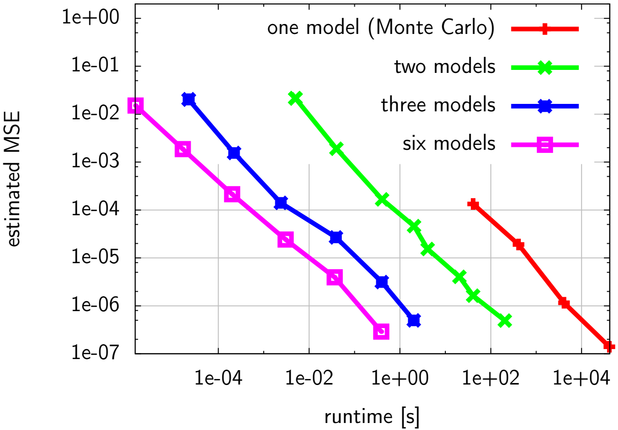
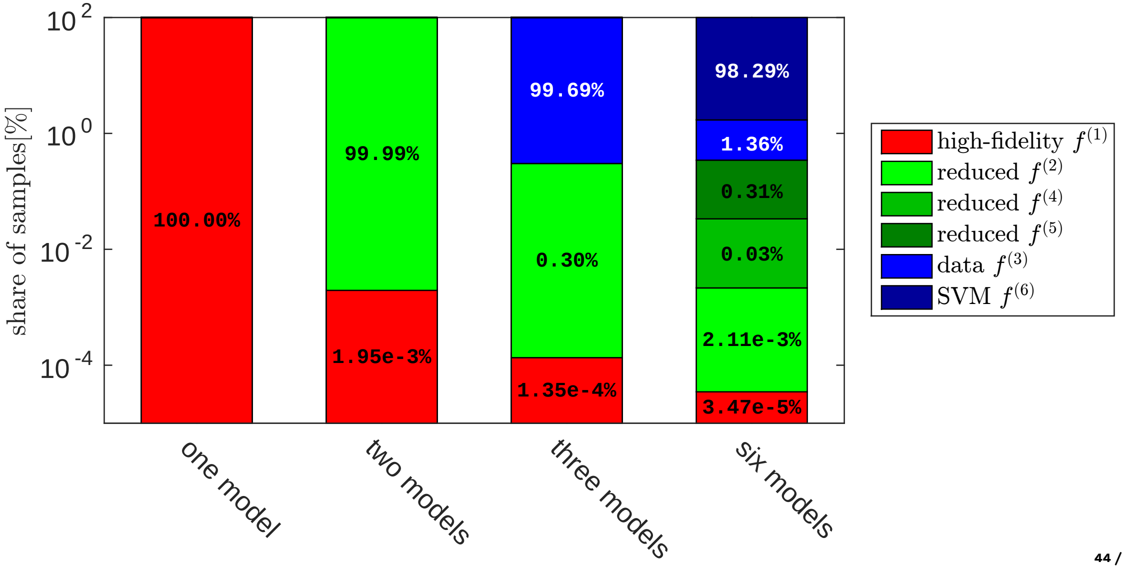
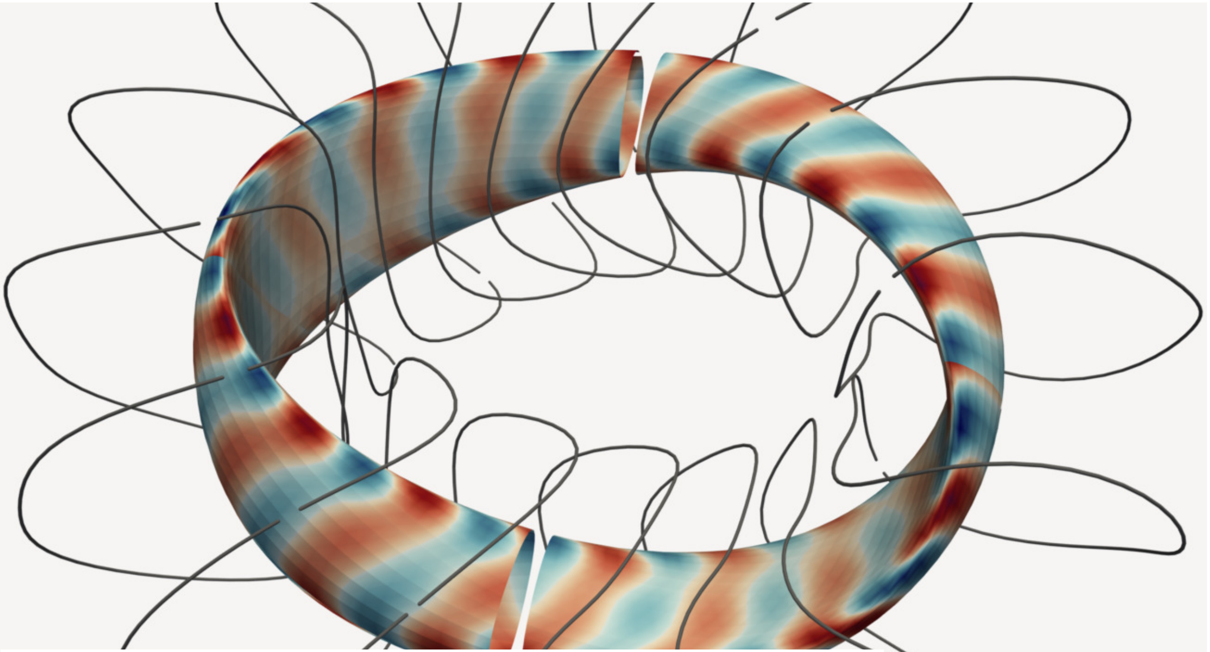
MFMC: Combining many models



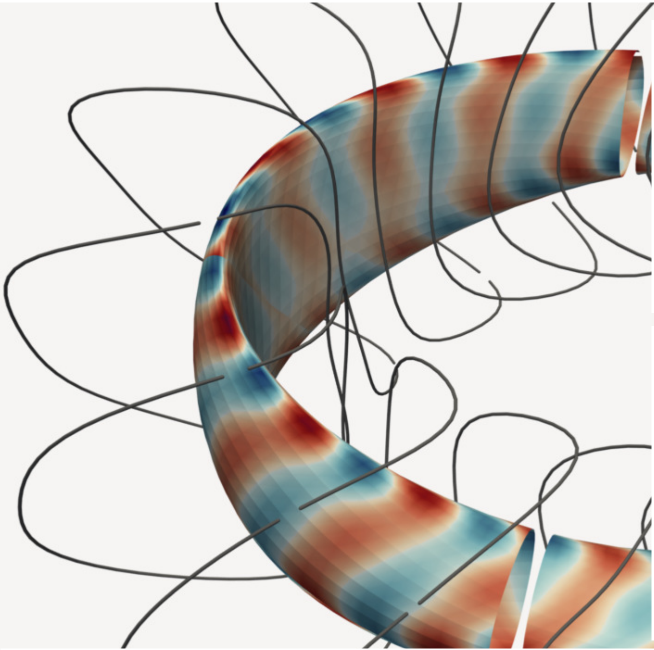
- Largest improvement from "single → two" and "two → three"
- Adding yet another reduced/SVM model reduces variance only slightly

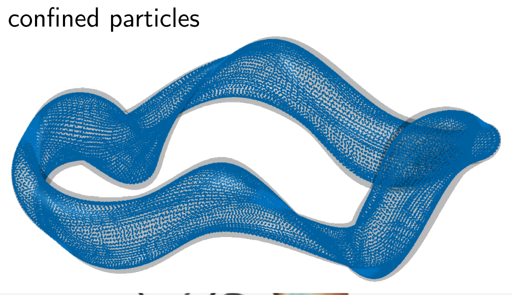
MFMC: Distribution of model evaluations

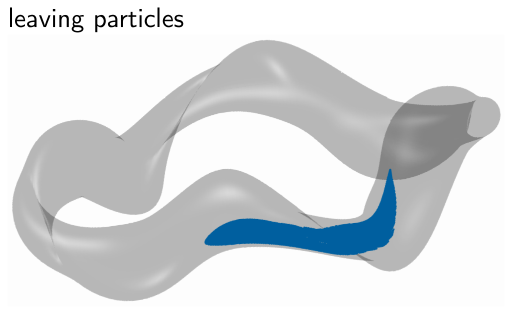




[with Frederick Law, Ionut Farcas, Antoine Cerfon, Georg Stadler, Frank Jenko, Tobias Neckel, Hans-Joachim Bungartz]

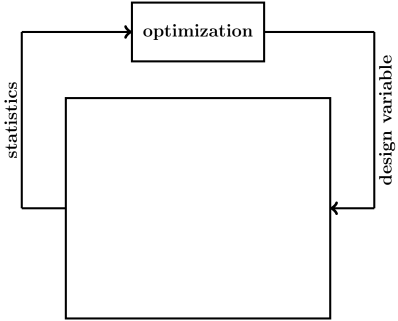






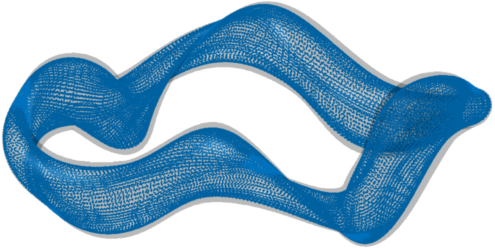
[with Frederick Law, Ionut Farcas, Antoine Cerfon, Georg Stadler, Frank Jenko, Tobias Neckel, Hans-Joachim Bungartz]

Multi-fidelity speed up (Lonestar6/TACC)
72 days $\rightarrow$ 4 hours

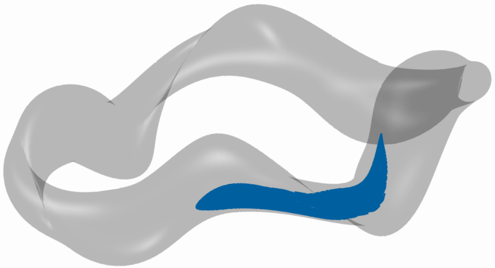


Enables UQ in design, e.g., *robust* coils to maximize confinement in fusion devices

confined particles

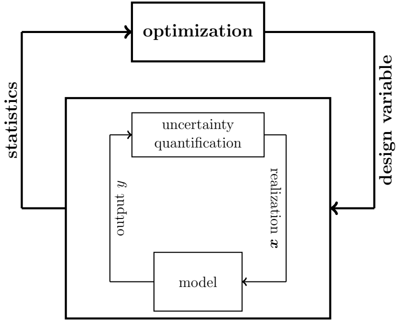


leaving particles



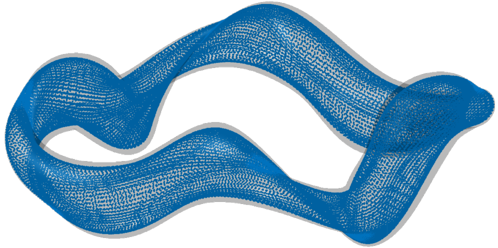
[with Frederick Law, Ionut Farcas, Antoine Cerfon, Georg Stadler, Frank Jenko, Tobias Neckel, Hans-Joachim Bungartz]

Multi-fidelity speed up (Lonestar6/TACC)
72 days $\to$ 4 hours

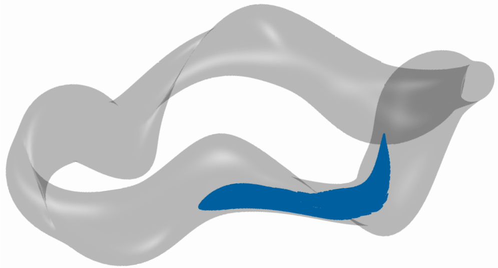


Enables UQ in design, e.g., *robust* coils to maximize confinement in fusion devices

confined particles

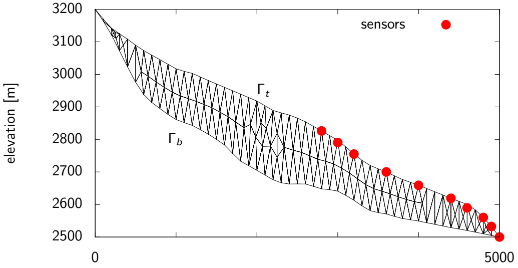


leaving particles

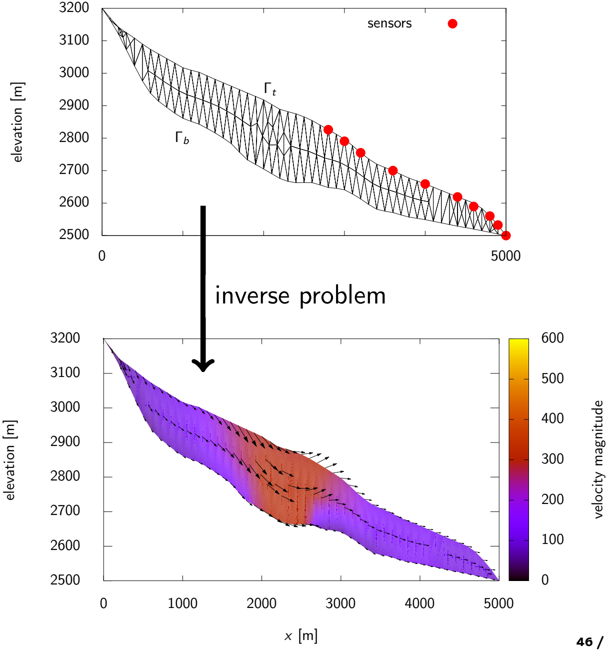


[with Frederick Law, Ionut Farcas, Antoine Cerfon, Georg Stadler, Frank Jenko, Tobias Neckel, Hans-Joachim Bungartz]

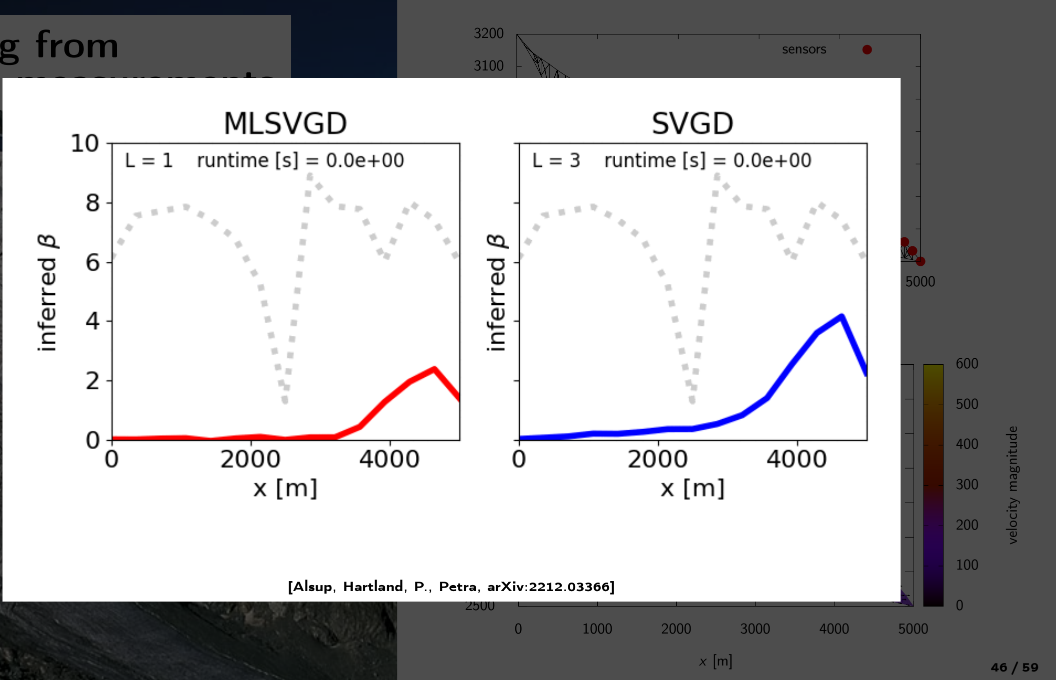
Learning from indirect measurements



Learning from indirect measurements



Learning from indirect measurements



[Alsup, Hartland, P., Petra, arXiv:2212.03366]

Multi-fidelity Monte Carlo in the wild

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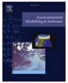

Multifidelity prediction in wildfire spread simulation: Modeling, uncertainty quantification and sensitivity analysis

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[a] Department of Meteorology and Climate Science, San José State University, San José, CA, 95192, USA
[b] Center for Turbulence Research, Stanford University, Stanford, CA, 94305, USA
[c] Department of Fluid Mechanics, Technical University of Catalonia - BarcelonaTech, Barcelona, 08019, Spain

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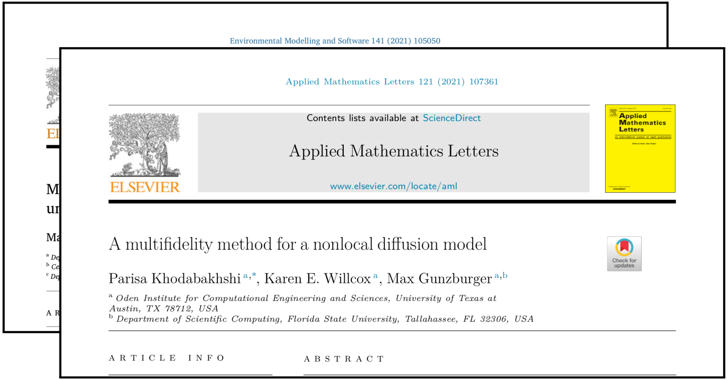
ABSTRACT

Multi-fidelity Monte Carlo in the wild



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A multifidelity method for a nonlocal diffusion model

Parisa Khodabakhshi [a,*], Karen E. Willcox [a], Max Gunzburger [a,b]

[a] Oden Institute for Computational Engineering and Sciences, University of Texas at Austin, TX 78712, USA
[b] Department of Scientific Computing, Florida State University, Tallahassee, FL 32306, USA

ARTICLE INFO

ABSTRACT

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Nucl. Fusion **62** (2022) 076019 (15pp) https://doi.org/10.1088/1741-4326/ac4777

Accelerating the estimation of collisionless energetic particle confinement statistics in stellarators using multifidelity Monte Carlo

Frederick Law*, **Antoine Cerfon** and **Benjamin Peherstorfer**

Courant Institute of Mathematics, New York University, United States of America

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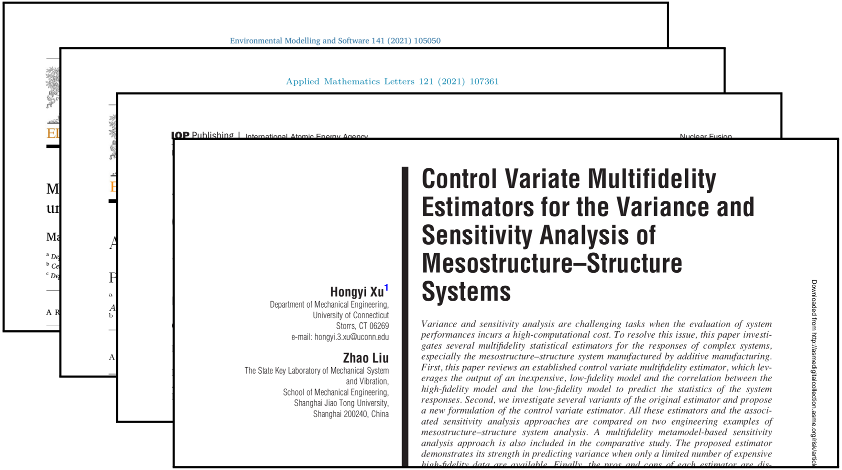
CrossMark

Abstract

Multi-fidelity Monte Carlo in the wild



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Nuclear Fusion

Control Variate Multifidelity Estimators for the Variance and Sensitivity Analysis of Mesostructure–Structure Systems

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Variance and sensitivity analysis are challenging tasks when the evaluation of system performances incurs a high-computational cost. To resolve this issue, this paper investigates several multifidelity statistical estimators for the responses of complex systems, especially the mesostructure–structure system manufactured by additive manufacturing. First, this paper reviews an established control variate multifidelity estimator, which leverages the output of an inexpensive, low-fidelity model and the correlation between the high-fidelity model and the low-fidelity model to predict the statistics of the system responses. Second, we investigate several variants of the original estimator and propose a new formulation of the control variate estimator. All these estimators and the associated sensitivity analysis approaches are compared on two engineering examples of mesostructure–structure system analysis. A multifidelity metamodel-based sensitivity analysis approach is also included in the comparative study. The proposed estimator demonstrates its strength in predicting variance when only a limited number of expensive

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Control Variate Multifidelity

Applications of Multifidelity Reduced Order Modeling to Single and Multiphysics Problems

Pengchao Song, X.Q. Wang and Marc P. Mignolet

AIAA 2020-2131
Session: Special Session: Managing Multiple Information Sources of Multi-Physics Systems

Published Online: 5 Jan 2020 • https://doi.org/10.2514/6.2020-2131

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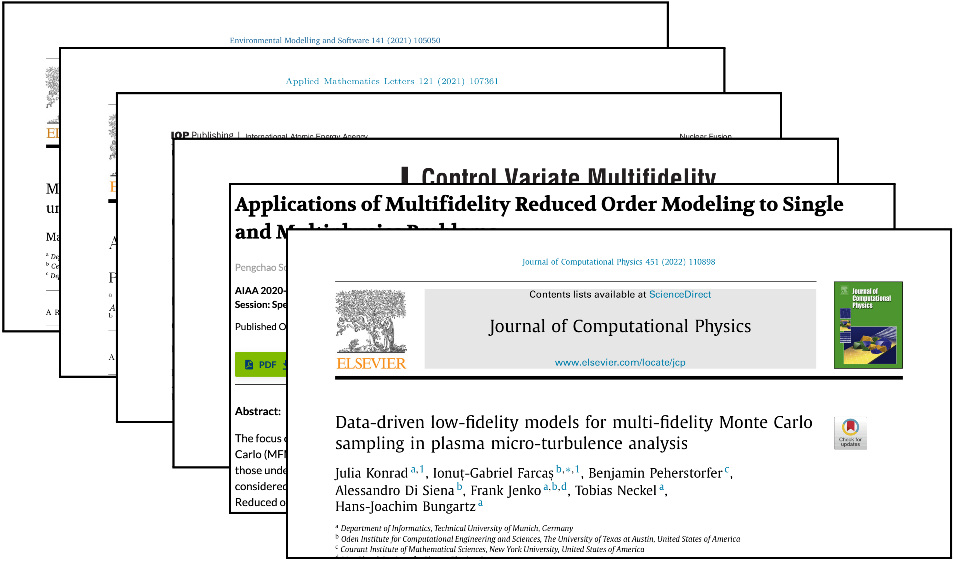
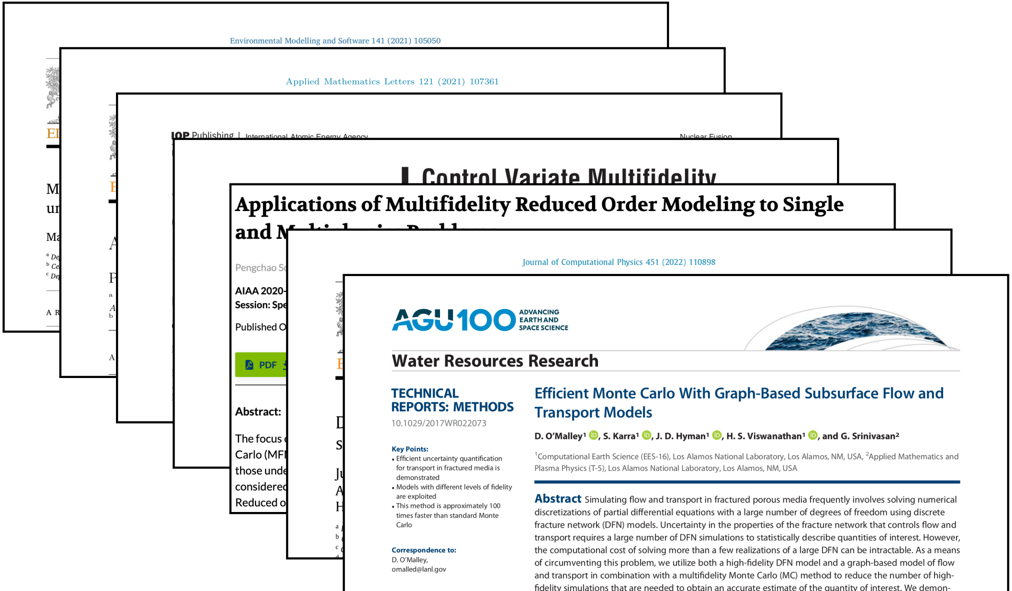
Abstract:

The focus of the present investigation is on assessing the applicability and performance of the recently introduced Multifidelity Monte Carlo (MFMC) for the computationally efficient prediction of the statistics of the random response of uncertain structures especially those undergoing large deformations and modeled within nonlinear reduced order models. Three such nonlinear applications are considered the first of which is a purely structural problem, a panel subjected to a large loads inducing nonlinear geometric effects. Reduced order models with different fidelities are then generated by reducing the size of the basis from a given set of basis functions.

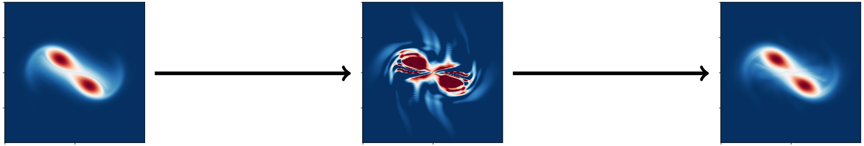
Multi-fidelity Monte Carlo in the wild



Multi-fidelity Monte Carlo in the wild



Learning surrogate models (from data) is key for making tractable outer-loop applications



... but they typically come without accuracy guarantees.

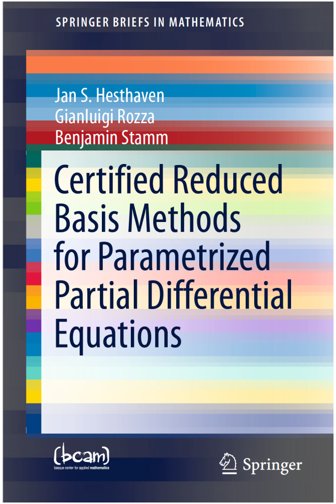
Certify outer-loop results with multi-fidelity methods

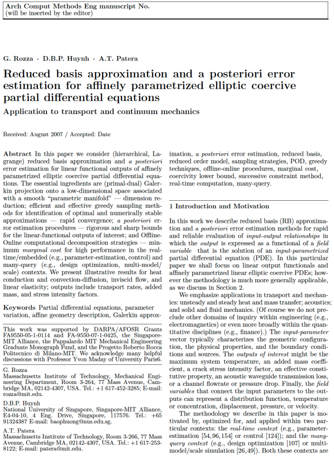
high-fidelity model + surrogate model | surrogate model | ... | surrogate model

... to establish trust for making high-consequence decision and enabling downstream tasks.

Summary and additional resources

Summary: Introduction material on reduced basis method





Arch Comput Methods Eng manuscript No.
(will be inserted by the editor)

G. Rozza · D.B.P. Huynh · A.T. Patera

Reduced basis approximation and a posteriori error estimation for affinely parametrized elliptic coercive partial differential equations

Application to transport and continuum mechanics

Received: August 2007 / Accepted: Date

Abstract In this paper we consider (hierarchical, Lagrange) reduced basis approximation and *a posteriori* error estimation for linear functional outputs of affinely parametrized elliptic coercive partial differential equations. The essential ingredients are (primal-dual) Galerkin projection onto a low-dimensional space associated with a smooth "parametric manifold" — dimension reduction; efficient and effective greedy sampling methods for identification of optimal and numerically stable approximations — rapid convergence; *a posteriori* error estimation procedures — rigorous and sharp bounds for the linear-functional outputs of interest; and Offline-Online computational decomposition strategies — minimum *marginal cost* for high performance in the real-time/embedded (e.g., parameter-estimation, control) and many-query (e.g., design optimization, multi-model/scale) contexts. We present illustrative results for heat conduction and convection-diffusion, inviscid flow, and linear elasticity; outputs include transport rates, added mass, and stress intensity factors.

Keywords Partial differential equations, parameter variation, affine geometry description, Galerkin approximation, *a posteriori* error estimation, reduced basis, reduced order model, sampling strategies, POD, greedy techniques, offline-online procedures, marginal cost, coercivity lower bound, successive constraint method, real-time computation, many-query.

This work was supported by DARPA/AFOSR Grants FA9550-05-1-0114 and FA-9550-07-1-0425, the Singapore-MIT Alliance, the Pappalardo MIT Mechanical Engineering Graduate Monograph Fund, and the Progetto Roberto Rocca Politecnico di Milano-MIT. We acknowledge many helpful discussions with Professor Yvon Maday of University Paris6.

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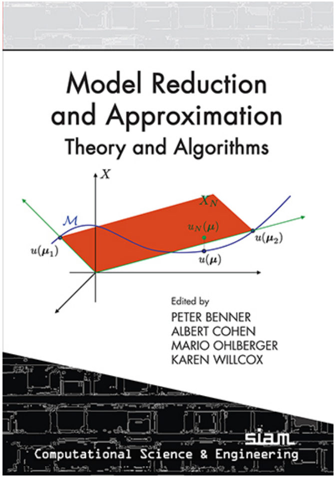
1 Introduction and Motivation

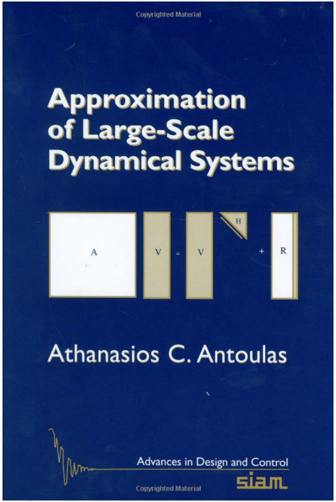
In this work we describe reduced basis (RB) approximation and *a posteriori* error estimation methods for rapid and reliable evaluation of *input-output relationships* in which the *output* is expressed as a functional of a *field variable* that is the solution of an *input-parametrized* partial differential equation (PDE). In this particular paper we shall focus on linear output functionals and affinely parametrized linear elliptic coercive PDEs; however the methodology is much more generally applicable, as we discuss in Section 2.

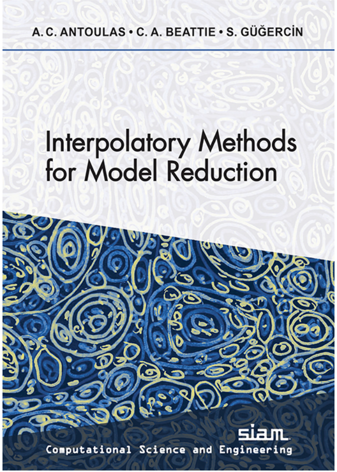
We emphasize applications in transport and mechanics: unsteady and steady heat and mass transfer; acoustics; and solid and fluid mechanics. (Of course we do not preclude other domains of inquiry within engineering (e.g., electromagnetics) or even more broadly within the quantitative disciplines (e.g., finance).) The *input-parameter* vector typically characterizes the geometric configuration, the physical properties, and the boundary conditions and sources. The *outputs of interest* might be the maximum system temperature, an added mass coefficient, a crack stress intensity factor, an effective constitutive property, an acoustic waveguide transmission loss, or a channel flowrate or pressure drop. Finally, the *field variables* that connect the input parameters to the outputs can represent a distribution function, temperature or concentration, displacement, pressure, or velocity.

The methodology we describe in this paper is motivated by, optimized for, and applied within two particular contexts: the *real-time context* (e.g., parameter-estimation [54,96,154] or control [124]); and the *many-query context* (e.g., design optimization [107] or multi-model/scale simulation [26,49]). Both these contexts are



Summary: Introduction material on systems approaches





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A Survey of Projection-Based Model Reduction Methods for Parametric Dynamical Systems*

Peter Benner†
Serkan Gugercin‡
Karen Willcox§

Abstract. Numerical simulation of large-scale dynamical systems plays a fundamental role in studying a wide range of complex physical phenomena; however, the inherent large-scale nature of the models often leads to unmanageable demands on computational resources. Model reduction aims to reduce this computational burden by generating reduced models that are faster and cheaper to simulate, yet accurately represent the original large-scale system behavior. Model reduction of linear, nonparametric dynamical systems has reached a considerable level of maturity, as reflected by several survey papers and books. However, parametric model reduction has emerged only more recently as an important and vibrant research area, with several recent advances making a survey paper timely. Thus, this paper aims to provide a resource that draws together recent contributions in different communities to survey the state of the art in parametric model reduction methods.

Parametric model reduction targets the broad class of problems for which the equations governing the system behavior depend on a set of parameters. Examples include parameterized partial differential equations and large-scale systems of parameterized ordinary differential equations. The goal of parametric model reduction is to generate low-cost but accurate models that characterize system response for different values of the parameters. This paper surveys state-of-the-art methods in projection-based parametric model reduction, describing the different approaches within each class of methods for handling parametric variation and providing a comparative discussion that lends insights to potential advantages and disadvantages in applying each of the methods. We highlight the important role played by parametric model reduction in design, control, optimization, and uncertainty quantification—settings that require repeated model evaluations over different parameter values.

Key words. dynamical systems, parameterized model reduction, (Petrov–)Galerkin projection, Krylov subspace method, moments, interpolation, proper orthogonal decomposition, balanced truncation, greedy algorithm

AMS subject classifications. 35B30, 37M99, 41A05, 65K99, 93A15, 93C05

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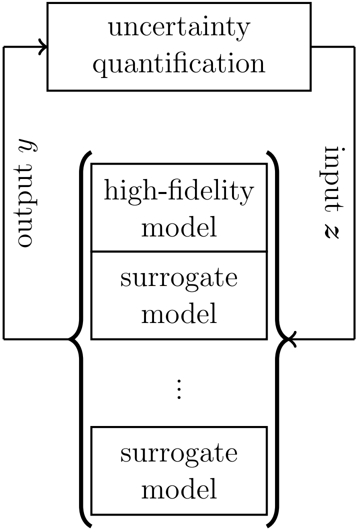
‡Department of Mathematics, Virginia Tech, Blacksburg, VA 24061-0123 (gugercin@math.vt.edu). The work of this author was supported by NSF grant DMS-1217156 (Program Manager L.M. Jameson).

§Department of Aeronautics & Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139 (kwillcox@mit.edu). The work of this author was supported by AFOSR Computational Mathematics grant FA9550-12-1-0420 (Program Manager F. Fahroo) and the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research, Applied Mathematics program under awards DE-FG02-08ER2585 and DE-SC0009297 (Program Manager A. Landsberg).

Summary: Multi-fidelity methods to *certify* outer-loop results



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Survey of Multifidelity Methods in Uncertainty Propagation, Inference, and Optimization*

Benjamin Peherstorfer†
Karen Willcox‡
Max Gunzburger§

Abstract. In many situations across computational science and engineering, multiple computational models are available that describe a system of interest. These different models have varying evaluation costs and varying fidelities. Typically, a computationally expensive high-fidelity model describes the system with the accuracy required by the current application at hand, while lower-fidelity models are less accurate but computationally cheaper than the high-fidelity model. Outer-loop applications, such as optimization, inference, and uncertainty quantification, require multiple model evaluations at many different inputs, which often leads to computational demands that exceed available resources if only the high-fidelity model is used. This work surveys multifidelity methods that accelerate the solution of outer-loop applications by combining high-fidelity and low-fidelity model evaluations, where the low-fidelity evaluations arise from an explicit low-fidelity model (e.g., a simplified physics approximation, a reduced model, a data-fit surrogate) that approximates the same output quantity as the high-fidelity model. The overall premise of these multifidelity methods is that low-fidelity models are leveraged for speedup while the high-fidelity model is kept in the loop to establish accuracy and/or convergence guarantees. We categorize multifidelity methods according to three classes of strategies: adaptation, fusion, and filtering. The paper reviews multifidelity methods in the outer-loop contexts of uncertainty propagation, inference, and optimization.

Key words. multifidelity, surrogate models, model reduction, multifidelity uncertainty quantification, multifidelity uncertainty propagation, multifidelity statistical inference, multifidelity optimization

AMS subject classifications. 65-02, 62-02, 49-02

DOI. 10.1137/16M1082469

Summary: Software

https://pymor.org/

https://github.com/pressio/pressio

Operator Inference

https://pypi.org/project/rom-operator-inference/

RBmatlab

https://www.morepas.org/software/rbmatlab/

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Equations

$$\ldots \tag{2}$$

$$\ldots \tag{3}$$

$$\ldots \tag{4}$$