Randomized Model Order Reduction

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joint work with
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Model Reduction of Parametrized Systems (MoRePaS IV)

Motivation/Outline

- Motivation: Randomized methods have got a steadily growing deal of attention in recent years, especially for problems in large-scale data analysis.
  Two most important benefits:
  - They can result in faster algorithms, either in worst-case asymptotic theory and/or numerical implementation,
  - they allow very often for (novel) tight error bounds
- Topic of this talk: Show how we can benefit from randomized methods in model order reduction

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- Topic of this talk: Show how we can benefit from randomized methods in model order reduction
- Outline:
  1. Short overview on randomized methods
  2. Projection-based model order reduction
  3. Present randomized a posteriori error estimator for projection-based model reduction error that does not require the computation/ estimation of stability constants
  4. Build adaptively a reduced space in localized model order reduction that converges at a quasi-optimal rate

Randomized Numerical Linear Algebra

- produce random "sketch" of a matrix and then use the sketch as a surrogate for computations
  - sketch is a smaller or sparser matrix that represents the essential information in the original matrix
  - generated by random sampling
- How to generate a sketch?
  - Element-wise sampling (unfavorable error bounds)
  - Row/column sampling $\rightarrow$ CUR decomposition
  - apply given matrix to random matrix $\rightarrow$ SVD, QR decomposition

For an overview on algorithms and associated error estimates see for instance: [Halko et al 2011], [Mahoney 2011], [Drineas, Mahoney, 2016]

Why can randomization work?

- Goal: Given a matrix $B \in \mathbb{R}^{m \times n}$ and an integer k find an orthonormal matrix Q of rank k such that $B \approx QQ^*B$.
- Approach:
- Draw k random vectors $r_j \in \mathbb{R}^n$ (say standard Gaussian)
- Form sample vectors $y_j = Br_j \in \mathbb{R}^m \quad j = 1, \ldots, k$.
- Orthonormalize $y_j \longrightarrow q_j, = 1, \ldots, k$ and define $Q = [q_1, \ldots, q_k]$
- Result: If B has exactly rank k then $q_j, = 1, \ldots, k$ span the range of B at probability 1. But also in the general case $q_j, = 1, \ldots, k$ often perform nearly as good as the k leading left singular vectors of B
- Compute randomized SVD:
- Form $C = Q^*B$ which yields $B \approx QC$
- Compute SVD of of the small matrix $C = \widetilde{U}\Sigma V^*$ and set $U = Q\widetilde{U}$

Subspace embeddings and concentration inequalities

Proposition (Concentration inequality; Johnson-Lindenstrauss)

- *Choose rows of a matrix* $\Phi : \mathbb{R}^{\mathcal{N}} \to \mathbb{R}^{K}$ *say as* K *independent copies of standard Gaussian random vectors scaled by* $1/\sqrt{K}$
- $0 < \varepsilon < 1$
- $\mathcal{S} \subset \mathbb{R}^{\mathcal{N}}$ *a finite set*
- *assume* $K \geqslant (C(z)/\varepsilon^2)\log(\#\mathcal{S}/\delta)$.

Then we have

$$\mathbb{P}\left\{(1-\varepsilon)\|x-y\|_2^2 \leqslant \|\Phi x - \Phi y\|_2^2 \leqslant (1+\varepsilon)\|x-y\|_2^2 \quad \forall x, y \in \mathcal{S}\right\} \geqslant 1-\delta.$$

see for instance [Boucheron, Lugosi, Massart 2012], [Vershynin 2012], [Vershynin 2018+]

References for randomization in reduced order modelling

Exploiting randomization for construction of reduced spaces:

- Hochman et al 2014
- Alla, Kutz 2015
- Zahm, Nouy 2016
- Balabanov, Nouy 2018

Randomization within error estimation:

- Cao, Petzold 2004, Homescu, Petzold, Serban 2005
- Drohmann, Carlberg 2015, Trehan, Carlberg, and Durlofsky 2017
- Manzoni, Pagani, Lassila 2016
- Janon, Nodet, Prieur 2016
- Giraldi, Nouy 2017
- Balabanov, Nouy 2018

Projection-based model order reduction

Parametrized Partial Differential Equation

- Parameter vector $\mu \in \mathcal{P}$; compact parameter set $\mathcal{P} \subset \mathbb{R}^P$
- Parametrized PDE: Given any $\mu \in \mathcal{P}$, find $u(\mu) \in X$, s.th.

$$A(\mu)u(\mu) = f(\mu) \quad \text{in } X'.$$

- $\Omega \subset \mathbb{R}^3$: bounded domain with Lipschitz boundary $\partial\Omega$
- $H_0^1(\Omega)^d \subset X \subset H^1(\Omega)^d$ $(d = 1, 2, 3)$; X': dual space
- $A(\mu) : X \to X'$: inf-sup stable, continuous linear differential operator
- $f(\mu) : X \to \mathbb{R}$: continuous linear form

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- High-dimensional discretization:
- Introduce high-dimensional FE space $X^{\mathcal{N}} \subset X$ with $\dim(X^{\mathcal{N}}) = \mathcal{N}$ (assume small discretization error)
- High-dimensional approximation: Given any $\mu \in \mathcal{P}$, find $u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}}$, s.th.

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$$\underline{A}(\mu)\underline{u}^{\mathcal{N}}(\mu) = \underline{f}(\mu) \quad \underline{A}(\mu) \in \mathbb{R}^{\mathcal{N} \times \mathcal{N}}, \underline{f}(\mu) \in \mathbb{R}^{\mathcal{N}}.$$

Projection-based model order reduction

- Assume that we have given some reduced space $X^N \subset X^{\mathcal{N}}$ with $\dim(X^N) = N$.
- Galerkin projection on X^N: Given any $\mu \in \mathcal{P}$, find $u^N(\mu) \in X^N$, s.th.

$$A(\mu)u^N(\mu) = f(\mu) \quad \text{in } X^{N\prime}.$$

- Want to assess the approximation error $e(\mu) = u^{\mathcal{N}}(\mu) - u^N(\mu)$.

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Proposition (A posteriori error bound)

The error estimator $\widetilde{\Delta}_N(\mu) = \beta_{LB}(\mu)^{-1}\|f(\mu) - A(\mu)u^N(\mu)\|_{X^{\mathcal{N}\prime}}$ *with* $\beta_{LB}(\mu) \leqslant \beta_{\mathcal{N}}(\mu)$ *satisfies*

$$\|u^{\mathcal{N}}(\mu) - u^N(\mu)\|_X \leqslant \widetilde{\Delta}_N(\mu) \leqslant \frac{\gamma_{\mathcal{N}}(\mu)}{\beta_{LB}(\mu)}\|u^{\mathcal{N}}(\mu) - u^N(\mu)\|_X,$$

where $\beta_{\mathcal{N}}(\mu) := \inf_{v\in X^{\mathcal{N}}} \sup_{w\in X^{\mathcal{N}}} \frac{\langle A(\mu)v,w\rangle}{\|v\|_X\|w\|_X}$ *and* $\gamma_{\mathcal{N}}(\mu) = \sup_{v\in X^{\mathcal{N}}} \sup_{w\in X^{\mathcal{N}}} \frac{\langle A(\mu)v,w\rangle}{\|v\|_X\|w\|_X}$.

Randomized residual-based error estimators for parametrized equations

K. Smetana, O. Zahm, and A. T. Patera
Randomized residual-based error estimators for parametrized equations
arXiv:1807.10489

Goal/Motivation

- Goal: Develop a posteriori error estimator for projection-based model order reduction that does not contain constants whose estimation is expensive (inf-sup constant)
- Setting: We query a finite number of parameters in the online stage for which we want to estimate the approximation error.
- Approach: Exploit results for random subspace embeddings

Proposition (Concentration inequality, Johnson-Lindenstrauss)

Choose rows of matrix Φ say as K independent copies of standard Gaussian random vectors scaled by $1/\sqrt{K}$ and let $\mathcal{S} \subset \mathbb{R}^{\mathcal{N}}$ be a finite set. Moreover, assume $K \geqslant (C(z)/\varepsilon^2)\log(\#\mathcal{S}/\delta)$. Then we have

$$\mathbb{P}\left\{(1-\varepsilon)\|x-y\|_2^2 \leqslant \|\Phi x - \Phi y\|_2^2 \leqslant (1+\varepsilon)\|x-y\|_2^2 \quad \forall x, y \in \mathcal{S}\right\} \geqslant 1-\delta.$$

Assumptions on random vector

- $Z \in \mathbb{R}^{\mathcal{N}}$: random vector such that

$$\|v\|_\Sigma^2 = v^T \Sigma v = \mathbb{E}((Z^T v)^2) \quad \forall v \in \mathbb{R}^{\mathcal{N}},$$

where Σ is matrix e.g. associated with H^1- or L^2-inner product or a quantity of interest

$\Longrightarrow$ $(Z^T v)^2$ is an unbiased estimator of $\|v\|_\Sigma^2$

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- For simplicity: Assume $Z \sim \mathcal{N}(0, \Sigma)$ is a Gaussian vector with zero mean and covariance matrix Σ
- $Z_1, \ldots, Z_K$: K independent copies of Z
- Consider the following (unbiased) Monte-Carlo estimator of $\|v\|_{\Sigma}^2$

$$\frac{1}{K} \sum_{i=1}^{K} (Z_i^T v)^2.$$

Proposition (Concentration inequality)

For any given $w \in \mathbb{R}$, $w > \sqrt{e}$ and $K \geqslant 3$ we have for one fixed but arbitrary $\mu_j \in \mathcal{P}$

$$\mathbb{P}\left\{ \frac{\|\underline{e}(\mu_j)\|_{\Sigma}^2}{w^2} \leqslant \frac{1}{K}\sum_{i=1}^{K}(Z_i^T \underline{e}(\mu_j))^2 \leqslant w^2 \|\underline{e}(\mu_j)\|_{\Sigma}^2 \right\} \geqslant 1 - \left(\frac{\sqrt{e}}{w}\right)^K,$$

where $\underline{e}(\mu_j) = \underline{u}^{\mathcal{N}}(\mu_j) - \underline{u}^{N}(\mu_j)$.

Sketch of Proof:

- $\frac{K}{\|\underline{e}(\mu_j)\|_{\Sigma}^2}\left(\frac{1}{K}\sum_{i=1}^{K}(Z_i^T \underline{e}(\mu_j))^2\right) = \left(\sum_{i=1}^{K}\frac{(Z_i^T \underline{e}(\mu_j))^2}{\|\underline{e}(\mu_j)\|_{\Sigma}^2}\right)$ follows a chi-squared distribution with K degrees of freedom (denoted $\chi^2(K)$)
- Use cumulative distribution function of $\chi^2(K)$ distribution and Markov inequality

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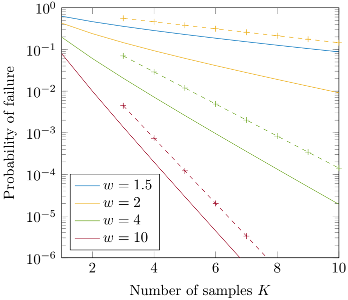

Proposition (Concentration inequality for set of vectors)

Given a finite set of parameters $\mathcal{S} = \{\mu_1, \ldots, \mu_S\} \subset \mathcal{P}$, a failure probability $0 < \delta < 1$, $w \in \mathbb{R}$, $w > \sqrt{e}$, we have for

$$K \geqslant \frac{\log(\#\mathcal{S}) + \log(\delta^{-1})}{\log(w/\sqrt{e})} \qquad \textit{that}$$

$$\mathbb{P}\left\{ \frac{\|\underline{e}(\mu_j)\|_\Sigma^2}{w^2} \leqslant \frac{1}{K}\sum_{i=1}^{K}(Z_i^T \underline{e}(\mu_j))^2 \leqslant w^2 \|\underline{e}(\mu_j)\|_\Sigma^2, \;\; \forall \mu_j \in \mathcal{S} \right\} \geqslant 1 - \delta.$$

Proof: union bound argument

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In contrast to Johnson-Lindenstrauss lemma a larger effectivity w allows us to use a smaller number of samples K.

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	$w=2$	$w=3$	$w=4$	$w=5$	$w=10$
$\#\mathcal{S}=1$	24	8	6	5	3
$\#\mathcal{S}=100$	48	16	11	9	6
$\#\mathcal{S}=1000$	60	20	13	11	7
$\#\mathcal{S}=10^6$	96	31	21	17	11

Table: Values for K that guarantee (1) for all $\mu_j \in \mathcal{S}$ with $\delta = 10^{-2}$.

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Define $\Delta(\mu) := \left(\frac{1}{K} \sum_{i=1}^{K} (Z_i^T \underline{e}(\mu))^2 \right)^{1/2}$

Problem: estimator $\Delta(\mu) = \left(\frac{1}{K} \sum_{i=1}^{K} (Z_i^T (\underline{u}^{\mathcal{N}}(\mu_j) - \underline{u}^N(\mu_j)))^2 \right)^{1/2}$

involves high-dimensional finite element solution

$\Longrightarrow$ Computationally infeasible in the online stage

A constant-free, randomized a posteriori error estimator

- Exploit error residual relationship

$$
\begin{aligned}
Z_i^T(\underline{u}^{\mathcal{N}}(\mu) - \underline{u}^N(\mu)) &= Z_i^T \underline{A}(\mu)^{-1}\underline{A}(\mu)(\underline{u}^{\mathcal{N}}(\mu) - \underline{u}^N(\mu)) \\
&= Z_i^T \underline{A}(\mu)^{-1}\underbrace{(\underline{f}(\mu) - \underline{A}(\mu)\underline{u}^N(\mu))}_{\text{residual}} \\
&= \underbrace{(\underline{A}(\mu)^{-T} Z_i)}_{\text{dual problem}}{}^T \underbrace{(\underline{f}(\mu) - \underline{A}(\mu)\underline{u}^N(\mu))}_{\underline{r}(\mu):=}
\end{aligned}
$$

- Define solutions of dual problem with random right-hand sides Z_i:
$\underline{y}_i^{\mathcal{N}}(\mu) := \underline{A}(\mu)^{-T} Z_i$

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- Define solutions of dual problem with random right-hand sides Z_i: $\underline{y}_i^{\mathcal{N}}(\mu) := \underline{A}(\mu)^{-T}Z_i$
- Rewrite randomized a posteriori error estimator

$$\Delta(\mu) = \left(\frac{1}{K}\sum_{i=1}^{K}(\underline{y}_i^{\mathcal{N}}(\mu)^T\underline{r}(\mu))^2\right)^{1/2}$$

A fast-to-evaluate randomized error estimator

- Approximation of the dual solutions via projection-based model order reduction:

$$\underline{y}_i^{\mathcal{N}}(\mu) \approx \underline{y}_i^{N_{du}}(\mu) \in Y^{N_{du}} \subset X^{\mathcal{N}},$$

  where $Y^{N_{du}}$ dual reduced space (we use one space for all K dual problems)
- Define fast-to-evaluate randomized error estimator

$$\Delta^{N_{du}}(\mu) := \left(\frac{1}{K} \sum_{i=1}^{K} (\underline{y}_i^{N_{du}}(\mu)^T \underline{r}(\mu))^2 \right)^{1/2}$$

- By using an auxiliary problem $\Delta^{N_{du}}(\mu)$ can be evaluated by solving one (and not K) linear system of equations of size N_{du}
  $\rightarrow$ computational complexity of $\Delta^{N_{du}}(\mu)$ in general $\mathcal{O}(N_{du}^3)$

A fast-to-evaluate randomized error estimator

Proposition

Choose $S \in \mathbb{N}$ in the offline stage. Then, in the online stage for any given $w > \sqrt{e}$ and $\delta > 0$ we have for S different parameters values μ_j, $j = 1, \ldots, S$ in a finite parameter set $\mathcal{S} = \{\mu_1, \ldots, \mu_S\}$ and

$$K \geqslant \frac{\log(S) + \log(\delta^{-1})}{\log(w/\sqrt{e})} \qquad \text{that} \qquad \Delta^{N_{du}}(\mu_j) := \left(\frac{1}{K} \sum_{i=1}^{K} (\underline{y}_i^{N_{du}}(\mu_j)^T \underline{r}(\mu_j))^2 \right)^{1/2}$$

satisfies

$$\mathbb{P}\Big\{ (\alpha w)^{-1} \Delta^{N_{du}}(\mu_j) \leqslant \|\underline{e}(\mu_j)\|_\Sigma \leqslant (\alpha w)\, \Delta^{N_{du}}(\mu_j), \quad \mu_j \in \mathcal{S}, \Big\} \geqslant 1 - \delta,$$

where

$$\alpha = \max_{\mu \in \mathcal{P}} \left(\max \left\{ \frac{\Delta(\mu)}{\Delta^{N_{du}}(\mu)}, \frac{\Delta^{N_{du}}(\mu)}{\Delta(\mu)} \right\} \right) \geqslant 1.$$

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satisfies

$$\mathbb{P}\left\{ (w+\varepsilon)^{-1} \Delta^{N_{du}}(\mu_j) \leqslant \|\underline{e}(\mu_j)\|_{\Sigma} \leqslant \frac{w}{1 - w\,\varepsilon} \Delta^{N_{du}}(\mu_j), \quad \forall \mu_j \in \mathcal{S} \right\} \geqslant 1 - \delta.$$

where

$$\varepsilon = \sup_{\mu \in \mathcal{P}} \left\{ \max_{1 \leqslant i \leqslant K} \|\underline{A}^T(\mu) \underline{y}_i^{\mathcal{N}}(\mu) - Z_i\|_{\Sigma^{-1}} \right\}$$

and we assume invertibility of Σ and that there holds almost surely $\varepsilon \leqslant w^{-1}$.

Algorithm 1: Greedy construction of the reduced space

input : Operator $A(\mu)$, size of the online parameter set S, covariance Σ, target effectivity parameters α, w, probability of failure δ, finite training set $\mathcal{P}^{train}$

output: The samples $Z_1, \ldots, Z_K$, the reduced space $Y^{N_{du}}$.

Initialize $Y^0 = \{0\}$, $l = 0$; Determine $K = (\log(S) + \log(\delta^{-1}))/\log(w/\sqrt{e})$

Draw the samples $Z_1, \ldots, Z_K \sim \mathcal{N}(0, \Sigma)$;

while $\alpha > \max_{\mu \in \mathcal{P}^{train}} \left(\max \left\{ \frac{\Delta_{ref}(\mu)}{\Delta^l(\mu)}, \frac{\Delta^l(\mu)}{\Delta_{ref}(\mu)} \right\} \right)$ **do**

Select parameter:

Find $\mu_{l+1} \in \underset{\mu \in \mathcal{P}^{\mathbf{train}}}{\operatorname{argmax}} \left(\max \left\{ \frac{\Delta_{ref}(\mu)}{\Delta^l(\mu)}, \frac{\Delta^l(\mu)}{\Delta_{ref}(\mu)} \right\} \right)$; $\quad \Delta_{\mathbf{ref}}(\mu) = \left(\frac{1}{K} \sum_{i=1}^{K} (Z_i^T \underline{e}_{\mathbf{ref}}(\mu))^2 \right)^{1/2}$;

Enrich space:

Define $\underline{y}^{\mathcal{N}}(\mu_{l+1}) := \sum_{i=1}^{K} \lambda_i \underline{y}_i^{\mathcal{N}}(\mu_{l+1})$, where $\lambda = (\lambda_1, \ldots, \lambda_K)$ solves

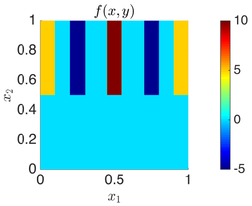
$$\lambda_{l+1} = \underset{\lambda \in \mathbb{R}^K, \|\lambda\|_2 = 1}{\operatorname{argmax}} \left\| \frac{1}{K} \sum_{i=1}^{K} \lambda_i (\underline{y}_i^{\mathcal{N}}(\mu_{l+1}) - \underline{y}_i^{N_{du}}(\mu_{l+1})) \right\|_2.$$

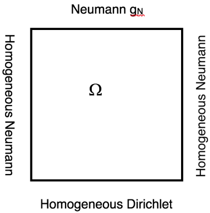
Update the reduced space $Y^{l+1} = Y^l + \operatorname{span}\{\underline{y}^{\mathcal{N}}(\mu_{l+1})\}$;

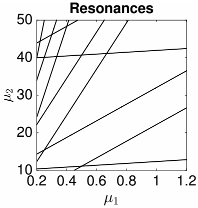
$l \leftarrow l + 1$

end

Numerical experiments: acoustics in 2D

- $\Omega = (0,1) \times (0,1)$
- $X = \{v \in H^1(\Omega) \; : \; v(0, x_2) = 0, x_2 \in (0,1)\}$
- $A(\mu) := -\partial_{x_1 x_1} - \mu_1 \partial_{x_2 x_2} - \mu_2$,
- $\mathcal{P} = [0.2, 1.2] \times [10, 50]$
- Neumann b.c. on top: $g_N = \cos(\pi x)$
- 

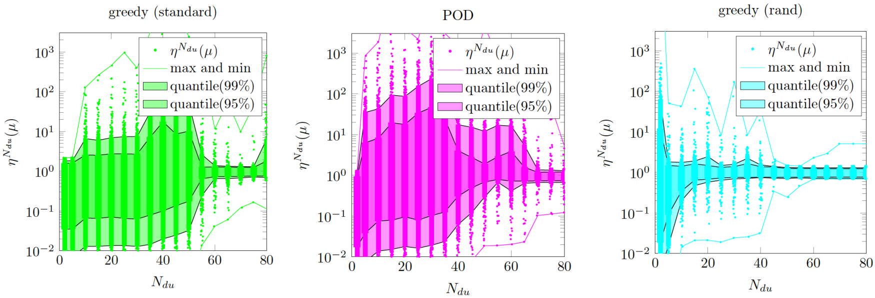




- high dimensional discretization: linear FE, $h = 0.01$ in each direction

Numerical experiments: acoustics in 2D

Effectivity $\eta^{N_{du}}(\mu) = \Delta^{N_{du}}(\mu)/\|e(\mu)\|_{H^1(\Omega)}$ for increasing N_{du} for 1 realization, $K = 20$



Numerical experiments: acoustics in 2D

Dimension of $Y^{N_{du}}$ for standard greedy[1]

	$tol = 0.5$	$tol = 5$	$tol = 50$
$K = 2$	$30.9\,(\pm 1.56)$	$28\,(\pm 2.55)$	$12.6\,(\pm 9.91)$
$K = 5$	$47.9\,(\pm 1.85)$	$39.1\,(\pm 3.61)$	$29.8\,(\pm 10.7)$
$K = 10$	$74\,(\pm 1.84)$	$57.2\,(\pm 4.38)$	$47.4\,(\pm 7.71)$
$K = 20$	> 80	> 80	$63.1\,(\pm 9.9)$

Table: Stopping criterion: max of ε over $\mathcal{P}^{\text{train}}$ is $\leqslant tol$

	$tol = 0.5$	$tol = 5$	$tol = 50$
$K = 2$	$29.3\,(\pm 2.01)$	$25.8\,(\pm 2.19)$	$7.9\,(\pm 5.52)$
$K = 5$	$46.3\,(\pm 1.47)$	$36.6\,(\pm 3.05)$	$21.1\,(\pm 8.3)$
$K = 10$	$72\,(\pm 1.59)$	$55.7\,(\pm 4.34)$	$37.4\,(\pm 9.12)$
$K = 20$	> 80	> 80	$56.1\,(\pm 8.88)$

Table: Stopping criterion: 99% quantile of ε over $\mathcal{P}^{\text{train}}$ is $\leqslant tol$

[1] index of random right-hand side is additional parameter

Numerical experiments: acoustics in 2D

Dimension of $Y^{N_{du}}$ for greedy with error estimator as quantity of interest

	$N = 10$	$N = 20$	$N = 30$
$K = 2$	16.4 (±13.5)	32.4 (±29.3)	28.4 (±23.3)
$K = 5$	19.8 (±6.64)	23.9 (±9.75)	13.6 (±10.1)
$K = 10$	15.4 (±6.07)	31.3 (±10.3)	19.3 (±10.7)
$K = 20$	15.2 (±5.53)	25.6 (±10.9)	26.2 (±11.7)

Table: Stopping criterion: max of α over $\mathcal{P}^{\text{train}}$ is $\leqslant 3$

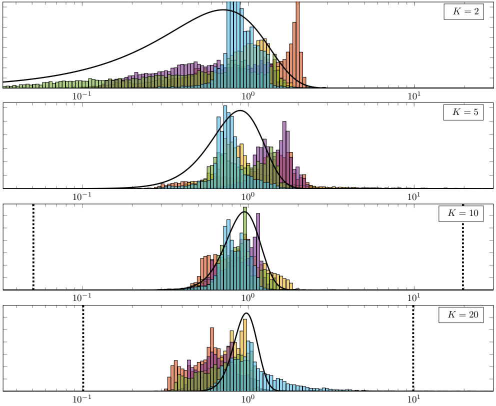
	$N = 10$	$N = 20$	$N = 30$
$K = 2$	6.1 (±5.4)	6.7 (±4.58)	6.6 (±4.64)
$K = 5$	7.9 (±4.39)	8.35 (±4.13)	6.95 (±2.11)
$K = 10$	9 (±2.38)	12.8 (±4.89)	10.7 (±3.5)
$K = 20$	10 (±2.62)	14.4 (±3.38)	15.1 (±4.35)

Table: Stopping criterion: 99% quantile of α over $\mathcal{P}^{\text{train}}$ is $\leqslant 3$

Numerical experiments: acoustics in 2D, $S = 10000$ queries

Histograms of $\Delta^{N_{du}}(\mu)/\|e(\mu)\|_{H^1(\Omega)}$ for 5 different realizations, $N = 20$, 99% quantile

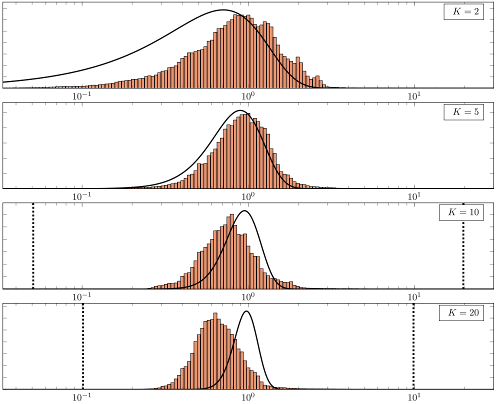
- Continuous line: pdf of $\sqrt{\frac{1}{K}\chi^2(K)}$
- Dashed lines: value of $(\alpha w)^{-1}$ and αw such that concentration inequality holds with $\delta = 10^{-2}$ and $S = 10^4$



Numerical experiments: acoustics in 2D, $S = 10000$ queries

Histograms of $\Delta^{N_{du}}(\mu)/\|e(\mu)\|_{H^1(\Omega)}$ for 40 realizations, $N = 20$, 99% quantile

- Continuous line: pdf of $\sqrt{\frac{1}{K}\chi^2(K)}$
- Dashed lines: value of $(\alpha w)^{-1}$ and αw such that concentration inequality holds with $\delta = 10^{-2}$ and $S = 10^4$



Randomized local model order reduction

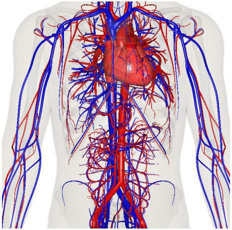
(joint work with A. Buhr)

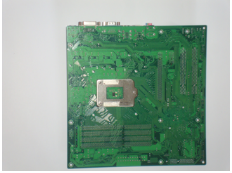
A. Buhr and K. Smetana,
Randomized local model order reduction,
SIAM J. Sci. Comput., accepted for publication

Localized model order reduction

Limitations of standard model order reduction approach:

- Curse of parameter dimensionality: many parameters require prohibitively large reduced spaces
- No topological flexibility (although geometric variation is possible)
- Possibly high computational costs in the offline stage





Localized model order reduction

Limitations of standard model order reduction approach:

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- Possibly high computational costs in the offline stage

$\longrightarrow$ **Localized model order reduction**

Further advantages:

- Allows to use different (sizes of) reduced spaces in different parts of the domain (similar to hp-methods)
- (Local) changes of the PDE, the geometry in the online stage are possible

Many localized model order reduction approaches:

- Component Mode Synthesis: [Bampton, Craig 68], [Hurty 65], [Bourquin 92], [Hetmaniuk, Lehoucq 10], [Jakobsson, Bengzon, Larson 11], [Hetmaniuk, Klawonn 14], ...
- Generalized Finite Element Method: [Babuška, Caloz, Osborn 94], [Babuška, Melenk 97], [Strouboulis, Babuška, K. Copps 01], [Babuška, Lipton 11], ...
- Reduced Basis Element Method: [Maday, Rønquist 02,04], ...
- Multiscale Reduced Basis Method: [Nguyen 08]
- Reduced Basis Hybrid Method: [Iapichino, Quarteroni, Rozza 12]
- Localized Reduced Basis Multiscale Method: [Schindler, Haasdonk, Kaulmann, Ohlberger 12], [Ohlberger, Schindler 15], ...
- Static Condensation Reduced Basis Element Method: [Huynh, Knezevic, Patera 13], [Eftang, Patera 13], [Smetana 15], [Smetana, Patera 16], ...
- Generalized Multiscale Finite Element Method: [Efendiev, Galvis, Hou 13], [Calo, Efendiev, Galvis, Li 16], ...

Many localized model order reduction approaches:

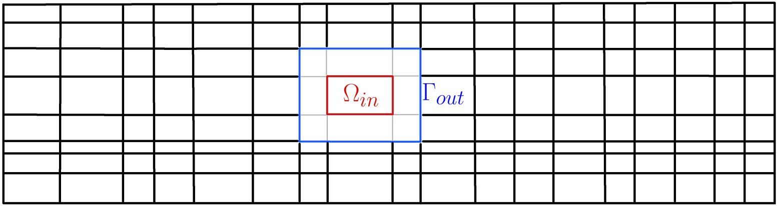
- Reduced Basis Multiscale Finite Element Methods: [Hesthaven, Zhang, X. Zhu 15]
- Reduced Basis methods combined with a Dirichlet-Neumann scheme: [Maier Haasdonk 14]
- Reduced Basis methods combined with a heterogeneous Domain Decomposition scheme: [Martini, Rozza, Haasdonk 15]
- ArbiLoMod: [Buhr, Engwer, Ohlberger, Rave 15], ...
- RDF method: [Iapichino, Quarteroni, Rozza 16]
- Discontinuous Galerkin Reduced Basis Element Method: [Antonietti, Pacciarini, Quarteroni 16], ...
- and many, many more ...

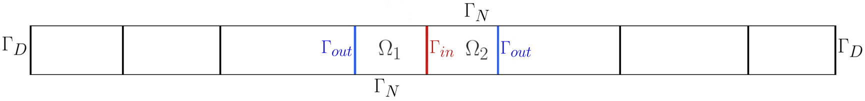
Localized model order reduction

Challenges:

- We can only exploit that the global solution solves PDE locally
- But: No knowledge of the trace of the global solution on Γ_{out}

$\Longrightarrow$ Infinite dimensional parameter space





Localized model order reduction

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- We can only exploit that the global solution solves PDE locally
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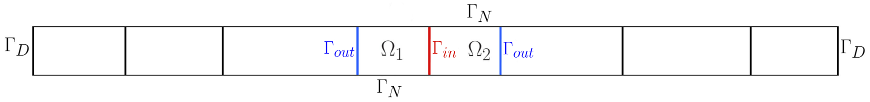
$\Longrightarrow$ Infinite dimensional parameter space

[Babuška, Lipton 11] for space on Ω_{in}, [Smetana, Patera 16] for space on Γ_{in}:

- Restrict to space of functions that solve the PDE locally on Ω for arbitrary boundary conditions on Γ_{out}
- Exploit that for those local solutions we have a very fast decay of higher frequencies from Γ_{out} to Ω_{in}, Γ_{in} ($\rightarrow$ Caccioppoli inequality)
- yields optimal local approximation spaces in the sense of Kolmogorov



The space of all local solutions of the PDE on Ω

- Consider the space of all local solutions of the PDE[2] on Ω

$$\mathcal{H} := \{w \in H^1(\Omega) : \text{with } \; Aw = 0 \quad \in X'\}.$$

- global solution of the PDE restricted to Ω lies in $\mathcal{H}$!
- We are interested in $u|_{\Gamma_{in}}$ or $u|_{\Omega_{in}}$ and thus introduce

$$R := \{w|_{\Gamma_{in}}, \; w \in \mathcal{H}\} \quad \text{or} \quad R := \{w|_{\Omega_{in}}, \; w \in \mathcal{H}\},$$
$$\text{and} \quad S := \{w|_{\Gamma_{out}}, \; w \in \mathcal{H}\}.$$

[2]For theoretical purposes one needs to consider the quotient space $\tilde{\mathcal{H}} := \mathcal{H}/\ker(A)$ at certain instances.

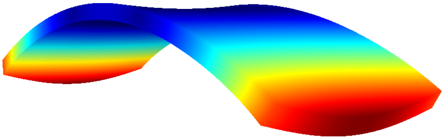
Transfer operator

- We introduce a transfer operator

$$T : S \to R$$

- For $w \in \mathcal{H}$ and thus $w|_{\Gamma_{out}} \in S$ we define

$$T(w|_{\Gamma_{out}}) := w|_{\Gamma_{in}} \quad \text{or} \quad T(w|_{\Gamma_{out}}) := w|_{\Omega_{in}}.$$



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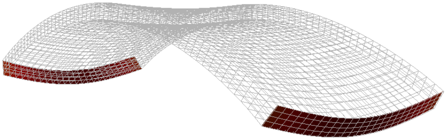

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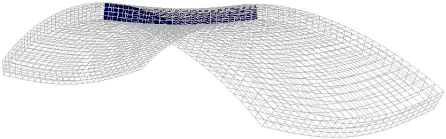

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- T is compact thanks to the Caccioppoli inequality.
- Introduce adjoint operator T^* and consider the eigenvalue problem

$$T^* Tw|_{out} = \lambda w|_{out} \quad \text{for} \;\; w \in \mathcal{H}.$$

- Equivalent formulation: Find $(\varphi_j, \lambda_j) \in (\mathcal{H}, \mathbb{R}^+)$ such that

$$(\varphi_j|_{D_{in}} , w|_{D_{in}})_R = \lambda_j (\varphi_j|_{\Gamma_{out}} , w|_{\Gamma_{out}})_S \;\; \forall w \in \mathcal{H}, D_{in} = \Gamma_{in}, \Omega_{in}$$

Transfer eigenvalue problem

Proposition (Transfer eigenvalue problem)

- φ_j *and* λ_j*: eigenfunctions and eigenvalues of the transfer eigenvalue problem: Find* $(\varphi_j, \lambda_j) \in (\mathcal{H}, \mathbb{R}^+)$ *such that*

$$\left(\varphi_j|_{D_{in}} \; , \; w|_{D_{in}} \right)_R = \lambda_j \; \left(\varphi_j|_{\Gamma_{out}} \; , \; w|_{\Gamma_{out}} \right)_S \;\; \forall w \in \mathcal{H}, D_{in} = \Gamma_{in}, \Omega_{in}$$

- *List* λ_j *such that* $\lambda_1 \geqslant \lambda_2 \geqslant \ldots$*, and* $\lambda_j \to 0$ *as* $j \to \infty$*.*
- *The optimal space on* Γ_{in} *or* Ω_{in} *is given by*

$$R^n := \operatorname{span}\{\phi_1^{sp}, \ldots, \phi_n^{sp}\}, \;\; \phi_j^{sp} = T\varphi_j|_{\Gamma_{out}}, \quad j = 1, \ldots, n.$$

- $$d_n(T(S); R) = \sup_{\xi \in S} \inf_{\zeta \in R^n} \frac{\|T\xi - \zeta\|_R}{\|\xi\|_S} = \sqrt{\lambda_{n+1}}$$

Exponential convergence of optimal modes

- Heat conduction, linear elasticity: [Babuška, Lipton 11], [Babuška, Huang, Lipton 2014]: Proof that eigenvalues of the transfer eigenvalue problem decay almost exponentially, i.e. superalgebraically
- Numerical Experiments: Eigenvalues converge exponentially even for irregular domains [Smetana, Patera 16]:

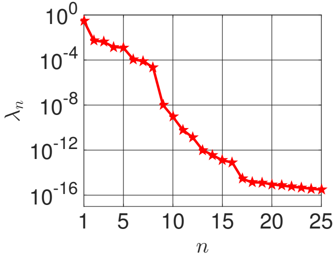


Figure: eigenvalues λ_n

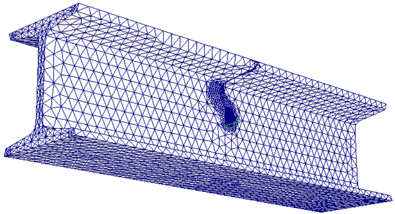


Figure: mesh in Ω_i

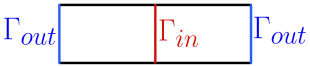
Computing an approximation of the transfer eigenvalue problem

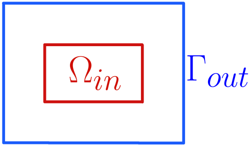
Transfer eigenvalue problem: Find $(\varphi_j, \lambda_j) \in (\mathcal{H}, \mathbb{R}^+)$ such that

$$\left(T^h(\varphi_j|_{\Gamma_{out}}) \ , \ T^h(w|_{\Gamma_{out}}) \right)_R = \lambda_j \left(\varphi_j|_{\Gamma_{out}} \ , \ w|_{\Gamma_{out}} \right)_S \quad \forall w \in \mathcal{H}$$

$\mathcal{H} = \{$ set of all local solutions of the PDE with arbitrary Dirichlet b. c. $\}$

1. Introduce a FE discretization with $\mathcal{N}_{out}$ degrees of freedom (DOFs) on Γ_{out} and $\mathcal{N}_{in}$ DOFs on Γ_{in} or Ω_{in}
2. Solve for each basis function on Γ_{out} the PDE locally
   $\Longrightarrow$ number of required local solutions of the PDE scales with the number of DOFs on Γ_{out} and thus depends on the discretization
3. Assemble and solve generalized eigenvalue problem





Computing an approximation of the transfer eigenvalue problem

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$$\left(\; T^h(\varphi_j|_{\Gamma_{out}}) \;,\; T^h(w|_{\Gamma_{out}}) \; \right)_R = \lambda_j \; \left(\; \varphi_j|_{\Gamma_{out}} \;,\; w|_{\Gamma_{out}} \right)_S \quad \forall w \in \mathcal{H}$$

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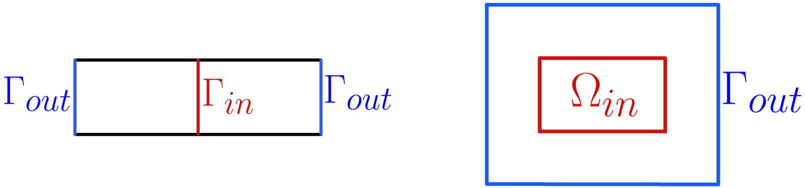
3. Assemble and solve generalized eigenvalue problem

Problem: For large number of DOFs on Γ_{out} the approximation of the transfer eigenvalue problem can be very/prohibitively expensive especially in 3D

Approximating optimal local spaces with Randomized Linear Algebra[3]

- Prescribe random boundary conditions; in detail choose every coeffcient of a FEM basis function on Γ_{out} as a (mutually independent) Gaussion random variable with zero mean and variance one
- Solve PDE for random boundary conditions numerically and store evaluation of local solution of PDE $u^h|_{\Gamma_{in}}$ or $u^h|_{\Omega_{in}}$.
- Define reduced space R^n_{rand} as the span of n such evaluations $u^h|_{\Gamma_{in}}$ or $u^h|_{\Omega_{in}}$



[3] for a review see [Halko, Martinsson, Tropp 11]

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Questions: What is the quality of such an approximation?
(How) can we determine the dimension of the reduced space for a given tolerance?

[3] for a review see [Halko, Martinsson, Tropp 11]

Probalistic a priori error bound[4]

Proposition (A priori error bound (Buhr, Smetana 17))

Under the above assumptions there holds for $n, p \geqslant 2$

$$\mathbb{E}\left[\sup_{\xi \in S^h} \inf_{\zeta \in R^{n+p}_{rand}} \frac{\|T^h\xi - \zeta\|_R}{\|\xi\|_S}\right] \leqslant \underbrace{C_h \left\{\left(1 + \frac{\sqrt{n}}{\sqrt{p-1}}\right)\sqrt{\lambda^h_{n+1}} + \frac{e\sqrt{n+p}}{p}\left(\sum_{j>n} \lambda^h_j\right)^{1/2}\right\}}_{\sim c\sqrt{n}\sqrt{\lambda^h_{n+1}}}$$

Optimal convergence rate achieved with transfer eigenvalue problem:

$$d_n(T(S); R) = \sup_{\xi \in S} \inf_{\zeta \in R^n} \frac{\|T\xi - \zeta\|_R}{\|\xi\|_S} = \sqrt{\lambda_{n+1}}$$

[4] based on results in [Halko, Martinsson, Tropp 11]

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where

- $C_h = \sqrt{\frac{\lambda_{max}(\underline{M}_R)}{\lambda_{min}(\underline{M}_R)}} \sqrt{\frac{\lambda_{max}(\underline{M}_S)}{\lambda_{min}(\underline{M}_S)}}$
- $(\underline{M}_R)_{i,j} = (\psi_j, \psi_i)_R$, ψ_i: *FE basis functions*
- $(\underline{M}_S)_{i,j} = (\psi_j, \psi_i)_S$, ψ_i: *FE basis functions*
- p: *oversampling parameter*

Probablistic a posteriori error bound[5]

Proposition (Probablistic a posteriori error bound (Buhr, Smetana 2017))

- $\{\underline{\omega}^{(i)} : i = 1, 2, \dots, n_t\}$: *standard Gaussian vectors*
- $D_S : \mathbb{R}^{\mathcal{N}_{out}} \to S^h$; $(c_1, \dots, c_{\mathcal{N}_{out}}) \mapsto \chi$, $\chi = \sum_{i=1}^{\mathcal{N}_{out}} c_i \psi_i$, ψ_i : *FE basis functions*
- N_T : *bound for the dimension of the range of operator* T^h

Define

$$\Delta(n_t, \delta_{\mathrm{tf}}) := \frac{c_{\mathrm{est}}(n_t, \delta_{\mathrm{tf}})}{\sqrt{\lambda_{min}^{M_S}}} \max_{i \in 1,\dots,n_t} \left(\inf_{\zeta \in R^n_{rand}} \| T^h D_S \underline{\omega}^{(i)} - \zeta \|_R \right)$$

Then there holds

$$\sup_{\xi \in S^h} \inf_{\zeta \in R^n_{rand}} \frac{\| T^h \xi - \zeta \|_R}{\|\xi\|_S} \leqslant \Delta(n_t, \delta_{\mathrm{tf}}) \leqslant \left(\frac{\lambda_{max}^{M_S}}{\lambda_{min}^{M_S}} \right)^{1/2} c_{\mathrm{eff}}(n_t, \delta_{\mathrm{tf}}) \sup_{\xi \in S^h} \inf_{\zeta \in R^n_{rand}} \frac{\| T^h \xi - \zeta \|_R}{\|\xi\|_S}$$

with a probability of at least $1 - \delta_{\mathrm{tf}}$.

[5] Estimator extends results in [Halko, Martinsson, Tropp 11]; effectivity bound new

Algorithm 2: Adaptive randomized range finder

input : T^h, N_T, target tolerance `tol`, number of test vectors n_t, maximum failure probability δ_{algofail}

output: R^n_{rand} such that $P\left(\sup_{\xi \in S^h} \inf_{\zeta \in R^n_{rand}} \frac{\|T\xi - \zeta\|_R}{\|\xi\|_S} \leqslant \texttt{tol}\right) \geqslant 1 - \delta_{\text{algofail}}$.

Initialize n_t test functions: $\tau^{(i)} = T^h D_S \underline{\omega}^{(i)}$, $i = 1, \ldots, n_t$, $\underline{\omega}^{(i)}$: standard Gaussian vector

$\delta_{\text{tf}} = \delta_{\text{algofail}}/N_T$. Initialize $j = 0$.

while $\Delta(n_t, \delta_{\text{tf}}) > tol$ **do**

  $j = j + 1$

  Compute a new basis function:

  $\zeta^{(j)} = T^h D_S \underline{\omega}^{(j+n_t)}$, $\underline{\omega}^{(j+n_t)}$: standard Gaussian vector

  $\zeta^{(j)} \leftarrow \zeta^{(j)} - \sum_{l=1}^{j-1} (\phi_l^{rand}, \zeta^{(j)})_R \phi_l^{rand}$

  $\phi_j^{rand} = \zeta^{(j)} / \|\zeta^{(j)}\|_R$

  Update test functions $\tau^{(i)}$ and therefore $\Delta(n_t, \delta_{\text{tf}})$:

  $\tau^{(i)} \leftarrow \tau^{(i)} - (\phi_j^{rand}, \tau^{(i)})_R \phi_j^{rand}$, $i = 1, \ldots, n_t$

end

$n = j$; $R^n_{rand} = \text{span}\{\phi_1^{rand}, \ldots, \phi_n^{rand}\}$

Numerical Experiments for analytic test problem

Numerical Experiments: interfaces

- local (oversampling) domain $\Omega := (-1,1) \times (0,1)$
- Consider PDE: $-\Delta u = 0$ in Ω
- Goal: Construct reduced space on Γ_{in}

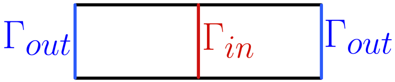


Figure: Ω

Heat conduction: $-\Delta u = 0$ on $\Omega = (-1, 1) \times (0, 1)$

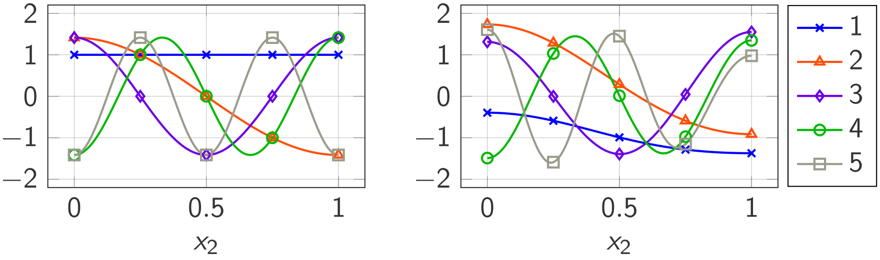
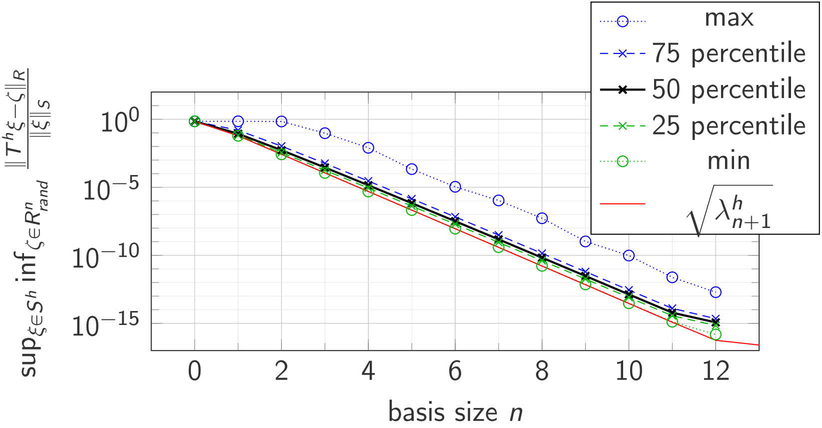


Figure: optimal basis — basis generated by randomized range finder algorithm

Heat conduction: $-\Delta u = 0$ on $\Omega = (-1, 1) \times (0, 1)$



Heat conduction: $-\Delta u = 0$ on $\Omega = (-1,1) \times (0,8)$

CPU times

Properties of basis generation

	Algorithm 2	Scipy/ARPACK
(resulting) basis size n	39	39
operator evaluations	59	79
adjoint operator evaluations	0	79
execution time in s (without factorization)	20.4 s	47.9 s

Table: CPU times; Target accuracy `tol`$= 10^{-4}$, number of testvectors $n_t = 20$, failure probability $\delta_{\mathrm{algofail}} = 10^{-15}$; unknowns of corresponding problem 638,799

Numerical Experiments for a transfer operator with slowly decaying singular values

Numerical Experiments: subdomains

- local (oversampling) domain $\Omega := (-2, 2) \times (-0.25, 0.25) \times (-2, 2)$
- Consider PDE: linear elasticity in Ω (isotropic, homogeneous)
- Goal: Construct reduced space on $\Omega_{in} = (-0.5, 0.5) \times (-0.25, 0.25) \times (-0.5, 0.5)$

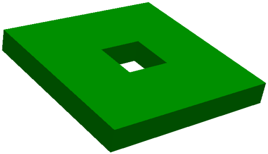
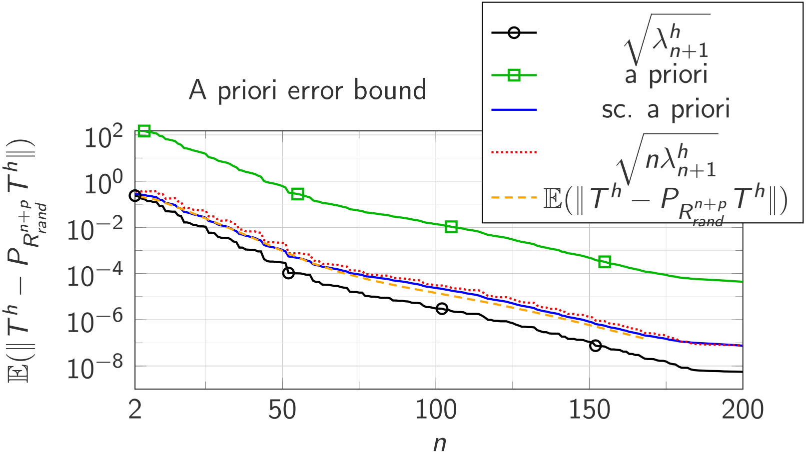


Figure: $\Omega \backslash \Omega_{in}$

Linear elasticity on $\Omega := (-2,2) \times (-0.25, 0.25) \times (-2,2)$



Linear elasticity on $\Omega := (-2,2) \times (-0.5,0.5) \times (-2,2)$

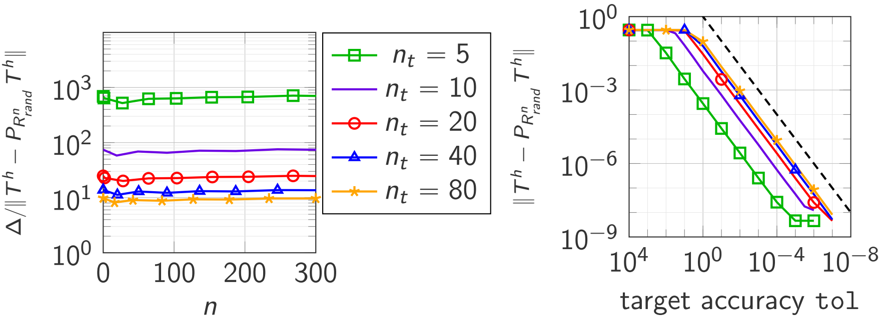


Figure: Convergence behavior of adaptive algorithm (left) and effectivity of a posteriori error estimator $\Delta/\| T^h - P_{R^n_{rand}} T^h \|$ (right) for increasing number of test vectors n_t.

Summary

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  - ... is based on concentration inequalities, error-residual relationship, and random dual problem
  - ... does only contain computable constants
  - ... is reliable and efficient at high (given) probability
  - ... has a favorable computational complexity as N_{du} can be chosen relatively small
- Reduced local approximation spaces generated by methods from Randomized Linear Algebra
  - Probabilistic a priori error bound/Numerical experiments: convergence rate is only slightly worse compared to the optimal rate (factor $\sqrt{n}$).
  - Probabilistic a posteriori error bound allows to build the reduced space adaptively
  - required number of local solutions of PDE scale (roughly) with size of the reduced space; Numerical experiments: faster than Lanczos

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Thank you very much for your attention!

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- target error: $\|s(\mu) - L\underline{u}^{N}(\mu)\|_W$ for a quantity of interest $s(\mu) = L\underline{u}^{\mathcal{N}}(\mu) \in \mathbb{R}^m$, where $\|\cdot\|_W = \sqrt{(\cdot)^T R_W (\cdot)}$ is a given (natural) norm on $\mathbb{R}^m \quad \longrightarrow \quad$ choose $\Sigma = L^T R_W L$

A fast-to-evaluate randomized error estimator

Proposition

Assume Σ is invertible. The a posteriori error estimator $\Delta^{N_{du}}(\mu)$ satisfies

$$\frac{|\Delta(\mu) - \Delta^{N_{du}}(\mu)|}{\|\underline{u}^{\mathcal{N}}(\mu) - \underline{u}^{N_{du}}(\mu)\|_{\Sigma}} \leqslant \max_{1 \leqslant i \leqslant K} \|\underline{A}^{T}(\mu)\underline{y}_i(\mu) - Z_i\|_{\Sigma^{-1}} \quad \forall \mu \in \mathcal{P}.$$