Reduced Basis Methods for Parametrized Partial Differential Equations

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Overview Part 1–3

- Introduction
  - Motivation of model reduction, basic idea and notions
- Model Problem
  - Thermal block, solution structure
- Abstract Problem
  - Uniform coercivity, continuity, parameter separability
  - Full problem, solution manifold, examples, regularity
- RB Problem
  - "Primal" formulation, error bounds, effectivities
- Experiments

Overview Part 1–3

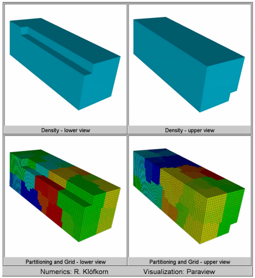
- Offline/Online Decomposition
  - RB-Problem, error estimators
  - Min-theta procedure
- Basis Generation
  - Lagrangian basis
  - Greedy, convergence rates
  - Orthonormalization
  - Adaptivity
- Primal-Dual RB Approach
  - Output correction
  - Improved error estimation
- Nonlinear RB Approach
  - Quadratically nonlinear problems

Overview Part 1–3

- RB Methods for Instationary Problems
  - Projection, error estimation, basis generation
- RB Methods for Nonlinear Problems
  - Empirical Operator Interpolation
  - Applications: Burgers equation, 2PF in porous media
- Offline Adaptivity
  - Adaptive training set refinement
  - Adaptive parameter domain partitioning
  - Adaptive time domain partitioning
- Online Adaptivity
  - Online N adaptation and online greedy
- Summary and Conclusion

Introduction

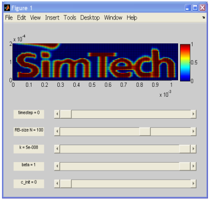
Motivation of Model Reduction



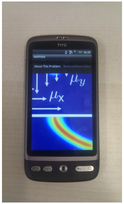
- Today: High resolution simulation schemes
  - Multitude of applications
  - High dimensional models (PDEs, ODEs)
  - Development of accurate schemes
    Adaptive grids, higher order schemes
    Parallelization and HPC
  - High runtime- and hardware requirements
- Goal: Reduced models
  - Smaller model dimension, reduced requirements
  - Similar precision, error control
  - Automatic reduction, not „manual‟
- Realization of complex simulation scenarios
  - Multi-query, real-time, „Cool‟-computing platforms

Motivation of Model Reduction

- „Real Time" Scenarios
  - Real-time control of processes
  - Graphical user interfaces
    - Man-machine-interaction
    - Interactive design
    - Parameter exploration



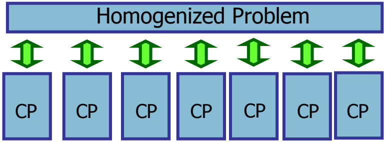
- „Cool" Computing Platforms
  - Simple industrial controllers
  - Web-applications / Applets
  - Ubiquitous Computing:
    Mobile phone, smart devices

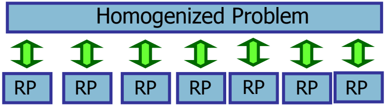


Motivation of Model Reduction

„Multi-Query“, High-Level Simulation Scenarios

- Parameter studies, statistical investigations
- Design, Parameter optimization, inverse problems
- Multiscale Settings: Reduced Models as Microsolvers





- Stochastic PDEs: Monte Carlo with Reduced Models

SPDE $u(x, \omega)$

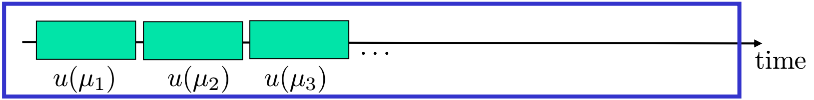
$$\bar{u}_n(x) = \frac{1}{n}\left(\boxed{\text{RP}} + \boxed{\text{RP}} + \ldots + \boxed{\text{RP}}\right)$$

$$\bar{u}(x) := \int_\Omega u(x,\omega) p(\omega)$$

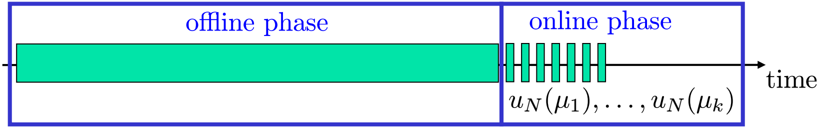
Motivation of Model Reduction

- Offline/Online Computational Procedure
  - Accept computationally intensive „offline phase" (reduced model generation, etc.)
  - Amortization of runtime cost in view of multiple online phases i.e. simulations with reduced model

Multi-query with high dimensional model:

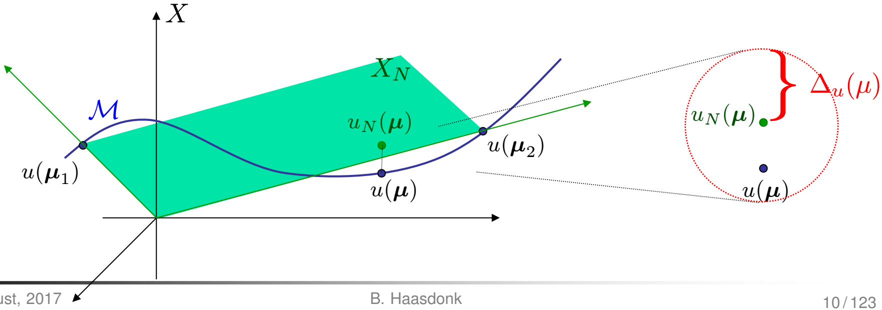


Multi-query with reduced model:



Motivation of RB-Methods

- Parametric problems:
  - Parameter domain $\mathcal{P} \subset \mathbb{R}^p$, parameter vector $\mu \in \mathcal{P}$
  - solution $u(\mu) \in X$, Hilbert space (HS)
  - Manifold of solutions $\mathcal{M}$ „parametrized" by $\mu \in \mathcal{P}$
  - Low-dimensional subspace $X_N \subset X$ („RB-Space")
  - Approximation $u_N(\mu) \in X_N$ and error bound $\Delta_u(\mu)$



Motivation of RB-Methods

- Simple Example: $\mu \in \mathcal{P} = [0,1]$
  - Find $u(\mu) \in C^2([0,1])$ (not a HS) satisfying

$$(1+\mu)u'' = 1 \text{ in } (0,1), \quad u(0) = u(1) = 1$$

  - „Snapshots": $u_0 := u(\mu = 0) = \frac{1}{2}x^2 - \frac{1}{2}x + 1$

$$u_1 := u(\mu = 1) = \frac{1}{4}x^2 - \frac{1}{4}x + 1$$

$$X_N = \text{span}\{u_0, u_1\}$$

  - Reduced Solution $u_N(\mu) = \alpha_0(\mu)u_0 + \alpha_1(\mu)u_1$

$$\alpha_0(\mu) = \frac{2}{\mu+1} - 1, \quad \alpha_1(\mu) = 2 - \frac{2}{\mu+1}$$

  - Exact approximation: $u_N(\mu) = u(\mu)$ for $\mu \in \mathcal{P}$
  - $\mathcal{M}$ is contained in 2-dimensional subspace (more precisely: $\mathcal{M}$ is convex hull of u_0, u_1)

Motivation of RB-Methods

- Questions that need to be addressed:
  - How to construct good spaces X_N? Can such „procedures" be provably good?
  - How to obtain approximation $u_N(\mu) \in X_N$? Can we do better than interpolation?
  - Efficiency: How can $u_N(\mu)$ be computed rapidly?
  - Stability with growing N?
  - Can we bound the error? Are bounds „rigorous", i.e. provable upper bounds?
  - Are error bounds largely overestimating the error or can the „effectivity" be bounded?
  - For which problem classes is low dimensional approximation expected to be successful?

Motivation of RB-Methods

General References on the Topic

- Electronical Book (PR07)

  A.T. Patera and G. Rozza: “Reduced Basis Approximation and A Posteriori Error Estimation for Parametrized Partial Differential Equations, V 1.0, Copyright MIT 2007, to appear in (tentative rubric) MIT Pappalardo Graduate Monographs in Mechanical Engineering.

- RB-Tutorial (Ha14)

  B. Haasdonk: Reduced Basis Methods for Parametrized PDEs – A Tutorial Introduction for Stationary and Instationary Problems. Chapter in P. Benner, A. Cohen, M. Ohlberger and K. Willcox (eds.): “Model Reduction and Approximation: Theory and Algorithms”, SIAM, Philadelphia, 2017.

- Recent RB Books (Rozza&al 2016, Manzoni&al 2016)

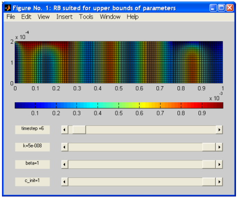
Motivation of RB-Methods

- Websites:
  - augustine.mit.edu: MIT-website
  - www.morepas.org: german RB activities
  - www.modelreduction.org: german MOR Wiki
  - www.eu-mor.net: COST EU-MORNET network
- Software:
  - rbMIT: http://augustine.mit.edu
  - RBmatlab, Dune-rb: www.morepas.org
  - pyMOR: http://pymor.org
- Course Material:

  www.haasdonk.de/data/durham2017

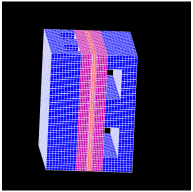
Software

- RBmatlab
  - MATLAB discretization and RB-library
  - 2d-Grids, adaptive n-D grids
  - Linear, Nonlinear Evolution Problems
  - FV, FEM, LDG Discretizations, RB Algorithms



Download & Documentation:
www.morepas.org

RBmatlab ⇄ DUNE-RB



- DUNE-RB
  - Detailed Parametrized Models, C++ Template lib.
  - Extension of Dune-FEM (www.dune-project.org)
  - Discrete Function Lists, Parametrized Operators
  - Interface to RBmatlab

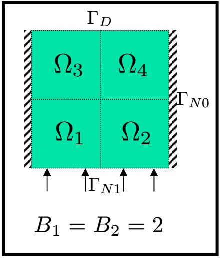
Dune
Distributed and Unified Numerics Environment

Model Problem: Thermal Block

Model Problem

- Thermal Block
  - Slight modification of [PR06]
  - Heat conduction in solid block
  - Computational domain $\Omega = (0,1)^2$
  - Partition in B_1 horiz., B_2 vert. subblocks

$$\Omega = \bigcup_{i=1}^{p} \Omega_i \qquad p := B_1 \cdot B_2$$



  - Parameters: heat conductivity coefficients

$$\mu = (\mu_i)_{i=1}^{p} \in [\mu_{min}, \mu_{max}]^p, \quad \mu_{min} = \frac{1}{\mu_{max}} \in (0,1)$$

  - Governing PDE

$$\begin{aligned} -\nabla \cdot k(\boldsymbol{\mu})\nabla u &= 0 \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \Gamma_D \\ k(\boldsymbol{\mu})\nabla u \cdot n &= i \quad \text{on } \Gamma_{Ni}, \quad i = 0,1 \end{aligned}$$

$$k(x;\boldsymbol{\mu}) = \sum_i \mu_i \chi_{\Omega_i}(x)$$

Model Problem

- Weak Form:
  - Solution space

$$X = H^1_{\Gamma_D}(\Omega) := \{\, v \in H^1(\Omega) \,|\, v|_{\Gamma_D} = 0\}$$

  - Weak form: find $u(\mu) \in X$ such that

$$\underbrace{\int_\Omega k(\boldsymbol{\mu}) \nabla u(\boldsymbol{\mu}) \cdot \nabla v}_{a(u(\mu),v;\mu)} = \underbrace{\int_{\Gamma_{N1}} v}_{f(v;\mu)}, \quad v \in X$$

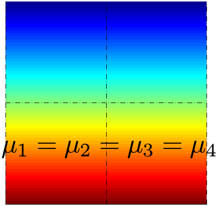
- Possible output of interest: average bottom temperature

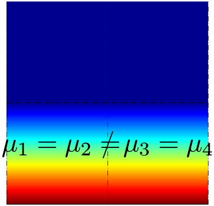
$$s(\mu) := \int_{\Gamma_{N,1}} u(x;\mu)dx = l(u(\mu);\mu)$$

- Compactly written by means of bilinear form $a(\cdot,\cdot;\mu)$ and linear forms $f(\cdot;\mu), l(\cdot;\mu) \in X'$

Model Problem

- Solution Variety:
  - Simple solution structure:
    if $B_1 = 1$ (or $B_1 \geq 1$ and all μ_i in each row identical) the solution exhibits horizontal symmetry, is piecewise linear, can be exactly represented in a finite dimensional space, although the full problem is infinite dimensional.

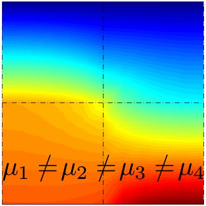


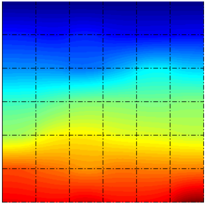


> Exercise 1: Find and prove an explicit solution representation in a B_2-dimensional linear space

Model Problem

- Solution Variety:
  - Complex solution structure: if $B_1 > 1$ the solution is in general nonsymmetric, complexity increasing with B_1, B_2





  - Parameter redundancy: manifold is invariant with respect to scaling of the parameter vector:

$$\bar{\mu} := c\mu \in \mathcal{P}, c > 0 \quad \Rightarrow \quad u(\bar{\mu}) = \frac{1}{c} u(\mu).$$

    Important insight: More/many parameters do not necessarily imply complex manifold structure

Exercise 2: Provide a different parametrization of $k(x;\mu)$ in the thermal block, such that the model has arbitrary large number $p > B_1 \cdot B_2$ of parameters, but only 1-dimensional solution manifold.

Abstract Problem

Abstract Problem

- Notation
  - X Hilbert space (real, separable), scalar product $\langle \cdot, \cdot \rangle$, norm

$$\|v\| := \sqrt{\langle v, v \rangle}, \quad v \in X$$

  - Dual space X' with norm

$$\|g\|_{X'} := \sup_{v \in X \setminus \{0\}} \frac{g(v)}{\|v\|}, \quad g \in X'$$

  - For all $g \in X'$ denote Riesz-Representer by $v_g \in X$:

$$g(v) = \langle v_g, v \rangle, \quad v \in X \qquad \text{(Representer property)}$$

$$\|g\|_{X'} = \|v_g\| \qquad \text{(Isometry of Riesz-map)}$$

  - Parameter domain $\mathcal{P} \subset \mathbb{R}^p$
  - bilinear form and linear forms

$$a(\cdot, \cdot; \mu) : X \times X \to \mathbb{R} \qquad f(\cdot; \mu), l(\cdot; \mu) \in X', \quad \mu \in \mathcal{P}$$

Abstract Problem

- (A1): Uniform Boundedness and Coercivity of $a(\cdot,\cdot;\mu)$
  - $a(\cdot,\cdot;\mu)$ is assumed to be coercive, i.e.

$$\alpha(\mu) := \inf_{v \in X \setminus \{0\}} \frac{a(v,v;\mu)}{\|u\|^2} > 0$$

and the coercivity is uniform wrt. μ, i.e. there exists $\bar{\alpha}$ with

$$\alpha(\mu) \geq \bar{\alpha} > 0, \quad \mu \in \mathcal{P}.$$

  - $a(\cdot,\cdot;\mu)$ is assumed to be bounded (continuous), i.e.

$$\gamma(\mu) := \sup_{u,v \in X \setminus \{0\}} \frac{a(u,v;\mu)}{\|u\| \, \|v\|} < \infty$$

and boundedness is uniform wrt. μ, i.e. there exists a $\bar{\gamma}$ s.th.

$$\gamma(\mu) \leq \bar{\gamma} < \infty, \quad \mu \in \mathcal{P}.$$

- Remark: $a(\cdot,\cdot;\mu)$ may possibly be nonsymmetric

Abstract Problem

- (A2): Uniform Boundedness of $f(\cdot;\mu), l(\cdot;\mu)$
  - $f(\cdot;\mu), l(\cdot;\mu)$ are assumed to be uniformly bounded wrt. μ :

$$\|f(\cdot;\mu)\|_{X'} \leq \bar{\gamma}_f, \quad \|l(\cdot;\mu)\|_{X'} \leq \bar{\gamma}_l, \quad \mu \in \mathcal{P}.$$

    for suitable constants $\bar{\gamma}_l, \bar{\gamma}_f$

- Remark: Possible Discontinuity wrt. μ
  - Example: $X = \mathbb{R}, \mathcal{P} := [0,2]$

$$l(x;\mu) := x \cdot \chi_{[1,2]}(\mu)$$

    $l(\cdot;\mu)$ is linear and bounded, hence a continuous linear functional with respect to x, but it is discontinuous with respect to μ

Abstract Problem

- (A3): Parameter Separability
  - We assume the forms a, f, l to be parameter separable:

$$a(u,v;\mu) = \sum_{q=1}^{Q_a} \theta_q^a(\mu) a_q(u,v), \quad u,v \in X, \mu \in \mathcal{P}$$

    for suitable bilinear, continuous components $a_q : X \times X \to \mathbb{R}$ coefficient functions $\theta_q^a : \mathcal{P} \to \mathbb{R}, q = 1, \ldots, Q_a$, and similar expansions for f, l with linear functionals f_q, l_q and coefficient functions θ_q^f, θ_q^l and expansion sizes Q_f, Q_l

- Remark:
  - Q_a, Q_f, Q_l should be preferably small, as they will enter the online computational complexity.
  - This property also is referred to as „affine" parameter dependence (which is slightly misleading)

Abstract Problem

Sufficient Criteria for (A1), (A2)

Assume that we have parameter separability (A3) then

- If coefficient functions $\theta_q^a, \theta_q^f, \theta_q^l$ are bounded, then the forms a, f, l are uniformly bounded with respect to μ :

$$|\theta_q^f(\mu)| \leq C \quad \Rightarrow \quad \|f(\cdot;\mu)\|_{X'} \leq \sum_{q=1}^{Q_f} C\,\|f_q\|_{X'} =: \bar{\gamma}_f$$

- If coefficient functions are strictly positive, $\theta_q^a(\mu) \geq \bar{\theta} > 0, \quad \forall \mu, q$ components a_q are positive semidefinite, $a_q(v,v) \geq 0, \quad \forall v, q$ and $a(\cdot,\cdot;\bar{\mu})$ is coercive for at least one $\bar{\mu} \in \mathcal{P}$, then a is uniformly coercive wrt. μ

Exercise 3: Prove sufficient criteria for uniform coercivity

Abstract Problem

- Definition: Full Problem (P)
  - For $\mu \in \mathcal{P}$ find a solution $u(\mu) \in X$ and output $s(\mu) \in \mathbb{R}$ such that

$$a(u(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X$$

$$s(\mu) = l(u(\mu); \mu)$$

- Well-posedness: Existence, Uniqueness & Boundedness
  - Assuming (A1),(A2) then a unique solution of (P) exists and is uniformly bounded

$$\|u(\mu)\| \leq \frac{\|f(\cdot;\mu)\|_{X'}}{\alpha(\mu)} \leq \frac{\bar{\gamma}_f}{\bar{\alpha}}, \quad |s(\mu)| \leq \|l(\cdot;\mu)\|_{X'} \|u(\mu)\| \leq \frac{\bar{\gamma}_l \bar{\gamma}_f}{\bar{\alpha}}.$$

  - Proof: Lax Milgram & uniform boundedness/coercivity

Abstract Problem

- (P) Can both represent
  - analytical problem, infinite dimensional (interesting from approximation theoretic viewpoint, manifold properties)
  - discretized problem, high dimensional (important for practical application of RB-methods), also denoted „detailed problem“ and „detailed solution“

- Examples of Instantiations of (P):
  - Thermal Block

Exercise 4: Prove, that the bilinear and linear forms of the thermal block model are separable parametric, uniformly bounded and uniformly coercive. In particular, provide the corresponding constants, coefficients, components.

Abstract Problem

- Examples of Instantiations of (P)
  - Parametric Matrix-Equation:
    For $\mu \in \mathcal{P}$ find a solution $u(\mu) \in \mathbb{R}^H$ of
    $$\boldsymbol{A}(\mu)u(\mu) = \boldsymbol{b}(\mu), \quad \boldsymbol{A}(\mu) \in \mathbb{R}^{H\times H}, \boldsymbol{b}(\mu) \in \mathbb{R}^H$$
    Corresponds to (P) by choosing
    $$X := \mathbb{R}^H, \quad a(u,v;\mu) := u^T \boldsymbol{A}(\mu)v, \quad f(v) := \boldsymbol{b}(\mu)^T v, \quad u,v \in \mathbb{R}^H$$
  - Forms by given manifold:
    Choose X and arbitrary complicated (discontinuous, nonsmooth) $u : \mathcal{P} \to X$. Then $u(\mu)$ is the solution of (P) by
    $$a(v,v';\mu) := \langle v, v' \rangle \quad f(v) := \langle u(\mu), v \rangle \quad v, v' \in X$$
- Note:
  - (A1)-(A3) are not addressed here, output is ignored
  - (P) can be used for MOR of finite dimensional matrix equations, (P) may have arbitrary complex solutions

Abstract Problem

- Solution Manifold

$$\mathcal{M} := \{u(\mu), |u(\mu) \text{ solves (P) }, \mu \in \mathcal{P}\} \subset X$$

- Finite dimensional manifold for $Q_a = 1$

Exercise 5: If a consists of a single component, $Q_a = 1$ show, that $\mathcal{M}$ is contained in an (at most) Q_f -dimensional linear space.

- Boundedness of Manifold

$$\mathcal{M} \subseteq B_{\frac{\bar{\gamma}_f}{\bar{\alpha}}}(0)$$

  - Is consequence of the well-posedness-result.

Abstract Problem

- Lipschitz-Continuity (extension of [EPR10])
  - Assume that (A1),(A2),(A3) hold and additionally the coefficient functions are Lipschitz-continuous,

$$|\theta_q^a(\mu) - \theta_q^a(\mu')| \leq L \|\mu - \mu'\| \quad \text{etc.}$$

  - Then the forms a, f, l are Lipschitz-continuous wrt. μ

$$|a(u,v;\mu) - a(u,v;\mu')| \leq L_a \|u\| \|v\| \|\mu - \mu'\|, \quad L_a = L \sum_q \gamma_{a_q}$$

  - and the solutions u and s are Lipschitz-continuous with respect to μ

$$\|u(\mu) - u(\mu')\| \leq L_u \|\mu - \mu'\|, \quad L_u = \frac{L_f}{\bar{\alpha}} + \frac{\bar{\gamma}_f L_a}{\bar{\alpha}^2}$$

$$\|s(\mu) - s(\mu')\| \leq L_s \|\mu - \mu'\|, \quad L_s = \frac{L_l \bar{\gamma}_f}{\bar{\alpha}} + \bar{\gamma}_l L_u$$

Exercise 6: Prove the Lipschitz-constants for u and s.

Abstract Problem

- Differentiability (cf. [PR06])
  - Assume that (A1),(A2),(A3) hold and additionally the coefficient functions are differentiable wrt. μ.
  - Then the solution $u : \mathcal{P} \to X$ is differentiable with respect to μ and the partial derivatives $\partial_{\mu_i} u(\mu) \in X$ are the solution of

$$(*) \qquad a(\partial_{\mu_i} u(\mu), v; \mu) = \tilde{f}_i(v; u(\mu), \mu), \quad v \in X$$

with u-dependent right hand side

$$\tilde{f}_i(\cdot; u(\mu), \mu) := \sum_{q=1}^{Q_f} (\partial_{\mu_i} \theta_q^f(\mu)) f_q(\cdot) - \sum_{q=1}^{Q_a} (\partial_{\mu_i} \theta_q^a(\mu)) a_q(u(\mu), \cdot; \mu) \in X'.$$

  - Proof (sketch): Solution of (*) uniquely exists with Lax Milgram, and satisfies conditions for being derivative of u.

Abstract Problem

- Remarks
  - The partial derivatives are also denoted „sensitivity derivatives" and the variational problem (*) the „sensitivity PDE".
  - Similar statements are possible for higher order derivatives: right hand side of sensitivity PDE depending on lower order derivatives.
  - Sensitivity derivatives are useful for Parameter Optimization: RB model for sensitivity PDEs yields gradient information [DH13,DH13b].
  - The more smooth the coefficient functions, the more smooth the solution manifold
  - With increasing smoothness of the manifold, we may hope and expect better approximability by an RB-approach.

RB Method

RB Method

- Reduced Basis / RB-Space
  - Let parameter samples be given
$$S_N = \{\mu^{(1)}, \dots, \mu^{(N)}\} \subset \mathcal{P}$$
  - Define „Lagrangian“ RB-Space and Basis
$$X_N := \mathrm{span}\{u(\mu^{(i)})\}_{i=1}^N = \mathrm{span}\Phi_N, \quad \Phi_N := \{\varphi_1, \dots, \varphi_N\}$$
- Remarks:
  - RB may be identical to snapshots, or orthogonalized.
  - Other MOR-Techniques: A RB-space may also be chosen completely different/arbitrary, as long as it is a N-dimensional subspace: Proper Orthogonal Decomposition (POD) [Vo13], Balanced Truncation, Krylov-Supspaces, etc. [An05]
  - For now: Simple choice of samples: Random or equidistant samples, assuming linear independence of snapshots.
  - Later: More clever choice: a-priori analysis / greedy

RB Method

- Definition: Reduced Problem (P_N)
  - For $\mu \in \mathcal{P}$ find a solution $u_N(\mu) \in X_N$ and output $s_N(\mu) \in \mathbb{R}$ such that

$$a(u_N(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X_N$$

$$s_N(\mu) = l(u_N(\mu); \mu)$$

- Remarks:
  - The above is called „Galerkin" projection, as Ansatz and test space are identical (in contrast to „Petrov-Galerkin" required for non-coercive problems)
  - Improved output estimation is possible by primal-dual technique: see later section.
  - „Galerkin Orthogonality": Error is a-orthogonal to RB-space:

$$a(u - u_N, v) = a(u, v) - a(u_N, v) = f(v) - f(v) = 0, \quad v \in X_N$$

RB Method

- Well-posedness: Existence, Uniqueness & Boundedness
  - Identical statement as for (P), even with same constants:
  - Assuming (A1),(A2), then a unique solution of (P_N) exists, and is uniformly bounded

$$\|u_N(\mu)\| \leq \frac{\|f(\cdot;\mu)\|_{X'}}{\alpha(\mu)} \leq \frac{\bar{\gamma}_f}{\bar{\alpha}}, \quad |s_N(\mu)| \leq \|l(\cdot;\mu)\|_{X'} \|u(\mu)\| \leq \frac{\bar{\gamma}_l \bar{\gamma}_f}{\bar{\alpha}}.$$

  - Proof: Lax-Milgram is applicable, as continuity and coercivity is inherited to subspaces:

$$\inf_{u \in X_N \setminus \{0\}} \frac{a(u,u;\mu)}{\|u\|^2} \geq \inf_{u \in X \setminus \{0\}} \frac{a(u,u;\mu)}{\|u\|^2} = \alpha(\mu)$$

$$\sup_{u,v \in X_N \setminus \{0\}} \frac{a(u,v;\mu)}{\|u\| \, \|v\|} \leq \sup_{u,v \in X \setminus \{0\}} \frac{a(u,v;\mu)}{\|u\| \, \|v\|} = \gamma(\mu)$$

then same argumentation as for (P) applies.

RB Method

Discrete Form of RB Problem

- For given $\mu \in \mathcal{P}$ and basis $\Phi_N = \{\varphi_i\}_{i=1}^N$ define

$$\boldsymbol{A}_N(\mu) := (a(\varphi_j, \varphi_i; \mu))_{i,j=1}^N \in \mathbb{R}^{N \times N}$$

$$\boldsymbol{f}_N(\mu) := (f(\varphi_i; \mu))_{i=1}^N, \quad \boldsymbol{l}_N(\mu) := (l(\varphi_i; \mu))_{i=1}^N \in \mathbb{R}^N$$

- Solve the following linear system for $\boldsymbol{u}_N(\mu) = (u_{Nj})_{j=1}^N \in \mathbb{R}^N$

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

- Then the solution of (P_N) is obtained by

$$u_N(\mu) = \sum_{j=1}^N u_{Nj}\varphi_j, \quad s_N(\mu) = \boldsymbol{l}(\mu)^T \boldsymbol{u}_N(\mu)$$

- Proof: This representation of $u_N(\mu)$ fulfills (P_N) by linearity

RB Method

- Algebraic Stability by Using Orthonormal Basis
  - If $a(\cdot,\cdot;\mu)$ is symmetric and Φ_N is orthonormal, then the condition number of $\boldsymbol{A}_N(\mu)$ is bounded (independent of N)

$$\mathrm{cond}_2(\boldsymbol{A}_N(\mu)) = \|\boldsymbol{A}_N(\mu)\| \left\|\boldsymbol{A}_N(\mu)^{-1}\right\| \leq \frac{\gamma(\mu)}{\alpha(\mu)}$$

  - Proof: symmetry $\Rightarrow \mathrm{cond}_2(\boldsymbol{A}_N) = \lambda_{max}/\lambda_{min}$

Let $\boldsymbol{u} = (u_i)_{i=1}^N$ be EV for λ_{max} and set $u := \sum_{i=1}^N u_i\varphi_i \in X$

Orthonormality yields

$$\|u\|^2 = \left\langle \sum_i u_i\varphi_i, \sum_j u_j\varphi_j \right\rangle = \sum_{i,j} u_i u_j \langle \varphi_i, \varphi_j\rangle = \sum_i u_i^2 = \|\boldsymbol{u}\|^2$$

Definition of $\boldsymbol{A}_N$ and continuity yields

$$\lambda_{max} \|\boldsymbol{u}\|^2 = \boldsymbol{u}^T \boldsymbol{A}_N \boldsymbol{u} = a\left(\sum_i u_i\varphi_i, \sum_j u_j\varphi_j\right) = a(u,u) \leq \gamma(\mu)\|u\|^2$$

Hence $\lambda_{max} \leq \gamma(\mu)$, similar $\lambda_{min} \geq \alpha(\mu)$

RB Method

- Remark: Difference FEM/RB
  - Let $\boldsymbol{A}(\mu)$ denote the FEM (or Finite Volume, Discontinuous Galerkin) matrix
  - The RB matrix $\boldsymbol{A}_N(\mu) \in \mathbb{R}^{N \times N}$ is small but typically dense in contrast to the typically sparse but large matrix $\boldsymbol{A}(\mu) \in \mathbb{R}^{H \times H}$
  - The condition of $\boldsymbol{A}_N(\mu)$ does not deteriorate with N (if using orthonormal basis, e.g. by Gram Schmidt), while the condition number of $\boldsymbol{A}(\mu)$ typically grows polynomial in H.

RB Method

- Relation to Best-Approximation (Lemma of Cea)
  - For all $\mu \in \mathcal{P}$ holds

$$\|u(\mu) - u_N(\mu)\| \leq \frac{\gamma(\mu)}{\alpha(\mu)} \inf_{v \in X_N} \|u(\mu) - v\|$$

  - Proof: For all $v \in X_N$ continuity and coercivity result in

$$\begin{aligned}
\alpha \|u - u_N\|^2 &\leq a(u - u_N, u - u_N) \\
&= a(u - u_N, u - v) + \underbrace{a(u - u_N, v - u_N)}_{=0} \\
&= a(u - u_N, u - v) \leq \gamma \|u - u_N\| \, \|v - u_N\|
\end{aligned}$$

Where $a(u - u_N, v - u_N) = 0$ follows from Galerkin orthogonality as $v - u_N \in X_N$

RB Method

- Remarks:
  - „Quasi-optimality": RB-scheme is as good as best-approximation up to a constant.
  - Implication: Approximation scheme and space are decoupled: Find a good approximating space (without RB-scheme) you are sure, that the RB-scheme performs well.
  - Similar best-approximation bounds are known for interpolation techniques (via „Lebesgue"-constant). But for interpolation techniques (e.g. polynomial) these constants diverge to infinity for growing dimension of the approximation space.
  - In contrast: the bounding constant in RB-approximation does not grow to infinity with growing dimension. This is a conceptional advantage of Galerkin projection over interpolation techniques.

Exercise 7: Assuming symmetric a, the Lemma of Cea can be sharpened by a squareroot in the constants. (Hint: Energy norm, introduced soon)

RB Method

Error-Residual Relation

- The error satisfies a variational problem with residual as right hand side:
- For $\mu \in \mathcal{P}$ we define the residual $r(\cdot;\mu) \in X'$ via

$$r(v;\mu) := f(v;\mu) - a(u_N(\mu), v;\mu), \quad v \in X$$

  Then the error $e(\mu) := u(\mu) - u_N(\mu)$ satisfies

$$a(e(\mu), v;\mu) = r(v;\mu), \quad v \in X$$

- Proof:

$$a(e,v) = a(u,v) - a(u_N,v) = f(v) - a(u_N,v) = r(v), \quad v \in X$$

- Remark: Residual vanishes on the RB-space:

$$v \in X_N \Rightarrow r(v) := f(v) - a(u_N,v) = a(u_N,v) - a(u_N,v) = 0$$

RB Method

- Reproduction of Solutions
  - If $u(\mu) \in X_N$ for some $\mu \in \mathcal{P}$ then $u_N(\mu) = u(\mu)$
  - Proof: $e(\mu) = u(\mu) - u_N(\mu) \in X_N$ hence

$$\alpha \|e\|^2 \leq a(e,e) = r(e) = 0$$

- Remark:
  - Reproduction of solutions is a basic consistency property. Holds trivially, if error-bounds are available, but for some more complex RB-schemes this may be all you can get and a good initial consistency check.
  - Validation of Program Code: Choose Basis by snapshots

$$\varphi_i := u(\mu^{(i)}), i = 1, \ldots, N$$

Then we expect $\boldsymbol{u}_N(\mu^{(i)}) = \boldsymbol{e}_i \in \mathbb{R}^N$ to be a unit vector

RB Method

- Uniform Convergence of RB-approximation
  - Assume Lipschitz-continuity of coefficient functions, then $u(\mu)$ and $u_N(\mu)$ are Lipschitz-continuous with L_u independent of N.
  - Assume $\{S_N\}_{N\in\mathbb{N}}$ to be sample sets getting dense in $\mathcal{P}$,

    „fill distance" $h_N := \sup_{\mu\in\mathcal{P}} \text{dist}(\mu, S_N), \quad \lim_{N\to\infty} h_N = 0$
  - Then for all μ and „closest" $\mu^* := \arg\min_{\mu'\in S_N} \|\mu - \mu'\|$

$$\|u(\mu) - u_N(\mu)\| \leq \|u(\mu) - u(\mu^*)\| + \|u(\mu^*) - u_N(\mu^*)\| + \|u_N(\mu^*) - u_N(\mu)\|$$
$$\leq L_u \|\mu - \mu'\| + 0 + L_u \|\mu - \mu'\| \leq 2h_N L_u$$

  - Therefore, we obtain $\lim_{N\to\infty} \sup_{\mu\in\mathcal{P}} \|u(\mu) - u_N(\mu)\| = 0$
  - Note: Convergence rate linear in h_N is of no practical use

RB Method

- Coercivity Constant Lower Bound
  - We assume to have available a rapidly computable lower bound for the coercivity constant
    $$0 < \alpha_{LB}(\mu) \leq \alpha(\mu), \quad \mu \in \mathcal{P}$$
  - We assume this to be large, w.l.o.g. $\bar{\alpha} \leq \alpha_{LB}(\mu)$ (otherwise simply set $\alpha_{LB}(\mu) := \bar{\alpha}$)
- Continuity Constant Upper Bound
  - We assume to have available a rapidly computable upper bound for the continuity constant
    $$\gamma_{UB}(\mu) \geq \gamma(\mu), \quad \mu \in \mathcal{P}$$
  - We assume this to be small, w.l.o.g. $\bar{\gamma} \geq \gamma_{UB}(\mu)$ (otherwise simply set $\gamma_{UB}(\mu) := \bar{\gamma}$)

RB Method

- A-posteriori Error Bounds
  - For all $\mu \in \mathcal{P}$ holds

$$\|u(\mu) - u_N(\mu)\| \leq \Delta_u(\mu) := \frac{\|r(\cdot;\mu)\|_{X'}}{\alpha_{LB}(\mu)}$$

$$|s(\mu) - s_N(\mu)| \leq \Delta_s(\mu) := \|l(\cdot;\mu)\|_{X'} \Delta_u(\mu)$$

  - Proof: testing the error-residual eqn. with e yields

$$\alpha_{LB}(\mu)\,\|e\|^2 \leq a(e,e) = r(e) \leq \|r\|_{X'}\,\|e\|$$

    division then yields the bound for u.
    Bound for output error follows with continuity

$$|s - s_N| = |l(u) - l(u_N)| = |l(u - u_N)| \leq \|l(\cdot;\mu)\|_{X'} \Delta_u(\mu)$$

  - Note: Output bound is coarse, can be improved (see later)

RB Method

- Remark:
  - General pattern: Derive error-residual relation, then apply stability statement to obtain an error bound.
  - If u is the continous solution in infinite X, then the bound is „a-priori", as the residual norm is not computable.
  - In case of RB methods: If u is the FEM solution in finite-dimensional X, the residual norm is computable, hence the error bound turns into a computable quantity.
  - It is „a-posteriori": reduced solution must be available.
  - „Rigorosity": As the bound is a provable upper bound on the error, the bound is denoted „rigorous" in RB methods (corresponding to „reliable" error estimators in FEM literature)
  - RB method with a-posteriori error control is denoted a „certified" RB method

RB Method

- Vanishing Error Bound / Zero Error Prediction
  - If $u(\mu) = u_N(\mu)$ then $\Delta_u(\mu) = \Delta_s(\mu) = 0$
  - Proof:

$$e = 0 \Rightarrow 0 = a(e, v) = r(v) \Rightarrow \|r\|_{X'} = 0 \Rightarrow \Delta_u = 0 \Rightarrow \Delta_s = 0$$

- Remark:
  - Initial desired property of an error bound: Bound is zero if the error is zero. This may give hope, that the error bound is not too conservative, i.e. not too large overestimating the error.
  - The statement is trivial in case of „effective" error bounds as seen soon. But if no „effective" error bounds are available for a more complex RB scheme, this may be as much as you can get, or a useful initial property of an error estimator.
  - This property is again useful for validating program code

RB Method

- (Uniform) Effectivity Bound
  - The „effectivity" $\eta_u(\mu)$ of $\Delta_u(\mu)$ is defined and bounded by

$$\eta_u(\mu) := \frac{\Delta_u(\mu)}{\|u(\mu) - u_N(\mu)\|} \leq \frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)} \leq \frac{\bar{\gamma}}{\bar{\alpha}}, \quad \mu \in \mathcal{P}$$

  - Proof: Test error eqn. with Riesz-repr. $v_r \in X$ of residual:

$$\|v_r\|^2 = \langle v_r, v_r \rangle = r(v_r) = a(e, v_r) \leq \gamma_{UB}(\mu) \|e\| \|v_r\|$$

Therefore $\frac{\|v_r\|}{\|e\|} \leq \gamma_{UB}(\mu)$ and

$$\eta_u(\mu) = \frac{\Delta_u(\mu)}{\|e(\mu)\|} = \frac{\|v_r\|}{\alpha_{LB}(\mu)\|e\|} \leq \frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)} \leq \frac{\bar{\gamma}}{\bar{\alpha}}$$

- Remark
  - Upper bound on the effectivity can be evaluated rapidly
  - Related notion „efficiency" in FEM literature.
  - „Rigorosity" of error bound implies $\eta_u(\mu) \geq 1$

RB Method

- Relative Error Bound and Effectivity (cf. [PR06])
  - For all $\mu \in \mathcal{P}$ holds

$$\frac{\|u(\mu) - u_N(\mu)\|}{\|u(\mu)\|} \leq \Delta_u^{rel}(\mu) := 2 \cdot \frac{\|r(\cdot;\mu)\|_{X'}}{\alpha_{LB}(\mu)} \cdot \frac{1}{\|u_N(\mu)\|}$$

$$\eta_u^{rel}(\mu) := \frac{\Delta_u^{rel}(\mu)}{\|e(\mu)\| \,/\, \|u(\mu)\|} \leq 3 \cdot \frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)} \leq 3 \cdot \frac{\bar{\gamma}}{\bar{\alpha}}.$$

under the condition that $\Delta_u^{rel}(\mu) \leq 1$

Exercise 8: Prove this relative error bound and effectivity bound

- Remark:
  - Relative bounds are typically only valid if the bound is sufficiently small. If these are not small, the RB space should be improved.

RB Method

- Remark: No Effectivity for Output Error Bound
  - Without further assumptions, one cannot expect a bounded effectivity for the output error estimator $\Delta_s(\mu)$
  - Example: Choose X_N and μ such that $u_N(\mu) \neq u(\mu)$

    Then also $e(\mu), r(\mu), \Delta_u(\mu), \Delta_s(\mu)$ are nonzero.

    Now choose l such that

    $$l(u - u_N) = 0 \Rightarrow s(\mu) - s_N(\mu) = l(e) = 0$$

    Hence $\frac{\Delta_s(\mu)}{|s(\mu) - s_N(\mu)|}$ is not well defined.

- (A4) Symmetry:
  - For the remainder of this section, we additionally assume, that $a(\cdot, \cdot; \mu)$ is symmetric.

RB Method

- Energy norm
  - For symmetric, coercive, continuous $a(\cdot,\cdot;\mu)$ we define the (μ-dependent) energy scalar product and norm

$$\langle u, v\rangle_\mu := a(u,v;\mu) \qquad \|v\|_\mu := \sqrt{\langle v, v\rangle_\mu}, \quad u,v \in X$$

- Norm Equivalence
  - We have

$$\sqrt{\alpha(\mu)}\,\|u\| \leq \|u\|_\mu \leq \sqrt{\gamma(\mu)}\,\|u\|, \quad u \in X, \mu \in \mathcal{P}$$

  - Proof: Coercivity and Continuity imply

$$\alpha(\mu)\,\|u\|^2 \leq \underbrace{a(u,u;\mu)}_{=\|u\|_\mu^2} \leq \gamma(\mu)\,\|u\|^2$$

RB Method

- Energy Norm Error bound and Effectivity [PR06]
  - For $\mu \in \mathcal{P}$ holds

$$\|u(\mu) - u_N(\mu)\|_\mu \leq \Delta_u^{en}(\mu) := \frac{\|r(\cdot;\mu)\|_{X'}}{\sqrt{\alpha_{LB}(\mu)}}$$

$$\eta_u^{en}(\mu) := \frac{\Delta_u^{en}(\mu)}{\|u(\mu) - u_N(\mu)\|_\mu} \leq \sqrt{\frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)}} \leq \sqrt{\frac{\bar{\gamma}}{\bar{\alpha}}}, \quad \mu \in \mathcal{P}$$

  - As $\frac{\gamma(\mu)}{\alpha(\mu)} \geq 1$ this is an improvement by a squareroot

Exercise 9: Prove this energy error bound and effectivity bound

RB Method

- Remark: Possible Improvement by Changing Norm
  - By choosing $\bar{\mu} \in \mathcal{P}$ and setting $\|u\| := \|u\|_{\bar{\mu}}$ as new norm on X, we get
    $$\alpha(\bar{\mu}) = 1 = \gamma(\bar{\mu})$$
  - The RB-approximation is not affected
  - But the error bound and effectivities are improved:
    They are optimal in $\bar{\mu}$: $\Delta_u(\bar{\mu}) = \|e(\bar{\mu})\|, \quad \eta_u(\bar{\mu}) = 1$
    and (assuming continuity) almost optimal in the vicinity of $\bar{\mu}$

In the following: return to arbitrarily chosen norm on X

RB Method

- Improved Output Error Bound & Effectivity, Compliant Case
  - Assume that $a(\cdot,\cdot;\mu)$ is symmetric and $f = l$ (the so called „compliant" case), then we obtain the improved output error bound and effectivity

$$0 \leq s(\mu) - s_N(\mu) \leq \Delta_s'(\mu) := \frac{\|r(\cdot;\mu)\|_{X'}^2}{\alpha_{LB}(\mu)}$$

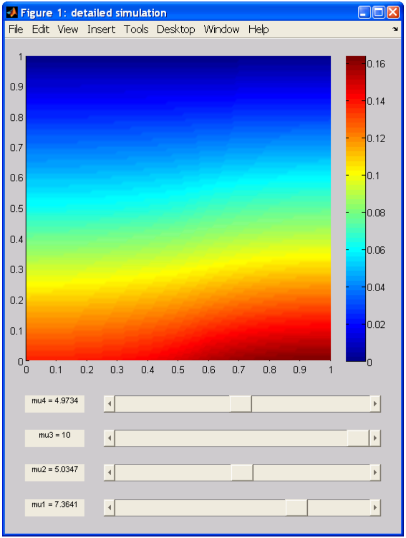
$$\eta_s'(\mu) := \frac{\Delta_s'(\mu)}{s(\mu) - s_N(\mu)} \leq \frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)} \leq \frac{\bar{\gamma}}{\bar{\alpha}}$$

- Remark:
  - Proof: Follows later from more general statement
  - The bound gives a definite sign on the error: $s_N(\mu) \leq s(\mu)$
  - This output error bound $\Delta_s'(\mu)$ is better as it is quadratic in $\|r\|_{X'}$ while $\Delta_s(\mu)$ is only linear
  - The thermal block is a „compliant" problem.

Experiments

Experiments

- Thermal Block
  - rb_tutorial(1): Full simulation, solution variety as seen earlier
  - rb_tutorial(2): Demo gui for full simulation:
  - rb_tutorial(3) All steps for generation of reduced model and timing

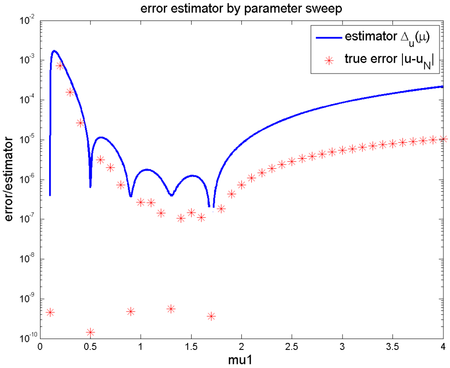


Experiments

Error Estimator and True Error

- rb_tutorial(4): Lagrangian basis for N=5 $B_1 = B_2 = 2$

$$S_N = (0.1, 0.1, 0.1, 0.1)$$
$$(0.5, 0.1, 0.1, 0.1)$$
$$(0.9, 0.1, 0.1, 0.1)$$
$$(1.3, 0.1, 0.1, 0.1)$$
$$(1.7, 0.1, 0.1, 0.1)$$



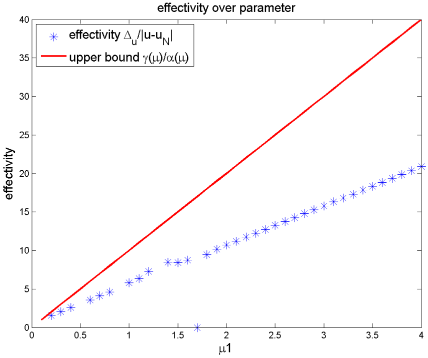
- Parameter sweep for estimator is cheap
- Estimator and error are zero for samples
- Estimator is upper bound of true error
- For small parameters larger error, hence more samples would be required

Experiments

- Effectivity and Bounds:
  - rb_tutorial(5)

$$\alpha(\mu) = \min(\mu_i) = 0.1$$
$$\gamma(\mu) = \max(\mu_i) = \mu_1$$

- Effectivities are good, only order of 10
- Effectivity upper bound is verified
- Effectivity undefined for basis samples (division by zero)

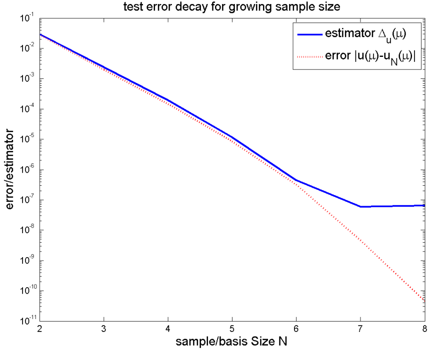


Experiments

- ## Error Convergence:
  - **rb_tutorial(6):** $B_1 = B_2 = 3, \quad \mu = (\mu_1, 1, 1, 1 \ldots, 1)$

- N equidistant samples $\mu_1 \in [0.5, 2]$
- Gram-Schmidt orth.
- Test-error/estimator: maximum over random test set

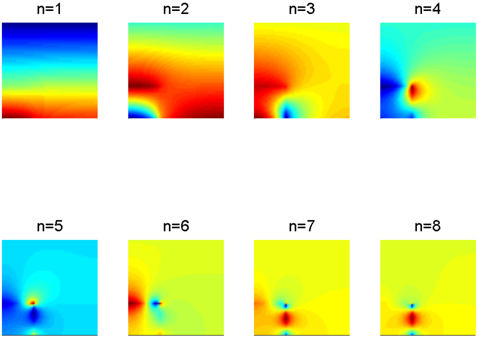
$S_{test} \subset \mathcal{P} \quad |S_{test}| = 100$



- Exponential error/bound convergence observed
- Upper bound very tight
- Numerical accuracy limit for estimators

Experiments

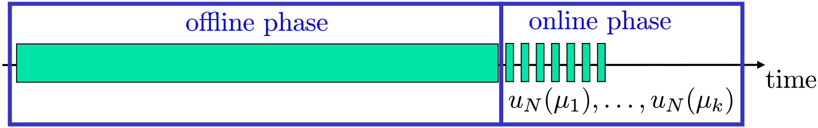
- Error Convergence:
  - Gram-Schmidt orthonormalized basis: rb_tutorial(7)



Offline/Online Decomposition

Offline/Online Decomposition

- Offline/Online Decomposition



- Offline Phase:
  - Possibly computationally intensive, depending on $H := \dim(X)$
  - Performed only once
  - Computation of snapshots, reduced basis, Riesz-representers and auxiliary parameter-independent low-dim. quantities
- Online Phase:
  - Rapid, i.e. complexity polynomial in N, Q_a, Q_f, Q_l, independent of H
  - Performed multiple times for different parameters
  - Assembly and solution of RB-system, computation of error estimators and effectivity bounds.

Offline/Online Decomposition

- Required: Discretization of (P)
  - Space $X = \mathrm{span}\{\psi_i\}_{i=1}^H$, high dimension $H := \dim(X)$
  - Inner Product Matrix $\boldsymbol{K} := (\langle \psi_i, \psi_j \rangle)_{i,j=1}^H \in \mathbb{R}^{H \times H}$
  - Assume component matrices and vectors

$$\boldsymbol{A}_q := (a_q(\psi_j, \psi_i))_{i,j=1}^H \in \mathbb{R}^{H \times H}$$

$$\boldsymbol{f}_q := (f_q(\psi_i))_{i=1}^H \in \mathbb{R}^H \qquad \boldsymbol{l}_q := (l_q(\psi_i))_{i=1}^H \in \mathbb{R}^H$$

  - For any $\mu \in \mathcal{P}$ evaluate coefficients & assemble full system

$$\boldsymbol{A}(\mu) := \sum_{q=1}^{Q_a} \theta_q^a(\mu) \boldsymbol{A}_q, \quad \boldsymbol{f}(\mu) := \sum_{q=1}^{Q_f} \theta_q^f(\mu) \boldsymbol{f}_q, \quad \boldsymbol{l}(\mu) := \sum_{q=1}^{Q_l} \theta_q^l(\mu) \boldsymbol{l}_q$$

  - Solve linear system $\boldsymbol{A}(\mu)\boldsymbol{u}(\mu) = \boldsymbol{f}(\mu)$ for $\boldsymbol{u}(\mu) = (u_i)_{i=1}^H \in \mathbb{R}^H$
  - Obtain solution of (P): $u(\mu) = \sum_{i=1}^H u_i \psi_i, \quad s(\mu) := \boldsymbol{l}^T \boldsymbol{u}$
- Remark:
  - Components may be nontrivial for third-party-software!

Offline/Online Decomposition

- Offline/Online Decomposition of (P_N)
  - Offline: After the computation of a basis $\Phi_N = \{\varphi_i\}_{i=1}^N$ construct the parameter-independent component matrices and vectors

$$\boldsymbol{A}_{N,q} := (a_q(\varphi_j, \varphi_i))_{i,j=1}^N \in \mathbb{R}^{N\times N}$$

$$\boldsymbol{f}_{N,q} := (f_q(\varphi_i))_{i=1}^N \in \mathbb{R}^N \qquad \boldsymbol{l}_{N,q} := (l_q(\varphi_i))_{i=1}^N \in \mathbb{R}^N$$

  - Online: For given $\mu \in \mathcal{P}$ evaluate the coefficient functions and assemble the matrix and vectors

$$\boldsymbol{A}_N(\mu) := \sum_{q=1}^{Q_a} \theta_q^a(\mu)\boldsymbol{A}_{N,q}, \quad \boldsymbol{f}_N(\mu) := \sum_{q=1}^{Q_f} \theta_q^f(\mu)\boldsymbol{f}_{N,q}, \quad \boldsymbol{l}_N(\mu) := \sum_{q=1}^{Q_l} \theta_q^l(\mu)\boldsymbol{l}_{N,q}$$

This exactly gives the discrete RB system $\boldsymbol{A}_N(\mu)\boldsymbol{u}_N(\mu) = \boldsymbol{f}_N(\mu)$ stated earlier, that can then be solved and gives $u_N(\mu), s_N(\mu)$

Offline/Online Decomposition

- Remark: Simple Computation of Reduced Components
  - The reduced component matrices/vectors do not require any space-integration, if the high dimensional components are available:
  - Assume expansion of reduced basis vectors

$$\varphi_j = \sum_{i=1}^{H} \varphi_{ij} \psi_i$$

With coefficient matrix

$$\mathbf{\Phi}_N := (\varphi_{ij})_{i,j=1}^{H,N} \in \mathbb{R}^{H \times N}$$

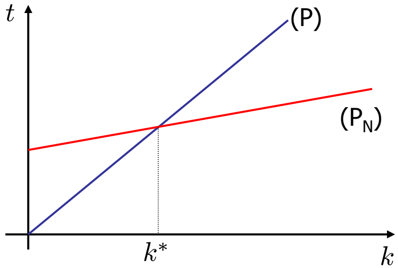
  - Reduced components are then simply obtained by matrix-matrix/matrix-vector multiplications

$$\boldsymbol{A}_{N,q} = \mathbf{\Phi}_N^T \boldsymbol{A}_q \mathbf{\Phi}_N, \quad \boldsymbol{f}_{N,q} = \mathbf{\Phi}_N^T \boldsymbol{f}_q, \quad \boldsymbol{l}_{N,q} = \mathbf{\Phi}_N^T \boldsymbol{l}_q$$

Offline/Online Decomposition

- Complexities of (P_N)
  - Offline: $\mathcal{O}(NH^2 + NH(Q_f + Q_l) + N^2 H Q_a)$
  - Online: $\mathcal{O}(N^3 + N(Q_f + Q_l) + N^2 Q_a)$ independent of H
- Runtime Diagram
  - Runtime for k simulations
  - With (P): $t = k \cdot t_{full}$
  - With (P_N): $t = t_{offline} + k \cdot t_{online}$
  - Intersection

$$k^* = \frac{t_{offline}}{t_{full} - t_{online}}$$

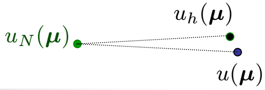


- ACHTUNG: RB Payoff only for „multiple“ requests
  - RB model offline time only pays off if sufficiently many $k \geq k^*$ reduced simulations are expected.

Offline/Online Decomposition

- Remark: No Distinction between u and u_h
  - Remember, we did not discriminate in (P) between the true weak (Sobolev) space solution u and the fine FEM solution, say u_h (we only do this for this slide). This can be motivated by two arguments:
  - 1. In view of the independency of the online phase on H, we can assume $\|u - u_h\|$ arbitrary small, hence H arbitrary large (just let the offline phase be sufficiently accurate) without affecting the online runtime.
  - 2. In practice, the reduction error will dominate the overall error, the FEM error is neglegible $\varepsilon := \|u - u_h\| \ll \|u_h - u_N\|$ Then it is sufficient to control $\|u_h - u_N\|$

$$\|u_h - u_N\| - \varepsilon \leq \|u - u_N\| \leq \|u_h - u_N\| + \varepsilon$$



Offline/Online Decomposition

- Requirements for Error and Effectivity Bounds

  We require offline/online decompositions of the following quantities if we want to compute a-posteriori and effectivity bounds rapidly:

  - Dual norm of the residual $\|r(\cdot;\mu)\|_{X'}$ for all error bounds
  - Dual norm of output functional $\|l(\cdot;\mu)\|_{X'}$ for output error bound $\Delta_s(\mu)$
  - Norm of RB-solution $\|u_N(\mu)\|$ for relative error bound $\Delta_u^{rel}(\mu)$
  - Lower coercivity constant bound $\alpha_{LB}(\mu)$ for all error and effectivy bounds
  - Upper bound for continuity constant $\gamma_{UB}(\mu)$ for effectivity upper bound

Offline/Online Decomposition

- Parameter Separability of Residual
  - Set $Q_r := Q_f + NQ_a$ and define $r_q \in X', q = 1, \dots, Q_r$ via
    $$(r_1, \dots, r_{Q_r}) := \big(f_1, \dots, f_{Q_f}, a_1(\varphi_1, \cdot), \dots, a_{Q_a}(\varphi_1, \cdot), \dots, a_1(\varphi_N, \cdot), \dots, a_{Q_a}(\varphi_N, \cdot)\big)$$
  - Let $u_N(\mu) = \sum_{i=1}^N u_{Ni}\varphi_i$ be solution of (P_N)
  - Define $\theta_q^r(\mu), q = 1, \dots, Q_r$ via
    $$(\theta_1^r, \dots, \theta_{Q_r}^r) := \Big(\theta_1^f, \dots, \theta_{Q_f}^f, -\theta_1^a \cdot u_{N1}, \dots, -\theta_{Q_a}^a \cdot u_{N1}, \dots, -\theta_1^a \cdot u_{NN}, \dots, -\theta_{Q_a}^a \cdot u_{NN}\Big)$$
  - Let $v_r, v_{r,q} \in X$ denote the Riesz-representers of r, r_q
  - Then r, v_r are parameter separable via
    $$r(v;\mu) = \sum_{q=1}^{Q_r} \theta_q^r(\mu) r_q(v), \quad v_r(\mu) = \sum_{q=1}^{Q_r} \theta_q^r(\mu) v_{r,q}, \quad \mu \in \mathcal{P}, v \in X$$
  - Proof: By definition and linearity

Offline/Online Decomposition

- Computation of Riesz-Representers
  - Recall: $X = \text{span}\{\psi_i\}_{i=1}^H$, $\boldsymbol{K} := (\langle \psi_i, \psi_j \rangle)_{i,j=1}^H$
  - For $g \in X'$ the coefficient vector $\boldsymbol{v} = (v_i)_{i=1}^H \in \mathbb{R}^H$ of its Riesz-representer $v_g = \sum_{i=1}^H v_i \psi_i \in X$ is obtained by solving the sparse linear system

    $$\boldsymbol{K}\boldsymbol{v} = \boldsymbol{g}$$

    with right hand side vector $\boldsymbol{g} = (g(\psi_i))_{i=1}^H$
  - Proof: For any $u = \sum_{i=1}^H u_i \psi_i$ with coefficient vector $\boldsymbol{u} = (u_i)_{i=1}^H$ we verify

$$g(u) = \sum_{i=1}^H u_i g(\psi_i) = \boldsymbol{u}^T \boldsymbol{g} = \boldsymbol{u}^T \boldsymbol{K} \boldsymbol{v} = \left\langle \sum_{i=1}^H u_i \psi_i, \sum_{j=1}^H v_j \psi_j \right\rangle = \langle v_g, u \rangle$$

Offline/Online Decomposition

- Offline/Online Decomposition of Dual Norm of Residual
  - Offline: After the offline-phase of (P_N) we compute the Riesz-representers $v_{r,q} \in X$ of the residual components $r_q \in X'$ and define the matrix

$$\boldsymbol{G}_r := (r_q(v_{r,q'}))_{q,q'=1}^{Q_r} \in \mathbb{R}^{Q_r \times Q_r}$$

  - Online: For given $\mu \in \mathcal{P}$ and RB-solution $u_N(\mu)$ compute the residual coefficient vector $\boldsymbol{\theta}_r(\mu) := (\theta_1^r(\mu), \ldots, \theta_{Q_r}^r(\mu))$ and

$$\|r(\cdot;\mu)\|_{X'} = \sqrt{\boldsymbol{\theta}_r(\mu)^T \boldsymbol{G}_r \boldsymbol{\theta}_r(\mu)}$$

  - Proof: G is symmetric as $r_q(v_{r,q'}) = \langle v_{r,q}, v_{r,q'} \rangle$, then

$$\|r(\cdot;\mu)\|_{X'}^2 = \|v_r\|^2 = \left\langle \sum_{q=1}^{Q_r} \theta_q^r(\mu) v_{r,q}, \sum_{q'=1}^{Q_r} \theta_{q'}^r(\mu) v_{r,q'} \right\rangle = \boldsymbol{\theta}_r(\mu)^T \boldsymbol{G}_r \boldsymbol{\theta}_r(\mu)$$

Offline/Online Decomposition

- Offline/Online Decomposition for $\|l(\cdot;\mu)\|_{X'}$
  - Completely analogous as for dual norm of residual:
  - Offline: compute the Riesz-representers $v_{l,q} \in X$ of the output functional components $l_q \in X'$ and define

$$\boldsymbol{G}_l := (l_q(v_{l,q'}))_{q,q'=1}^{Q_l} \in \mathbb{R}^{Q_l \times Q_l}$$

  - Online: For given $\mu \in \mathcal{P}$ compute the output coefficient vector $\boldsymbol{\theta}_l(\mu) := (\theta_1^l(\mu), \dots, \theta_{Q_l}^l(\mu))$ and

$$\|l(\cdot;\mu)\|_{X'} = \sqrt{\boldsymbol{\theta}_l(\mu)^T \boldsymbol{G}_l \boldsymbol{\theta}_l(\mu)}$$

Offline/Online Decomposition

- Offline/Online Decomposition for $\|u_N(\mu)\|$
  - Offline: After the basis generation, compute the reduced inner product matrix

$$\boldsymbol{K}_N := (\langle \varphi_i, \varphi_j \rangle)_{i,j=1}^N \in \mathbb{R}^{N \times N}$$

  - Online: For given $\mu \in \mathcal{P}$ and RB solution $u_N(\mu)$ with coefficient vector $\boldsymbol{u}_N(\mu) \in \mathbb{R}^N$ we obtain

$$\|u_N(\mu)\| = \sqrt{\boldsymbol{u}_N(\mu)^T \boldsymbol{K}_N \boldsymbol{u}_N(\mu)}$$

- Remark
  - Simple computation via basis matrix multiplication:

$$\boldsymbol{K}_N := \boldsymbol{\Phi}_N^T \boldsymbol{K} \boldsymbol{\Phi}_N$$

Offline/Online Decomposition

- „Min-Theta“ Approach for Coercivity Lower Bound
  - One approach that can be applied in certain cases:
  - Assume that the components satisfy $a_q(u,u) \geq 0, q = 1, \ldots, Q_a$ and the coefficients fulfill $\theta_q^a(\mu) > 0, q = 1, \ldots, Q_a$ Let $\bar{\mu} \in \mathcal{P}$ such that $\alpha(\bar{\mu})$ is available.
  - Then we have

$$0 < \alpha_{LB}(\mu) \leq \alpha(\mu), \quad \mu \in \mathcal{P}$$

with the lower bound

$$\alpha_{LB}(\mu) := \alpha(\bar{\mu}) \cdot \min_{q=1,\ldots,Q_a} \frac{\theta_q^a(\mu)}{\theta_q^a(\bar{\mu})}$$

  - (No symmetry required)

Offline/Online Decomposition

- Computation of $\alpha(\mu)$ for (P)
  - In offline-phase some evaluations of $\alpha(\mu)$ may be required, e.g. for Min-theta or other procedures.
  - Let $\boldsymbol{A} := (a(\psi_j, \psi_i; \mu))_{i,j=1}^H$ and $\boldsymbol{K} := (\langle \psi_i, \psi_j \rangle)_{i,j=1}^H$ be given. Define symmetric part $\boldsymbol{A}_s := \frac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^T)$, then

$$\alpha(\mu) = \lambda_{min}(\boldsymbol{K}^{-1}\boldsymbol{A}_s)$$

  - Proof: Assume $\boldsymbol{K} = \boldsymbol{L}\boldsymbol{L}^T$, use substitution $\boldsymbol{v} = \boldsymbol{L}^T\boldsymbol{u}$ in

$$\alpha(\mu) = \inf_{u \in X} \frac{a(u,u)}{\|u\|^2} = \inf_{\boldsymbol{u} \in \mathbb{R}^H} \frac{\boldsymbol{u}^T \boldsymbol{A}_s \boldsymbol{u}}{\boldsymbol{u}^T \boldsymbol{K} \boldsymbol{u}} = \inf_{\boldsymbol{v} \in \mathbb{R}^H} \frac{\boldsymbol{v}^T \boldsymbol{L}^{-1} \boldsymbol{A}_s \boldsymbol{L}^{-T} \boldsymbol{v}}{\boldsymbol{v}^T \boldsymbol{v}}$$

Hence, alpha minimizes Rayleigh-quotient, i.e.

$$\alpha(\mu) = \lambda_{min}(\boldsymbol{L}^{-1}\boldsymbol{A}_s\boldsymbol{L}^{-T})$$

$\boldsymbol{K}^{-1}\boldsymbol{A}_s$ and $\boldsymbol{L}^{-1}\boldsymbol{A}_s\boldsymbol{L}^{-T}$ are similar thus have identical λ_{min} :

$$\boldsymbol{L}^T(\boldsymbol{K}^{-1}\boldsymbol{A}_s)\boldsymbol{L}^{-T} = \boldsymbol{L}^T\boldsymbol{L}^{-T}\boldsymbol{L}^{-1}\boldsymbol{A}_s\boldsymbol{L}^{-T} = \boldsymbol{L}^{-1}\boldsymbol{A}_s\boldsymbol{L}^{-T}$$

Offline/Online Decomposition

- Remark: Prevent Inversion of K:
  - Inversion of K frequently badly conditioned, fill-in-effect, etc., hence prevention of inversion is recommended:
  - Reformulation as generalized Eigenvalue problem:

$$\boldsymbol{K}^{-1}\boldsymbol{A}_s\boldsymbol{u} = \lambda\boldsymbol{u} \quad \Leftrightarrow \boldsymbol{A}_s\boldsymbol{u} = \lambda\boldsymbol{K}\boldsymbol{u}$$

    and determine smallest generalized eigenvalue
- Remark: Computation of Continuity Constant & Bound
  - Similar: Computation of continuity constant via largest singular value of suitable matrix.
  - Then one can formulate max-theta approach for a continuity constant upper bound

Exercise 10: Formulate a Max-Theta approach for a continuity constant upper bound $\gamma_{UB}(\mu)$, under the assumptions, that $a(\cdot,\cdot;\mu)$ is symmetric, all $a_q(\cdot,\cdot)$ are positive semidefinite, $\theta_q^a(\mu) > 0$ and $\gamma(\bar{\mu})$ is available for one $\bar{\mu} \in \mathcal{P}$

Offline/Online Decomposition

- Complexities of Error Estimators $\Delta_u(\mu), \Delta_s(\mu)$ (Including Min-theta)
  - Offline: $\mathcal{O}(H^3 + H^2(Q_f + Q_l + NQ_a) + H(Q_f + NQ_a)^2 + HQ_l^2)$
  - Online: $\mathcal{O}((Q_f + NQ_a)^2 + Q_l^2 + Q_a)$ independent of H
  - Very clear: Online quadratic dependence on Q_a, Q_f, Q_l, this can become prohibitive in case of too large expansions
- Remark: Successive Constraint Method [HRSP07]
  - Alternative to Min-Theta
  - Offline: Computation of many $\alpha(\mu^{(i)}), i = 1, \ldots, M$
  - Online: solution of a small linear program for computing coercivity lower bound (or similar continuity upper bound)

Basis Generation

Basis Generation

- Recall: „Lagrangian" Reduced Basis
  - Let parameter samples be given $S_N = \{\mu^{(1)}, \ldots, \mu^{(N)}\} \subset \mathcal{P}$
  - Define „Lagrangian" RB-Space and Basis

$$X_N := \mathrm{span}\{u(\mu^{(i)})\}_{i=1}^N = \mathrm{span}\Phi_N, \quad \Phi_N := \{\varphi_1, \ldots, \varphi_N\}$$

- Remarks:
  - Good approximation globally in $\mathcal{P}$ is possible, subject to suitably distributed points.
  - This is in contrast to local approximation, e.g. first order Taylor basis as used in early RB literature [FR83]:

$$\Phi_N := \{u(\mu^{(0)}, \partial_{\mu_i} u(\mu^{(0)}, \ldots, \partial_{\mu_p} u(\mu^{(0)})))\}$$

- Central Questions:
  - How to select sample points? How good will the basis be? For which problems will it work?

Basis Generation

- Optimal RB Space

$$X_N := \arg \min_{\substack{Y \subset X \\ \dim(Y)=N}} E(X_N) \qquad E(X_N) := \sup_{\mu \in \mathcal{P}} \|u(\mu) - u_N(\mu)\|$$

  - Highly nonlinear optimization problem for N-dimensional space, practically infeasible
- Modifications for practical „Greedy Procedure“:
  - Iterative relaxation: Instead of one optimization problem for complete basis, incrementally search „next best vector“ and extend existing basis
  - Instead of optimization over parameter space perform maximum search over training set of parameters
  - Allow general error indicator $\Delta(Y,\mu) \in \mathbb{R}^+$ as substitute for $\|u(\mu) - u_N(\mu)\|$ (using $X_N := Y$)

Basis Generation

- Greedy Procedure [VPRP03]
  - Let $S_{train} \subseteq \mathcal{P}$ be a given training set of parameters and $\varepsilon_{tol} > 0$ a given error tolerance. Set $\Phi_0 := \emptyset, X_0 := \{0\}, S_0 := \emptyset$ and define iteratively
    - while $\varepsilon_n := \max\limits_{\mu \in S_{train}} \Delta(X_n, \mu) > \varepsilon_{tol}$

$$\mu^{(n+1)} := \arg \max_{\mu \in S_{train}} \Delta(X_n, \mu)$$

$$S_{n+1} := S_n \cup \{\mu^{(n+1)}\}$$

$$\varphi_{n+1} := u(\mu^{(n+1)})$$

$$\Phi_{n+1} := \Phi_n \cup \{\varphi_{n+1}\}$$

$$X_{n+1} := X_n + \text{span}\{\varphi_{n+1}\}$$

    - end while

    Finally set $N := n + 1$

Basis Generation

- Remarks:
  - First use of Greedy in RB in [VPRP03]
  - In literature also frequently first „search" is skipped by arbitrarily choosing $\mu^{(1)}$
  - The training set is mostly chosen as random or structured finite subset of $\mathcal{P}$
  - Orthonormalization by Gram-Schmidt can be added in loop
  - Termination: Simple criterion: If for all $\mu \in \mathcal{P}$ and all subspaces $Y \subset X$ holds

    $$u(\mu) \in Y \Rightarrow \Delta(Y, \mu) = 0$$

    then the Greedy algorithm terminates in at most $|S_{train}|$ steps. Reason: No sample will be selected twice.
  - Basis is hierarchical: $\Phi_n \subset \Phi_m, \quad n < m$

Basis Generation

- Choice of Error Indicators
  - i) Orthogonal projection error as indicator

$$\Delta(Y,\mu) := \inf_{v \in Y} \|u(\mu) - v\| = \|u(\mu) - P_Y u(\mu)\|$$

Motivation: If projection error is small then with „Cea" also RB-error is small

-Expensive to evaluate, high dimensional operations

-All snapshots for all training parameters must be computed and stored, $|S_{train}|$ thus limited.

+Termination criterion trivially satisfied

+Approximation space decoupled from RB scheme

+Can be applied without RB-scheme and without a-posteriori error estimators

Basis Generation

- Choice of Error Indicators
  - ii) True RB error as indicator

$$\Delta(Y,\mu) := \|u(\mu) - u_N(\mu)\|$$

Motivation: This directly is the error measure used in

$$E(X_N)$$

-Expensive to evaluate, high dimensional operations

-All snapshots for all training parameters must be computed and stored, $|S_{train}|$ thus limited.

+Termination criterion satisfied in case of „Reproduction of Solutions" property

+Can be applied without a-posteriori error estimators

Basis Generation

- Choice of Error Indicators
  - iii) A-posteriori error estimator as indicator:

$$\Delta(Y, \mu) := \Delta_u(\mu) \quad \text{(or energy or relative error bounds)}$$

Motivation: Minimizing this ensures that true RB-error also is small, if bounds are „rigorous"

+Cheap to evaluate, only low dimensional operations

+Only N snapshots must be computed, $|S_{train}|$ can be very large.

+Termination criterion satisfied in case of „Vanishing Error Bound" and „Reproduction of Solutions" property

-If a-posteriori error bound is overestimating the RB error much then the space may be not good

Basis Generation

- Goal-Oriented Indicators:
  - When using output-error or output error estimators

    $$\Delta(Y,\mu) := |s(\mu) - s_N(\mu)|$$

    in the greedy procedure, the procedure is called „goal oriented". The basis will be possibly quite small, very accurately approximating the output, but not necessarily approximating the field variable well.
  - When using field-oriented indicators

    $$\Delta(Y,\mu) := \Delta_u(\mu), \Delta_u^{rel}(\mu), \Delta_u^{en}(\mu)$$

    in the greedy procedure, the basis may be larger, well approximating both the field variable and the output.

Basis Generation

- Monotonicity
  - In general $\Delta(X_n, \mu) \leq \varepsilon \quad \not\Rightarrow \quad \Delta(X_{n+1}, \mu) \leq \varepsilon$
  - This means, that greedy error sequence $(\varepsilon_n)_{n \geq 1}$ may be non monotonic
  - If relation to best-approximation holds

    $$\Delta(X_n, \mu) \leq C \inf_{v \in X_n} \|u(\mu) - v\|$$

    at least a boundedness or even asymptotic decay can be expected
  - Monotonicity, however, can be proven in special cases:

Exercise 11: Prove that the Greedy algorithm produces monotonically decreasing error sequences $(\varepsilon_n)_{n \geq 1}$ if
i) $\Delta(Y, \mu) := \|u(\mu) - P_Y u(\mu)\|$, i.e. indicator chosen as orth. projection error
ii) in compliant case ($a(\cdot, \cdot; \mu)$ symmetric and $l = f$) and $\Delta(Y, \mu) := \Delta_u^{en}(\mu)$,
i.e. indicator chosen as energy error estimator.

Basis Generation

- Remark: Overfitting, Quality Measurement
  - In terms of statistical learning theory, S_{train} is a „training set“ of parameters and ε_N is the „training error“
  - S_{train} must represent $\mathcal{P}$ well, should be chosen as large as possible
  - If training set is chosen too small or unrepresentative „overfitting“ will occur, i.e.

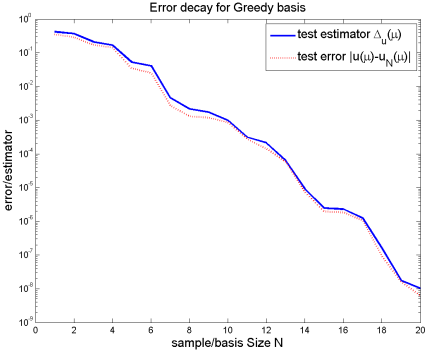
$$\max_{\mu \in \mathcal{P}} \Delta(X_N, \mu) \gg \varepsilon_N$$

  - => Low training error is a necessary but not a sufficient criterion for a good model (example „notepad“)
  - => Never compare models only by training error. Use error on independent „test-set“ instead.

Basis Generation

- Practice/Theory Gap:
  - Rb_tutorial(8): $B_1 = B_2 = 2, \quad \mu \in \mathcal{P} = [0.5, 2]^4$

- Greedy with random
  $S_{train} \subset \mathcal{P} \quad |S_{train}| = 1000$
- Estimator $\Delta(Y, \mu) := \Delta_u(\mu)$
- Gram-Schmidt orth.
- Test-error/estimator:
  maximum over
  random test set
  $S_{test} \subset \mathcal{P} \quad |S_{test}| = 100$
- Exponential error decay
  observed



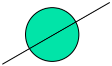
  - So Greedy is a well performing heuristic procedure
  - Formal convergence statements for analytical foundation?

Basis Generation

- Kolmogorov n-width $d_n(\mathcal{M})$
  - Maximum approximation error of best linear subspace

$$d_n(\mathcal{M}) := \inf_{\substack{Y \subset X \\ \dim(Y)=n}} \sup_{u \in \mathcal{M}} \|u - P_Y u\|$$

  - Decay indicates „approximability by linear subspaces“
  - $(d_n(\mathcal{M}))_{n\in\mathbb{N}}$ is a monotonically decreasing sequence
  - Examples
    - Unit balls: bad approximation, no decay



$$\mathcal{M} = \{u \,|\, \|u\| \leq 1\} \subset H^1([0,1]) \qquad d_n(\mathcal{M}) = 1, n \in \mathbb{N}$$

    - „Cereal Box“: good approximation, exponential decay

$$\prod_{i\in\mathbb{N}} [-2^{-i}, 2^{-i}] \subset l^2(\mathbb{R}) \qquad d_n(\mathcal{M}) \leq C \cdot 2^{-n}, n \in \mathbb{N}$$

Basis Generation

- Greedy Convergence Rates [BCDDPW10], [BMPPT09]
  - If $\mathcal{M}$ is well approximable by linear spaces, then the Greedy procedure will provide a quasi-optimal subspace:
  - Let $S_{train} = \mathcal{P}$ be compact and the greedy selection criterion guarantee (for suitable $\gamma \in (0,1]$)

$$\left\| u(\mu^{(n+1)}) - P_{X_n} u(\mu^{(n+1)}) \right\| \geq \gamma \sup_{u \in \mathcal{M}} \|u - P_{X_n} u\|$$

  - Then we can obtain algebraic convergence:

$$d_n(\mathcal{M}) \leq M n^{-\alpha}, n > 0 \quad \Rightarrow \quad \varepsilon_n \leq C M n^{-\alpha}, n > 0$$

  - Or exponential convergence:

$$d_n(\mathcal{M}) \leq M e^{-a n^{\alpha}}, n > 0 \quad \Rightarrow \quad \varepsilon_n \leq C M e^{-c n^{\beta}}, n > 0$$

(For suitable constants)

Basis Generation

- Strong vs. Weak Greedy
  - If $\gamma = 1$ it is a „Strong Greedy"
  - If $\gamma < 1$ it is a „Weak Greedy"
  - Strong Greedy can be realized by $\Delta(Y,\mu) := \|u(\mu) - P_Y u(\mu)\|$
- Error Estimator $\Delta(Y,\mu) := \Delta_u(\mu)$ Results in Weak Greedy!
  - Thanks to Cea, Effectivity and error bound properties:

$$\left\|u(\mu^{(n+1)}) - P_{X_n} u(\mu^{(n+1)})\right\| = \inf_{v \in X_N} \left\|u(\mu^{(n+1)}) - v\right\|$$

$$\geq \frac{\alpha(\mu)}{\gamma(\mu)} \left\|u(\mu^{(n+1)}) - u_N(\mu^{(n+1)})\right\| \geq \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \Delta_u(\mu^{(n+1)})$$

$$= \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \sup_{\mu \in \mathcal{P}} \Delta_u(\mu) \geq \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \sup_{\mu \in \mathcal{P}} \|u(\mu) - u_N(\mu)\|$$

$$\geq \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \sup_{\mu \in \mathcal{P}} \|u(\mu) - P_{X_N} u(\mu)\| \geq \frac{\bar{\alpha}^2}{\bar{\gamma}^2} \sup_{\mu \in \mathcal{P}} \|u(\mu) - P_{X_N} u(\mu)\|.$$

  - Hence, weakness factor $\gamma = (\bar{\alpha}/\bar{\gamma})^2 \in (0,1]$

Basis Generation

- Problem Reformulation
  - For which instantiations of (P) do we get exponential decaying Kolmogorov n-width?
  - Clearly not for all (P): imagine $\mathcal{M}$ a „sphere filling curve“
  - Positive example given by ([MPT02],[PR06]), specialization for the thermal block:
- Global Exponential Convergence for p=1
  - Consider (P) to be the thermal block with $B_1 = 2, B_2 = 1, \mu_1 = 1$ and single parameter $\mu = \mu_2 \in \mathcal{P}$
  - Let $\mathcal{P} := [\mu_{min}, \mu_{max}]$ and N_0 be sufficiently large
  - Choose $\mu_{min} = \mu^{(1)} < \ldots < \mu^{(N)} = \mu_{max}$ logarithmically equidistant and X_N the corresponding RB-space
  - Then
$$\frac{\|u(\mu) - u_N(\mu)\|_\mu}{\|u(\mu)\|_\mu} \leq e^{-\frac{N-1}{N_0-1}}, \mu \in \mathcal{P}, N \geq N_0.$$

Basis Generation

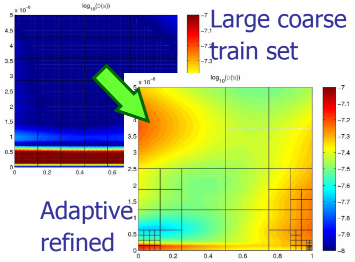
- Training Set Treatment
  - Multistage greedy [Se08]

    Decompose in coarser sets $S_{train}^{(0)} \subset \ldots \subset S_{train}^{(m)} := S_{train}$.

    Run Greedy on coarsest set, then start greedy on next larger set with first basis as starting basis, etc.
  - Adaptive Extension [HDO11]

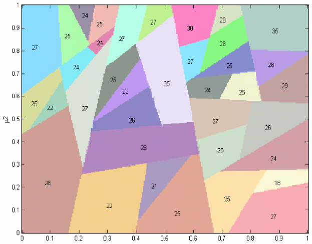
    Stop greedy when overfitting

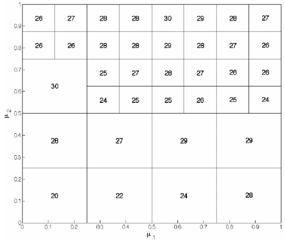
    Locally extend training set
  - Full Optimization: [UVZ12]
    - Optimization in greedy loop
  - Randomization [HSZ13]
    - In each greedy step new random training set



Basis Generation

- Parameter Domain Partitioning
  - Complex problems may require infeasibly large basis
    $N \leq N_{max}, \varepsilon_N \leq \varepsilon_{tol}$ can not simultaneously be satisfied
  - Solution: Partitioning of P, one basis per subdomain
    - hp-RB [EPR10]:
      - adaptive bisection
    - P-Partitioning: [HDO11]:
      - adaptive hexahedral refinement





Basis Generation

- Gramian Matrices Revisited
  - For $\{u_i\}_{i=1}^n \subset X$ we define the Gramian matrix

$$\boldsymbol{G} := (\langle u_i, u_j \rangle)_{i,j=1}^n \in \mathbb{R}^{n \times n}$$

  - We have seen such matrices play an important role in offline/online decomposition
  - They allow to perform some further operations independent of H
  - They have some nice properties: exercise

Exercise 12: Show that the following holds for the Gramian matrix:
i) G is symmetric and positive semidefinite
ii) $\mathrm{rank}(\boldsymbol{G}) = \dim(\mathrm{span}(\{u_i\}_{i=1}^n))$
iii) $\{u_i\}_{i=1}^n$ are linearly independent $\Leftrightarrow$ $\boldsymbol{G}$ is positive definite

Basis Generation

- Orthonormalization: Gram Schmidt
  - Useful for improving condition of the RB system matrix
  - Let basis $\Phi_N = \{\varphi_i\}_{i=1}^N \subset X$ be given with Gramian matrix $\boldsymbol{K}_N$
    Set $\boldsymbol{C} := (\boldsymbol{L}^T)^{-1}$ with $\boldsymbol{L}$ being a Cholesky factor of $\boldsymbol{K}_N = \boldsymbol{L}\boldsymbol{L}^T$
    Define the transformed basis $\tilde{\Phi}_N := \{\tilde{\varphi}_i\}_{i=1}^N \subset X$ by
    $$\tilde{\varphi}_j := \sum_{i=1}^N C_{ij}\varphi_i$$
    Then $\tilde{\Phi}_N$ is the Gram-Schmidt orthonormalization of Φ_N

Exercise 13: Prove that the above indeed performs Gram-Schmidt orthonormalization, i.e. set for $i = 1, \ldots, N$

$$v_i := \varphi_i - \sum_{j=1}^{i-1} \langle \bar{\varphi}_j, \varphi_i \rangle \bar{\varphi}_j \qquad \bar{\varphi}_i := v_i / \|v_i\|$$

And show that $\bar{\varphi}_j = \tilde{\varphi}_j, j = 1, \ldots, N$

Primal-Dual RB Approach

Primal-Dual RB Approach

- Recall:
  - For nonsymmetric, noncompliant case, we could only obtain an output-error estimator $\Delta_s(\mu)$, that only scaled linear with $\|r\|_{X'}$, and we showed the impossibility of obtaining effectivity bounds without further assumptions
  - In contrast, for the compliant case, the output error estimator $\Delta_s'(\mu)$ scaled quadratically in $\|r\|_{X'}$ and we obtained effectivity bounds.
- Goal of this section:
  - Improved output estimation for general nonsymmetric and/or noncompliant case by primal-dual techniques (but still no output effectivity bounds)
  - (P) and (P_N) are still required as „primal" problems

Primal-Dual RB Approach

- Definition: Full „Dual" Problem (P^{du})
  - For $\mu \in \mathcal{P}$ find a solution $u^{\mathrm{du}}(\mu) \in X$ satisfying

$$a(v, u^{\mathrm{du}}(\mu); \mu) = -l(v; \mu), \quad \forall v \in X$$

- Remark:
  - Obviously, the (negative) output functional is used as right hand side and the „arguments" are exchanged on the left.
  - Well-posedness (existence, uniqueness and stability) follow identical to „primal" Problem (P)
  - The dual problem only is required formally as reference, to which the dual error will be measured. Additionally, it can be used in practice to generate dual snapshots.

Primal-Dual RB Approach

- Dual RB Space
  - We assume to have a dual RB-space
    $$X_N^{\mathrm{du}} \subset X, \quad \dim X_N = N^{\mathrm{du}}$$
    that approximates the dual solutions $u^{\mathrm{du}}(\mu)$ well, possibly $N^{\mathrm{du}} \neq N$
  - Possible choice (without guarantee of success!) $X_N^{\mathrm{du}} = X_N$
  - Alternatives: Greedy procedure for (P^{du}) using snapshots of the full dual problem; Further alternative: combined approach; details explained at end of this section.

Primal-Dual RB Approach

- Definition: Primal-Dual Reduced Problem (P'_N)
  - For $\mu \in \mathcal{P}$ find the solution $u_N(\mu) \in X_N$ of (P_N), a solution $u_N^{\mathrm{du}}(\mu) \in X_N^{\mathrm{du}}$ satisfying

$$a(v, u_N^{\mathrm{du}}(\mu); \mu) = -l(v; \mu), \quad \forall v \in X_N^{\mathrm{du}}$$

    and the corrected output $s'_N(\mu) \in \mathbb{R}$

$$s'_N(\mu) := l(u_N(\mu); \mu) - r(u_N^{\mathrm{du}}(\mu); \mu)$$

- Remarks:
  - Well-posedness holds again via Lax-Milgram
  - „dual-weighted-residual" treatment as in goal-oriented FEM literature

Primal-Dual RB Approach

- Dual A-posteriori Error and Effectivity Bound
  - We introduce the dual residual $r^{\mathrm{du}}(\cdot;\mu) \in X'$

$$r^{\mathrm{du}}(v;\mu) := -l(v;\mu) - a(v, u_N^{\mathrm{du}}(\mu);\mu)), \quad v \in X$$

    and obtain the a-posteriori error bound

$$\left\| u^{\mathrm{du}}(\mu) - u_N^{\mathrm{du}}(\mu) \right\| \leq \Delta_u^{\mathrm{du}}(\mu) := \frac{\left\| r^{\mathrm{du}}(\cdot;\mu) \right\|_{X'}}{\alpha_{LB}(\mu)}$$

    with effectivity bound

$$\eta_u^{\mathrm{du}}(\mu) := \frac{\Delta_u^{\mathrm{du}}(\mu)}{\left\| u^{\mathrm{du}}(\mu) - u_N^{\mathrm{du}}(\mu) \right\|} \leq \frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)} \leq \frac{\bar{\gamma}}{\bar{\alpha}}$$

  - Proof: Completely analogous to the primal problem

Primal-Dual RB Approach

- Improved Output A-posteriori Error Bound
  - For $\mu \in \mathcal{P}$ holds

$$|s(\mu) - s'_N(\mu)| \leq \Delta'_s := \frac{\|r(\cdot;\mu)\|_{X'} \left\|r^{\mathrm{du}}(\cdot;\mu)\right\|_{X'}}{\alpha_{LB}(\mu)}$$

  - Proof: $s - s'_N = l(u) - l(u_N) + r(u_N^{\mathrm{du}}) = l(u - u_N) + r(u_N^{\mathrm{du}})$

$$= -a(u - u_N, u^{\mathrm{du}}) + \underbrace{f(u_N^{\mathrm{du}})}_{a(u,u_N^{\mathrm{du}})} - a(u_N, u_N^{\mathrm{du}})$$

$$= -a(u - u_N, u^{\mathrm{du}} - u_N^{\mathrm{du}}) =: -a(e, e^{\mathrm{du}})$$

Then

$$|s - s'_N| \leq |a(e, e^{\mathrm{du}})| = |r(e^{\mathrm{du}})| \leq \|r\|_{X'} \left\|e^{\mathrm{du}}\right\|$$

$$\leq \|r\|_{X'} \Delta_u^{\mathrm{du}} \leq \|r\|_{X'} \left\|r^{\mathrm{du}}\right\|_{X'} / \alpha_{LB}$$

Primal-Dual RB Approach

- Remark: Squared Effect
  - We see the desired „squared" effect by the product of the residual norms.
- Remark: No Effectivity for Output Error Bound Δ_s'
  - Without further assumptions, one cannot get output effectivity bounds for Δ_s' , as $s - s_N'$ may be zero, while $\Delta_s' \neq 0$, hence the quotient is not well defined.
  - Example: Choose $v_l \perp v_f \in X, \quad X_N = X_N^{\mathrm{du}} \perp \{v_f, v_l\}$

    $$a(u,v) := \langle u, v\rangle, \quad f(v) := \langle v_f, v\rangle, \quad l(v) := -\langle v_l, v\rangle$$

    then $u = v_f, \quad u^{\mathrm{du}} = v_l, \quad u_N = 0, \quad u_N^{\mathrm{du}} = 0$

    $$e = v_f, e^{\mathrm{du}} = v_l \quad \Rightarrow \quad r \neq 0, r^{\mathrm{du}} \neq 0 \quad \Rightarrow \quad \Delta_s' \neq 0$$

    but $s - s_N' = -a(e, e^{\mathrm{du}}) = \langle v_f, v_l\rangle = 0$
  - Reminder: „compliant" case gave output effectivity bounds

Primal-Dual RB Approach

- Remark: Dual Problem is Redundant for Compliant Case
  - For the compliant case, we claimed

$$0 \leq s(\mu) - s_N(\mu) \leq \Delta'_s(\mu) := \frac{\|r(\cdot;\mu)\|_{X'}^2}{\alpha_{LB}(\mu)}$$

  - The right ineq. is exactly a consequence of the primal-dual error bound, as $\|r\|_{X'} = \left\|r^{\mathrm{du}}\right\|_{X'}$ and $s_N = s'_N$:
    With $l = f$ and symmetry we obtain $u = -u^{\mathrm{du}}, u_N = -u_N^{\mathrm{du}}$
    and therefore $r = -r^{\mathrm{du}} \Rightarrow \|r\|_{X'} = \left\|r^{\mathrm{du}}\right\|_{X'}$
    Further, $r(u_N^{\mathrm{du}}) = -r(u_N) = 0 \Rightarrow s'_N = s_N$
  - The left ineq. Follows by coercivity:

$$s - s_N = s - s'_N = -a(e, e^{\mathrm{du}}) = a(e,e) \geq 0$$

  - The primal-dual approach only can lead to improvements in the non-compliant case, otherwise the simple primal approach is sufficient.

Primal-Dual RB Approach

- Remark: Output Effectivity Bound for Compliant Case
  - For the compliant case we claimed

$$\eta_s'(\mu) := \frac{\Delta_s'(\mu)}{s(\mu) - s_N(\mu)} \leq \frac{\gamma_{UB}(\mu)}{\alpha_{LB}(\mu)} \leq \frac{\bar{\gamma}}{\bar{\alpha}}$$

  - Proof: Cauchy-Schwarz and norm equivalence:

$$\|v_r\|^2 = \langle v_r, v_r \rangle = r(v_r) = a(e, v_r) = \langle e, v_r \rangle_\mu \leq \|e\|_\mu \|v_r\|_\mu \leq \|e\|_\mu \sqrt{\gamma_{UB}} \|v_r\|$$

$$\Rightarrow \|r\|_{X'} = \|v_r\| \leq \|e\|_\mu \sqrt{\gamma_{UB}}$$

  - Then we conclude using definitions

$$\eta_s' = \frac{\Delta_s}{s - s_N} = \frac{\|r\|_{X'}^2 / \alpha_{LB}}{a(e,e)} = \frac{\|r\|_{X'}^2}{\alpha_{LB} \|e\|_\mu^2} \leq \frac{\gamma_{UB} \|e\|_\mu^2}{\alpha_{LB} \|e\|_\mu^2} \leq \frac{\bar{\gamma}}{\bar{\alpha}}$$

Primal-Dual RB Approach

- Remarks: Offline/Online, Basis Generation
  - Offline/online procedure analogous to primal problem
  - Use of error estimation for basis generation:
    - Run separate greedy procedures for X_N, X_N^{du} using $\Delta_u, \Delta_u^{\mathrm{du}}$ with the same tolerance. Then the maximal primal and dual residuals will have similar order, indeed leading to a „squared" effect in the output error estimator Δ_s'
    - Alternative is a combined generation of primal and dual space: Run a greedy with the error bound Δ_s' and enrich both spaces simultaneously with corresponding snapshots of currently worst parameter.

Quadratically Nonlinear RB Approach

Quadratically Nonlinear RB Approach

- Example Reference [VPP03], [VRP03]
- Definition: Full Quadratical Problem (Q)
  - For $\mu \in \mathcal{P}$ find a solution $u(\mu) \in X$ and output $s(\mu) \in \mathbb{R}$ satisfying

$$a(u(\mu), u(\mu), v; \mu) + b(u(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X$$

$$s(\mu) = l(u(\mu); \mu)$$

  - with a, b, f, l continuous trilinear/bilinear/linear forms, continuity constants γ_a, γ_b , etc.
  - All forms being parameter separable
  - $a(\ldots)$ being symmetric w.r.t. first two arguments

$$a(u, v, w; \mu) = a(v, u, w; \mu), \quad \forall u, v, w \in X$$

Quadratically Nonlinear RB Approach

- Examples

  Find $u(\mu) \in H^1_0(\Omega)$ as solution of

  - Diffusion Eqn. with Nonlinear Reaction

$$-\mu_1 \Delta u + \mu_2 u^2 = q \quad \Longrightarrow \quad \underbrace{\mu_1 \int_\Omega \nabla u \cdot \nabla v}_{b(u,v;\mu)} + \underbrace{\mu_2 \int_\Omega u^2 v}_{a(u,u,v;\mu)} = \underbrace{\int_\Omega qv}_{f(v;\mu)}$$

  - Viscous Burgers Equation

$$-\mu_1 \Delta u + \nabla \cdot (cu^2) = q \quad \Longrightarrow \quad \underbrace{\mu_1 \int_\Omega \nabla u \cdot \nabla v}_{b(u,v;\mu)} + \underbrace{\int_\Omega u^2 (c \cdot \nabla v)}_{a(u,u,v;\mu)} = \underbrace{\int_\Omega qv}_{f(v;\mu)}$$

  - Nonlinear Diffusion
  - In 1D: Continuity of $a(\ldots)$ thanks to continuous embedding $H^1_0(\Omega) \to L^4(\Omega)$

Quadratically Nonlinear RB Approach

- Well-posedness
  - Existence/Uniqueness in general unclear: Multiple or no solutions possible
  - Existence/Uniqueness of the full problem will be concluded a-posteriori after successful RB solution
  - For simplicity: Assume well-posedness of full/reduced problem and its linearizations.

Quadratically Nonlinear RB Approach

Root finding formulation

- $u(\mu) \in X$ solves $F(u(\mu), \cdot; \mu) := 0 \in X'$ for
  $F(u(\mu), v; \mu) := a(u(\mu), u(\mu), v; \mu) + b(u(\mu), v; \mu) - f(v; \mu)$
- Derivative $DF|_u : X \to X'$

$$DF|_u(h) = \lim_{\delta \to 0} \frac{1}{\delta}(F(u + \delta h) - F(u)) = 2a(u, h, \cdot) + b(h, \cdot)$$

Solution of (Q) via Newton-Loop

- Choose $u^0 \in X$ and set k=0
- Repeat
  - Compute h^k as solution of $DF|_{u^k}(h^k) = -F(u^k)$, i.e.

$$2a(u^k, h^k, v) + b(h^k, v) = -a(u^k, u^k, v) - b(u^k, v) + f(v), \quad v \in X$$

  - Update solution $u^{k+1} := u^k + h^k$ and increment k
- Until convergence $\left\|u^{k+1} - u^k\right\| < \varepsilon_{tol}$

Quadratically Nonlinear RB Approach

- Definition: Reduced Quadratical Problem (Q_N)
  - For $\mu \in \mathcal{P}$ find a solution $u_N(\mu) \in X_N$ and output $s_N(\mu) \in \mathbb{R}$ satisfying

$$a(u_N(\mu), u_N(\mu), v; \mu) + b(u_N(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X_N$$

$$s_N(\mu) = l(u_N(\mu); \mu)$$

- Analogous Solution Steps:
  - Again formulation as Root-finding problem
  - Solution via Newton-loop, assuming solvability in each iteration and obtaining convergence.

Quadratically Nonlinear RB Approach

- Offline Phase:
  - Compute parameter independent component projections and reduced Gramian matrix:

$$\boldsymbol{A}_{N,q} := (a_q(\varphi_i, \varphi_j, \varphi_k))_{i,j,k=1}^N \in \mathbb{R}^{N\times N\times N}$$
$$\boldsymbol{B}_{N,q} := (b_q(\varphi_j, \varphi_i))_{i,j=1}^N \in \mathbb{R}^{N\times N}$$
$$\boldsymbol{f}_{N,q} := (f_q(\varphi_i))_{i=1}^N \in \mathbb{R}^{N}$$
$$\boldsymbol{l}_{N,q} := (l_q(\varphi_i))_{i=1}^N \in \mathbb{R}^{N}$$
$$\boldsymbol{K}_{N} := (\langle\varphi_i, \varphi_j\rangle)_{i,j=1}^N \in \mathbb{R}^{N\times N}$$

  - Obviously 3D-Tensors required: Size of N and Q_* considerably more critical

Quadratically Nonlinear RB Approach

- Online Phase:
  - For given $\mu \in \mathcal{P}$ perform linear combination of operators

$$\boldsymbol{A}_N(\mu) := \sum_{q=1}^{Q_a} \theta_q^a(\mu) \boldsymbol{A}_{N,q}, \quad \text{similarly} \quad \boldsymbol{B}_N(\mu), \boldsymbol{f}_N(\mu), \boldsymbol{l}_N(\mu)$$

  - Choose $\boldsymbol{u}_N^0 \in \mathbb{R}^N$
  - Repeat
    - Compute $\boldsymbol{h}_N^k \in \mathbb{R}^N$ as solution of

$$\left(2 \sum_{n=1}^{N} u_{N,n}^k \cdot (\boldsymbol{A}_N)_{n,:,:} + \boldsymbol{B}_N \right) \boldsymbol{h}_N^k = - \sum_{n,m=1}^{N} u_{N,n}^k u_{N,m}^k (\boldsymbol{A}_N)_{n,m,:} - \boldsymbol{B}_N \boldsymbol{u}_N^k + \boldsymbol{f}_N$$

    - Update solution $\boldsymbol{u}_N^{k+1} := \boldsymbol{u}_N^k + \boldsymbol{h}_N^k$ and increment k
  - Until convergence $(\boldsymbol{u}_N^{k+1} - \boldsymbol{u}_N^k)^T \boldsymbol{K}_N (\boldsymbol{u}_N^{k+1} - \boldsymbol{u}_N^k) < \varepsilon_{tol}^2$
  - set $\boldsymbol{u}_N(\mu) := \boldsymbol{u}_N^k, \quad s_N(\mu) = \boldsymbol{l}_N^T \boldsymbol{u}_N$

Quadratically Nonlinear RB Approach

- Existence of Solution for (Q)
  - Let $u_N(\mu) \in X_N$ be a reduced solution of (Q_N)
  - Define the dual norm of the residual

    $$\varepsilon := \|a(u_N(\mu), u_N(\mu), \cdot; \mu) + b(u_N(\mu), \cdot; \mu) - f(\cdot; \mu)\|_{X'}$$
  - and have a generalized stability constant

    $$0 < \beta_N(\mu) \leq 1/\left\|(DF|_{u_N})^{-1}\right\|_{X',X}$$
  - If the validity criterion holds, i.e. $\frac{8\varepsilon\gamma_a}{\beta_N^2} \leq 1$
  - then there exists a unique solution $u(\mu) \in B(u_N, 2\varepsilon/\beta_N)$ of (Q).
- Proof: Brezzi Rappaz Raviart (BRR) Theory
  - Verify assumptions of Thm 2.1 in [CR97]

Quadratically Nonlinear RB Approach

- Comments
  - We directly obtain an error bound

$$\|u(\mu) - u_N(\mu)\| \leq \Delta_u(\mu) := 2\varepsilon/\beta_N$$

  - $\beta_N(\mu)$ can be replaced by computable lower bound
  - If the validity criterion is not satisfied, the reduced basis should be improved to lower the residual norm.
  - Also effectivity of the bound can be proven

$$\Delta_u(\mu)/\|u(\mu) - u_N(\mu)\| \leq \rho(\mu) := \frac{4}{\beta_N}(2\gamma_a \|u_N\| + \gamma_b)$$

  - The „trilinearform" technique in principle generalizes to higher order polynomial nonlinearities in PDEs, that can be written as multilinear form. Limitation arises due to
    - Memory constraints for storing the tensors
    - online computation time for the increasingly demanding linear combinations.

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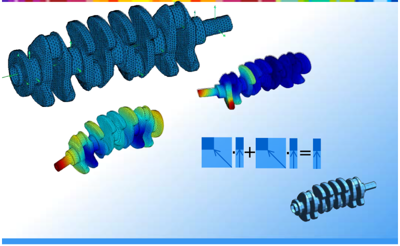

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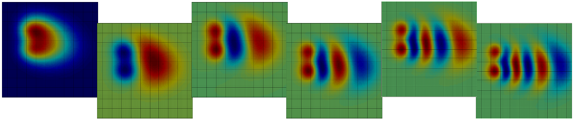

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