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

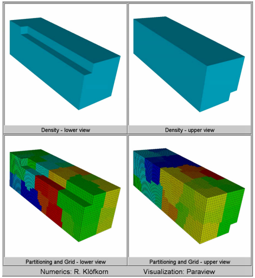
- Offline/Online Decomposition
  - RB-Problem, error estimators
  - Min-theta procedure
- Basis Generation
  - Lagrangian basis
  - Greedy, convergence rates
  - Orthonormalization
  - Adaptivity
- Primal-Dual RB Approach
  - Output correction
  - Improved error estimation
- Nonlinear RB Approach
  -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

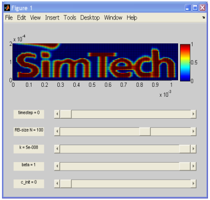
Motivation of Model Reduction



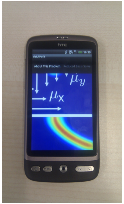
- Today: High resolution simulation schemes
  - Multitude of applications
  - High dimensional models (PDEs, ODEs)
  - Development of accurate schemes
    Adaptive grids, higher order schemes
    Parallelization and HPC
  - High runtime- and hardware requirements
- Goal: Reduced models
  - Smaller model 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



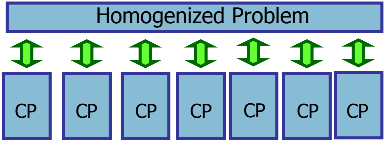
- „Cool" Computing Platforms
  - Simple industrial controllers
  - Web-applications / Applets
  - Ubiquitous Computing:
    Mobile phone, smart devices

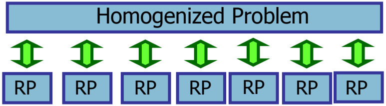


Motivation of Model Reduction

„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 $u(x, \omega)$

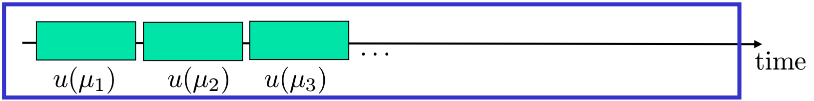
$$\bar{u}(x) := \int_\Omega u(x,\omega) p(\omega)$$

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

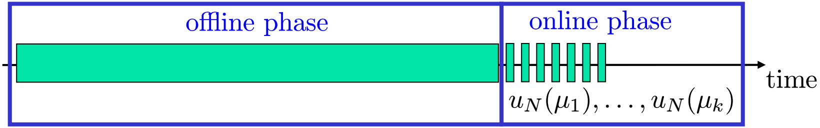
Motivation of Model Reduction

- 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:

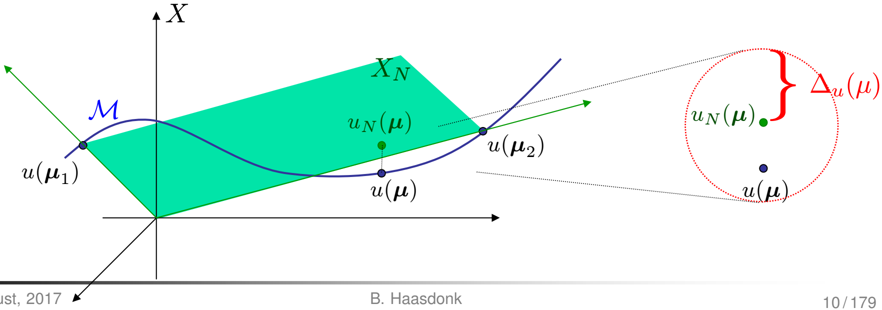


Multi-query with reduced model:



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 $u_N(\mu) = \alpha_0(\mu)u_0 + \alpha_1(\mu)u_1$
  $$\alpha_0(\mu) = \tfrac{2}{\mu+1} - 1, \quad \alpha_1(\mu) = 2 - \tfrac{2}{\mu+1}$$
  - 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)

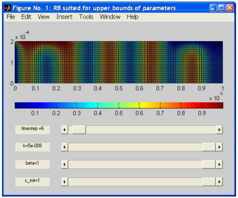
Motivation of RB-Methods

- 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:

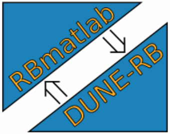
  www.haasdonk.de/data/durham2017

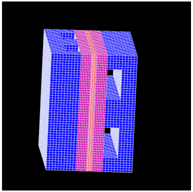
Software

- 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





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

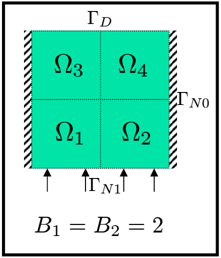
Dune
Distributed and Unified Numerics Environment

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

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

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

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

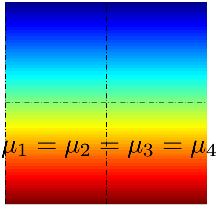
- Possible output of interest: average bottom temperature

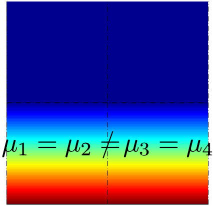
$$s(\mu) := \int_{\Gamma_{N,1}} u(x;\mu) dx = l(u(\mu);\mu)$$

- 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.

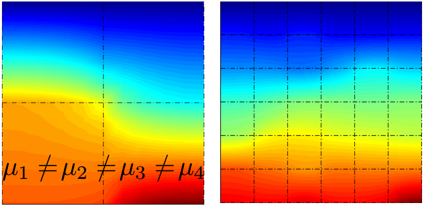




Exercise 1: Find and prove an explicit solution representation in a B_2-dimensional linear space

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" $h_N := \sup_{\mu\in\mathcal{P}} \mathrm{dist}(\mu, S_N), \quad \lim_{N\to\infty} h_N = 0$
  - 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

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

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

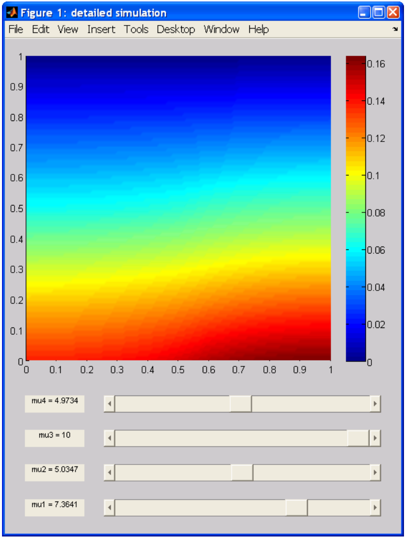
Remark:

- 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

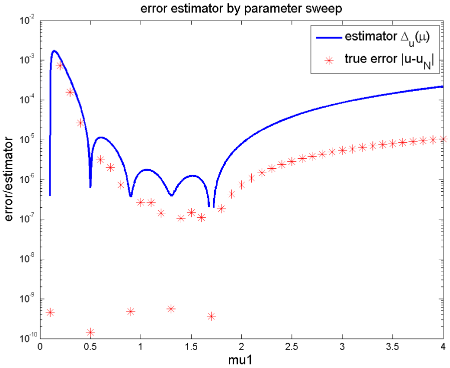
- Thermal Block
  - rb_tutorial(1):
    Full simulation, solution variety as seen earlier
  - rb_tutorial(2):
    Demo gui for full simulation:
  - rb_tutorial(3)
    All steps for generation of reduced model and timing



Experiments

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

$$S_N = \begin{array}{l}(0.1, 0.1, 0.1, 0.1)\\(0.5, 0.1, 0.1, 0.1)\\(0.9, 0.1, 0.1, 0.1)\\(1.3, 0.1, 0.1, 0.1)\\(1.7, 0.1, 0.1, 0.1)\end{array}$$

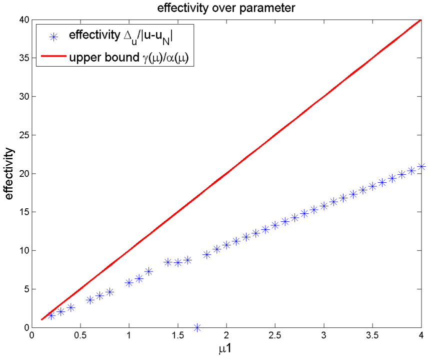


- Parameter sweep for estimator is cheap
- Estimator and error are zero for samples
- Estimator is upper bound of true error
- For small parameters larger error, hence more samples would be required

Experiments

- Effectivity and Bounds:
  - rb_tutorial(5)

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



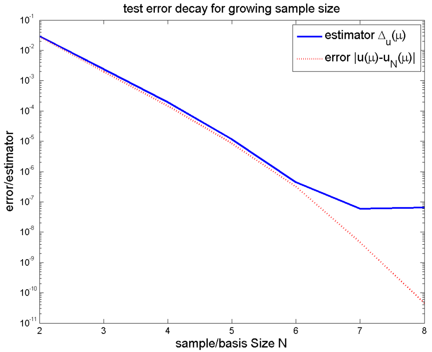
- Effectivities are good, only order of 10
- Effectivity upper bound is verified
- Effectivity undefined for basis samples (division by zero)

Experiments

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

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

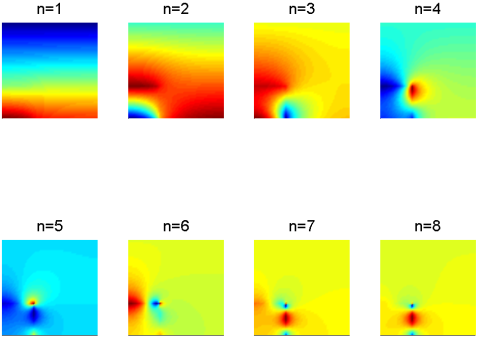
$S_{test} \subset \mathcal{P} \qquad |S_{test}| = 100$



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

Experiments

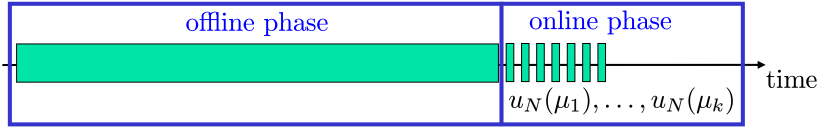
- Error Convergence:
  - Gram-Schmidt orthonormalized basis: rb_tutorial(7)



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

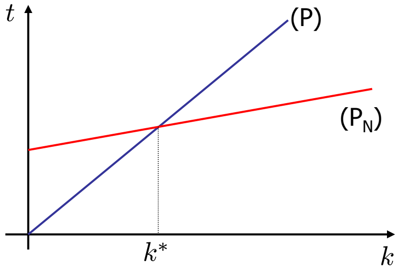
    $$\boldsymbol{\Phi}_N := (\varphi_{ij})_{i,j=1}^{H,N} \in \mathbb{R}^{H \times N}$$
  - Reduced components are then simply obtained by matrix-matrix/matrix-vector multiplications

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

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

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

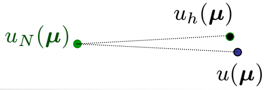


- ACHTUNG: RB Payoff only for „multiple“ requests
  - RB model offline time only pays off if sufficiently many $k \geq k^*$ reduced simulations are expected.

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: $X = \mathrm{span}\{\psi_i\}_{i=1}^H$, $\boldsymbol{K} := (\langle \psi_i, \psi_j \rangle)_{i,j=1}^H$
  - 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 $\boldsymbol{\theta}_l(\mu) := (\theta_1^l(\mu), \ldots, \theta_{Q_l}^l(\mu))$ 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 $S_N = \{\mu^{(1)}, \dots, \mu^{(N)}\} \subset \mathcal{P}$
  - 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:
  - 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]:

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

- 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 $\varepsilon_n := \max_{\mu \in S_{train}} \Delta(X_n, \mu) > \varepsilon_{tol}$

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

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

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

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

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

    - 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:

$\Delta(Y,\mu) := \Delta_u(\mu)$ (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 $\Delta(X_n,\mu)\leq\varepsilon \not\Rightarrow \Delta(X_{n+1},\mu)\leq\varepsilon$
  - 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.

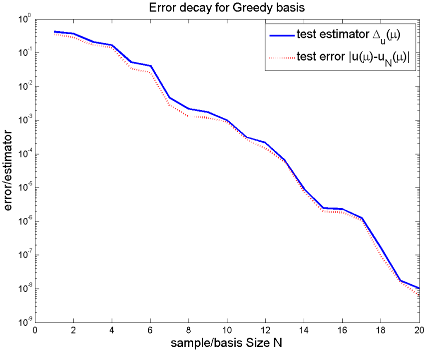
$$\max_{\mu\in\mathcal{P}} \Delta(X_N,\mu) \gg \varepsilon_N$$

  - => 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



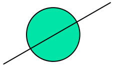
- So Greedy is a well performing heuristic procedure
- Formal convergence statements for analytical foundation?

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:

$$
\begin{aligned}
&\left\| u(\mu^{(n+1)}) - P_{X_n} u(\mu^{(n+1)}) \right\| = \inf_{v \in X_N} \left\| u(\mu^{(n+1)}) - v \right\| \\
&\geq \frac{\alpha(\mu)}{\gamma(\mu)} \left\| u(\mu^{(n+1)}) - u_N(\mu^{(n+1)}) \right\| \geq \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \Delta_u(\mu^{(n+1)}) \\
&= \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \sup_{\mu \in \mathcal{P}} \Delta_u(\mu) \geq \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \sup_{\mu \in \mathcal{P}} \|u(\mu) - u_N(\mu)\| \\
&\geq \frac{\alpha(\mu)}{\gamma(\mu)\eta_u(\mu)} \sup_{\mu \in \mathcal{P}} \|u(\mu) - P_{X_N} u(\mu)\| \geq \frac{\bar{\alpha}^2}{\bar{\gamma}^2} \sup_{\mu \in \mathcal{P}} \|u(\mu) - P_{X_N} u(\mu)\| .
\end{aligned}
$$

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

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

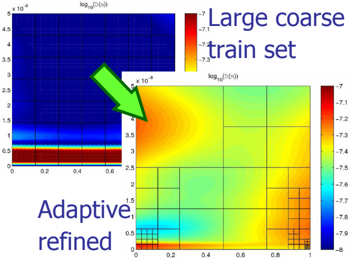
- Training Set Treatment
  - Multistage greedy [Se08]

    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]

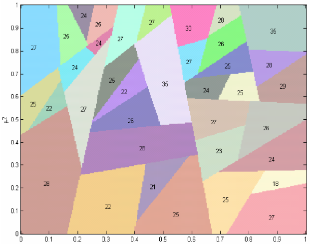
    Stop greedy when overfitting

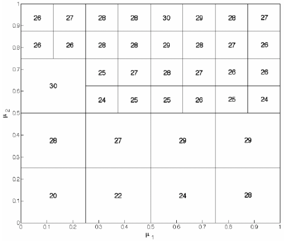
    Locally extend training set
  - Full Optimization: [UVZ12]
    - Optimization in greedy loop
  - Randomization [HSZ13]
    - In each greedy step new random training set



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:

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

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

  - Then we conclude using definitions

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

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
  - $a(\dots)$ 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

- 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

- Examples

  Find $u(\mu) \in H_0^1(\Omega)$ as solution of

  - Diffusion Eqn. with Nonlinear Reaction

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

  - 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 $H_0^1(\Omega) \to L^4(\Omega)$

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.

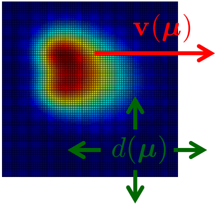
RB-Methods for Evolution Problems

RB for Param. Evolution

- Initial value problems (Porsching&Lee '87)
- Control of NS (Ito&Ravindran '98)
- POD (Volkwein, Hinze, Kunisch, ...)
- Linear, Nonlinear Parabolic problems (Grepl&Patera 2005), (Rovas&al,...)
- Instationary Burgers (Nguyen&al 2009), (Jung&al 2008)
- Linear FV (HO08)
- EOI: Empirical Operator Interpolation, Nonlinear Finite Volumes (HO08b), (DHO13)
- Space-time Galerkin Procedures (Urban&Patera, ...)
- GNAT (Carlberg, Farhat, Amsallem 2012)
- DEIM (Chaturantabut&Sorensen 2009)
- PMOR Review (Benner, Gugercin, Willcox)

RB-Method for Evolution Schemes

- Parametric PDE:
  - Parameter $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$: material-, geometry-, control-parameter
  - For $\boldsymbol{\mu} \in \mathcal{P}$ find solution $u(\cdot, t; \boldsymbol{\mu}) \in \mathcal{X}$ of

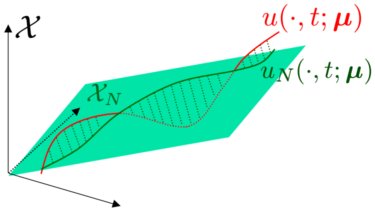


$$\partial_t u(\boldsymbol{\mu}) + \nabla \cdot (\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu}) - d(\boldsymbol{\mu}) \nabla u(\boldsymbol{\mu})) = 0 \text{ in } \Omega \times [0, T]$$

with suitable initial and boundary conditions

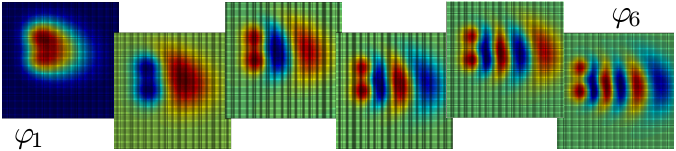
- Idea:
  - Approximate manifold by linear spaces spanned by „snapshots“

$$\mathcal{X}_N \subset \text{span}(u(\cdot; t_n, \boldsymbol{\mu}_n))$$



RB-Method for Evolution Schemes

- Reduced Basis
  - RB-Space $\mathcal{X}_N \subset \mathcal{X}$ of dimension N
  - Reduced Basis $\Phi_N = (\varphi_1, \dots, \varphi_N)^T$
- Basis generation:
  - Taylor-RB spaces [FR83] $\Phi_N := \{u(\boldsymbol{\mu}_0), \partial_{\mu_i} u(\boldsymbol{\mu}_0), \dots\}$
  - Lagrange-RB spaces [MPT02] $\Phi_N := \{u(\boldsymbol{\mu}_1), u(\boldsymbol{\mu}_2), \dots\}$
  - POD, Krylov, Greedy-schemes, Optimization
- Example: $N = 6$



u_0 + 5 POD-Modes of a Trajectory

- References: [NP80],[PL87],[PR07]

RB-Method for Linear Schemes

- Parametrized linear evolution equation [HO08]

For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ find $u : [0,T] \to \mathcal{X} \subset L^2(\Omega)$ s. th.

$$\partial_t u(t) + \mathcal{L}(\boldsymbol{\mu})[u(t)] = 0$$

$$u(0) = u_0(\boldsymbol{\mu})$$

- Space/time discrete implicit/explicit scheme

For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ find $\{u_h^k\}_{k=0}^K \subset \mathcal{X}_h \subset L^2(\Omega)$ s. th.

$$u_h^0 := P_h[u_0(\boldsymbol{\mu})]$$

$$(\mathrm{Id} + \Delta t \mathcal{L}_h^I)[u_h^{k+1}] = (\mathrm{Id} - \Delta t \mathcal{L}_h^E)[u_h^k] + \Delta t b_h^k$$

Ref: Haasdonk, Ohlberger: Reduced basis method for finite volume approximations of parametrized linear evolution equations, M2AN, 42(2):277-302, 2008.

RB-Method for Linear Schemes

- RB-Spaces

$$\mathcal{X}_N \subset \mathrm{span}(u_h(\cdot; t, \boldsymbol{\mu})) \subset \mathcal{X}_h \qquad N := \dim \mathcal{X}_N \ll \dim \mathcal{X}_h$$

- Reduced Operators
  - Orthogonal projection $P_N : \mathcal{X}_h \to \mathcal{X}_N$
  - Implicit/explicit space discretization operators

$$\mathcal{L}_N^E := P_N \circ \mathcal{L}_h^E \qquad \mathcal{L}_N^I := P_N \circ \mathcal{L}_h^I \qquad b_N^k := P_N[b_h^k]$$

- RB-Evolution-Scheme in Operator Form

For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ find $\{u_N^k\}_{k=0}^K \subset \mathcal{X}_N \subset X_h$ s. th.

$$u_N^0 := P_N[u_h^0(\boldsymbol{\mu})]$$

$$\left(\mathrm{Id} + \Delta t \mathcal{L}_N^I\right)[u_N^{k+1}] = \left(\mathrm{Id} - \Delta t \mathcal{L}_N^E\right)[u_N^k] + \Delta t b_N^k$$

see also: [GP05]

RB-Method for Linear Schemes

- Error-Analysis by Residuals
  - Definition of residuals

$$R_h^{k+1}(\boldsymbol{\mu}) := \frac{1}{\Delta t}\left(\mathcal{L}^I_{h,\Delta t}(t^k,\boldsymbol{\mu})[u_N^{k+1}] - \mathcal{L}^E_{h,\Delta t}(t^k,\boldsymbol{\mu})[u_N^k] - b_h(t^k,\boldsymbol{\mu})\right)$$

  - Norms are computable during RB-simulation

$$\left\|R_h^{k+1}\right\|^2_{L^2(\Omega)} := \frac{1}{(\Delta t)^2}\Big((\mathbf{a}^{k+1})^T\mathbf{K}_{II}\mathbf{a}^{k+1} - 2(\mathbf{a}^{k+1})^T\mathbf{K}_{IE}\mathbf{a}^k$$

$$+(\mathbf{a}^k)^T\mathbf{K}_{EE}\mathbf{a}^k + m - 2(\mathbf{a}^{k+1})^T\mathbf{m}_I + 2(\mathbf{a}^k)^T\mathbf{m}_E\Big)$$

  - With auxiliary matrices, vectors and scalars

$$(\mathbf{K}_{II}(t^k,\boldsymbol{\mu}))_{nm} := \int_\Omega \mathcal{L}^I_{h,\Delta t}(t^k,\boldsymbol{\mu})[\varphi_n]\mathcal{L}^I_{h,\Delta t}(t^k,\boldsymbol{\mu})[\varphi_m] \qquad m := \int_\Omega b_h^2$$

$$(\mathbf{K}_{IE})_{nm} := \int_\Omega \mathcal{L}^I_{h,\Delta t}[\varphi_n]\mathcal{L}^E_{h,\Delta t}[\varphi_m] \qquad (\mathbf{m}_I)_n := \int_\Omega \mathcal{L}^I_{h,\Delta t}[\varphi_n]b_h$$

$$(\mathbf{K}_{EE})_{nm} := \int_\Omega \mathcal{L}^E_{h,\Delta t}[\varphi_n]\mathcal{L}^E_{h,\Delta t}[\varphi_m] \qquad (\mathbf{m}_E^k)_n := \int_\Omega \mathcal{L}^E_{h,\Delta t}[\varphi_n]b_h$$

RB-Method for Linear Schemes

- Thm: A-Posteriori L²-Error Estimator [HO08]
  - Let constants $C_I, C_E \in \mathbb{R}^+$ be given such that

$$\left\| \mathcal{L}^E_{h,\Delta t}(t^k, \boldsymbol{\mu}) \right\| \leq C_E \qquad \left\| \mathcal{L}^I_{h,\Delta t}(t^k, \boldsymbol{\mu})^{-1} \right\| \leq C_I$$

    and initial data satisfy

$$P_h[u_0(\cdot; \boldsymbol{\mu})] \in \mathcal{X}_N$$

  - Then for all times the following estimate holds

$$\boxed{\left\| u_N^k(\boldsymbol{\mu}) - u_h^k(\boldsymbol{\mu}) \right\|_{L^2(\Omega)} \leq \Delta_N^k(\boldsymbol{\mu})}$$

  - The bound is effectively computable by

$$\Delta_N^k(\boldsymbol{\mu}) := \sum_{n=0}^{k-1} \Delta t \left\| R_h^{n+1} \right\| (C_E)^{k-1-n} (C_I)^{k-n}$$

RB-Method for Linear Schemes

- Basis generation: POD-Greedy [HO08]
  - Based on „Greedy“ for stationary RB problems [VPRP03]
  - Choose finite training parameter set $M_{\text{train}} \subset \mathcal{P}$
  - Iterative extension of initial basis $\Phi_{N_0} \subset \mathcal{X}_h$

While $\varepsilon := \max_{\boldsymbol{\mu} \in M_{\text{train}}} \Delta_N(\boldsymbol{\mu}) > \varepsilon_{tol}$

1. Find $\boldsymbol{\mu}^* := \operatorname{argmax}_{\boldsymbol{\mu} \in M_{\text{train}}} \Delta_N(\boldsymbol{\mu})$
2. Compute detailed trajectory $u_h(\boldsymbol{\mu}^*)$
3. Orthogonalize trajectory $e_h := u_h(\boldsymbol{\mu}^*) - P_{\mathcal{X}_N}(u_h(\boldsymbol{\mu}^*))$
4. Add principal components of proj. error as basis vectors

$$\Phi_{N+k} = \Phi_N \cup POD(e_h, k)$$

- Thm [Ha11]: Almost optimal Error Decay

$$d_n(\mathcal{F}) \leq M n^{-\alpha} \quad \Rightarrow \quad \sigma_{T,n}(\mathcal{F}_T) \leq C M n^{-\alpha}.$$

RB-Method for Linear Schemes

- Full Offline/Online-Decomposition:
  - Online-Phase: fast RB-simulation + error estimation, complexity completely independent of $H := \dim \mathcal{X}_h$
  - Offline-Phase: Precomputation of reduced basis and auxiliary quantities involving „expensive" operations of complexity polynomial in $\dim \mathcal{X}_h$
- Offline/Online for Operators:
  - Assumption of separable parameter dependence:

$$\mathcal{L}(t^k,\boldsymbol{\mu})[\cdot] = \sum_{q=1}^{Q} \theta^q(t^k,\boldsymbol{\mu})\mathcal{L}^q[\cdot] \quad \Rightarrow \quad (\mathbf{L}(t^k,\boldsymbol{\mu}))_{nm} := \int_\Omega \mathcal{L}(t^k,\boldsymbol{\mu})[\varphi_n]\varphi_m$$

$$= \sum_{q=1}^{Q} \theta^q(t^k,\boldsymbol{\mu}) \int_\Omega \mathcal{L}^q[\varphi_n]\varphi_m$$

$$= \boxed{\sum_{q=1}^{Q} \theta^q(t^k,\boldsymbol{\mu}) \boxed{(\mathbf{L}^q)_{nm}}}$$

Coefficients: space-independent

Components: parameter-independent

Online

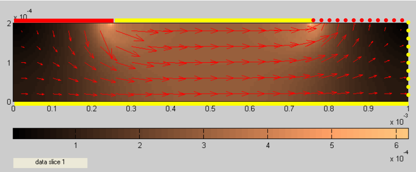
Offline

RB-Method for Linear Schemes

- Evolution Equation: Scalar Advection-Diffusion

$$\begin{aligned}
\partial_t u(\boldsymbol{\mu}) + \nabla \cdot (\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu}) - d(\boldsymbol{\mu}) \nabla u(\boldsymbol{\mu})) &= 0 \text{ in } \Omega \times [0,T] \\
u(\boldsymbol{\mu}, 0) &= u_0(\boldsymbol{\mu}) \text{ in } \Omega \\
u(\boldsymbol{\mu}) &= b_{\text{dir}}(\boldsymbol{\mu}) \text{ in } \Gamma_{\text{dir}} \times [0,T] \\
(\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu}) - d(\boldsymbol{\mu}) \nabla u(\boldsymbol{\mu})) \cdot \mathbf{n} &= b_{\text{neu}}(u; \boldsymbol{\mu}) \text{ in } \Gamma_{\text{neu}} \times [0,T]
\end{aligned}$$

- Geometry and Data
  - „Gas diffusion layer"
  - Velocity field precomputed
  - Diffusivity: k
  - Initial data: $u_0 = c_{\text{init}} \sin(\omega_x x)$
  - Neuman-boundary: noflow, outflow
  - Dirichlet-boundary: $b_{\text{dir}} = \beta \chi_{\boxed{\Gamma_1}} + (1-\beta)\chi_{\boxed{\Gamma_2}}$
  - Parameter $\boldsymbol{\mu} = (c_{\text{init}}, \beta, k) \in [0,1] \times [0,1] \times [0, 5 \cdot 10^{-8}]$



RB-Method for Linear Schemes

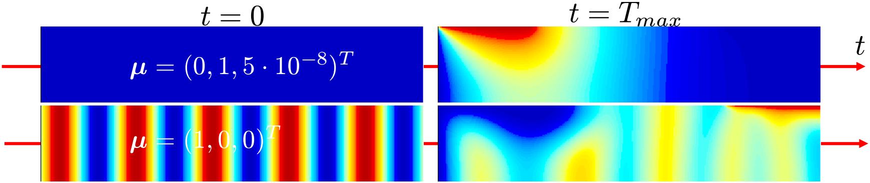
- Evolution Scheme: Linear Finite Volume Method

$$u_i^0 := \frac{1}{|T_i|}\int_{T_i} u_0(\boldsymbol{\mu})dx \qquad u_i^{k+1} = u_i^k - \frac{\Delta t_k}{|T_i|}\sum_{j\in\mathcal{N}(i)} h_{ij}^k(u_h^k, u_h^{k+1}; \boldsymbol{\mu})$$

$$h_{I,ij}^k(\boldsymbol{\mu})(u_H^{k+1}) := -d(\mathbf{s}_{ij})\frac{|e_{ij}|}{|\mathbf{s}_i - \mathbf{s}_j|}(u_j^{k+1} - u_i^{k+1})$$

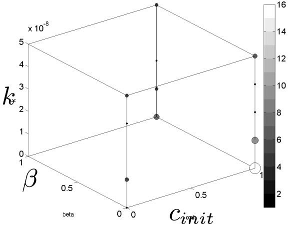
$$h_{E,ij}^k(\boldsymbol{\mu})(u^k) := \tfrac{1}{2}|e_{ij}|\left(\mathbf{v}(\mathbf{c}_{ij})\cdot\mathbf{n}_{ij}(u_j^k + u_i^k) - \tfrac{1}{\lambda}(u_j^k - u_i^k)\right)$$

- Examples of Solution Variety ($H = 400 \times 80$)

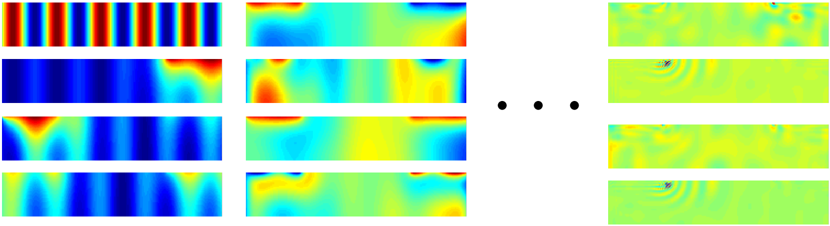


RB-Method for Linear Schemes

- Sample Selection
  - 5x5x5 train set
  - Nmax=100



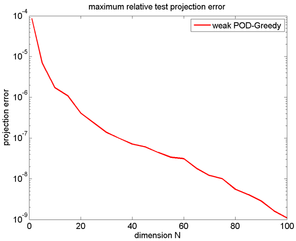
- Basis

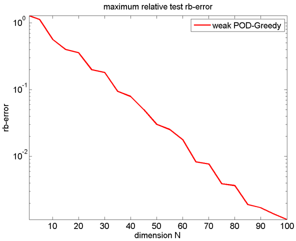


RB-Method for Linear Schemes

- Test Error Convergence
  - Max. rel. Projection error

Max. rel. RB error





- Offline Runtimes

	Train set	Runtime (sec)
Strong POD-Greedy	3x3x3	884.7067
Weak POD-Greedy	3x3x3	458.7860
Weak POD-Greedy	5x5x5	721.6122

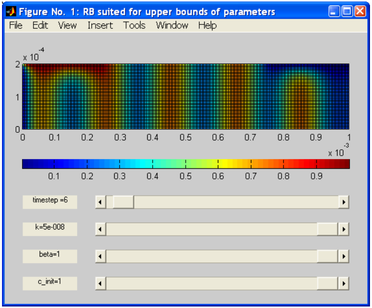
RB-Method for Linear Schemes

- Runtimes:
  - Detail- vs. RB-simulation with 20 basis vectors

Discretization: 40×200 **cells,** $K = 200$ **timesteps**

	Data non const in time			Data const in time		
	Detailed	RB online	RB offline	Detailed	RB online	RB offline
advection-diffusion	155.94s	16.67s	447.16s	45.67s	1.02s	2.41s
advection	105.97s	16.53s	437.20s	1.51s	0.79s	2.31s

- Online-Demo for Parameter-Variation
  - N=123 basis vectors
  - $\boldsymbol{\mu} = (c_{\text{init}}, \beta, k)$ variable in $[0,1] \times [0,1] \times [0, 5 \cdot 10^{-8}]$
  - $\Delta_N^K(\boldsymbol{\mu})$ < 1e-7 on 5x5x5 parameter-grid



RB-Method for Nonlinear Schemes

RB-Method for Nonlinear Schemes [HO08b,DHO10]

- Parametrized evolution equation

For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ find $u : [0,T] \to \mathcal{X} \subset L^2(\Omega)$ s. th.

$$\partial_t u(t) + \mathcal{L}(\boldsymbol{\mu})[u(t)] = 0$$

$$u(0) = u_0(\boldsymbol{\mu})$$

- Discrete implicit/explicit Newton scheme

For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ find $\{u_h^k\}_{k=0}^K \subset \mathcal{X}_h \subset L^2(\Omega)$ s. th.

$$u_h^0 := P_h[u_0(\boldsymbol{\mu})] \qquad u_h^{k+1} := u_h^{k+1,\nu_{\max(k)}}$$

with Newton iteration

$$u_h^{k+1,0} := u_h^k \qquad u_h^{k+1,\nu+1} := u_h^{k+1,\nu} + \delta_h^{k+1,\nu+1}$$

$$\left(\mathrm{Id} + \Delta t D\mathcal{L}_h^I|_{u_h^{k+1,\nu}}\right)[\delta_h^{k+1,\nu+1}] = u_h^k - u_h^{k+1,\nu} - \Delta t \left(\mathcal{L}_h^I[u_h^{k+1,\nu}] + \mathcal{L}_h^E[u_h^k]\right)$$

RB-Method for Nonlinear Schemes

- Reduced Operators:

  $P_N : \mathcal{X}_h \to \mathcal{X}_N$ L²-orthogonal projection

  $\mathcal{L}_N^I := P_N \circ \mathcal{I}_M \circ \mathcal{L}_h^I$

  $\mathcal{L}_N^E := P_N \circ \mathcal{I}_M \circ \mathcal{L}_h^E$ RB evolution operators

- Reduced Implicit/Explicit Evolution Scheme:

  For $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$ find $\{u_N^k\}_{k=0}^K \subset \mathcal{X}_N \subset \mathcal{X}_h$ s. th.

$$u_N^0 := P_N[u_h^0(\boldsymbol{\mu})] \qquad u_N^{k+1} := u_N^{k+1,\nu_{\max(k)}}$$

  with Newton iteration

$$u_N^{k+1,0} := u_N^k \qquad u_N^{k+1,\nu+1} := u_N^{k+1,\nu} + \delta_N^{k+1,\nu+1}$$

$$\left(\mathrm{Id} + \Delta t D\mathcal{L}_N^I(\boldsymbol{\mu})|_{u_N^{k+1,\nu}}\right)[\delta_N^{k+1,\nu+1}] = u_N^k - u_N^{k+1,\nu} - \Delta t\left(\mathcal{L}_N^I(\boldsymbol{\mu})[u_N^{k+1,\nu}] + \mathcal{L}_N^E(\boldsymbol{\mu})[u_N^k]\right)$$

RB-Method for Nonlinear Schemes

- Empirical Operator Interpolation (EOI) [HOR07]
  - Approximation of $\mathcal{L}_h(\boldsymbol{\mu}, t^k)$ by linear combinations

$$\mathcal{L}_h[u](x) \approx \mathcal{I}_M(\mathcal{L}_h)[u](x) := \sum_{m=1}^{M} \mathcal{L}_h[u](x_m)\xi_m(x) \qquad M << \dim(\mathcal{X}_h)$$

via collateral basis and „magic points"

$$\boldsymbol{\xi}_M = \{\xi_m\}_{m=1}^{M} \subset \mathcal{X}_h \qquad \{x_m\}_{m=1}^{M} \subset \Omega$$

  - Separable parameter dependency obtained
  - Generation of basis and points by snapshots & greedy
- Theory/analysis:
  - Convergence statements für EI [BMNP04], [CS09]
  - RB-schemes: Conservation [DHO12], error bounds [HOR07]

RB-Method for Nonlinear Schemes

- Offline/Online Decomposition for EI-Operators:

$$\int_\Omega \mathcal{I}_M(\mathcal{L}_h(\boldsymbol{\mu},t))[u_N]\varphi_n = \boxed{\sum_{m=1}^M \mathcal{L}_h(\boldsymbol{\mu},t^k)[u_N](x_m) \boxed{\int_\Omega \xi_m \varphi_n}}$$

Online Offline

- Offline/Online Decomp. for EI-Operator Derivatives:

$$\int_\Omega D(\mathcal{I}_M(\mathcal{L}_h(\boldsymbol{\mu},t)))|_{u_N}[\delta_N]\varphi_n$$

$$= \boxed{\sum_{m=1}^M D(\mathcal{L}_h(\boldsymbol{\mu},t^k)[\cdot](x_m))|_{u_N}[\delta_N] \boxed{\int_\Omega \xi_m \varphi_n}}$$

Online Offline

Required online: partial evaluation of Jacobian matrix

RB-Method for Nonlinear Schemes

- EI-Offline: Collateral Reduced Basis Generation
  - Finite training set of operator evaluation snapshots

$$L_{train} = \{\mathcal{L}_h(\boldsymbol{\mu}, t^k)[u_h^k(\boldsymbol{\mu})] | k = 0, \ldots, K, \boldsymbol{\mu} \in M_{train}\} \subset \mathcal{X}_h$$

  - Accumulatively collect interpolation functions and points

for $m = 1, \ldots, M$

1. have CRB-functions $\{q_i\}_{i=1}^{m-1}$ and points $\{x_i\}_{i=1}^{m-1}$
2. search worst approximated training example:

$$v_m := \arg \max_{v \in L_{train}} \|v - \mathcal{I}_{m-1}[v]\|_{L^\infty(\Omega)} \quad \text{(or } \|\cdot\|_{L^2}\text{)}$$

3. get interpolation residual $r_m := v_m - \mathcal{I}_{m-1}[v_m]$
4. define next interpolation point and CRB basis function

$$x_m := \arg \sup_{x \in X_H} |r_m(x)| \qquad q_m := r_m / r_m(x_m)$$

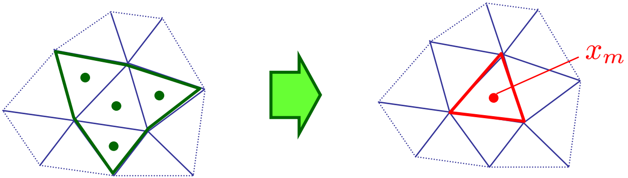
  - For notation: nodal basis $\boldsymbol{\xi}_M = \{\xi_m\}_{m=1}^M$

RB-Method for Nonlinear Schemes

- EI-Online: Local Evaluations
  - Problem: point evaluations in online phase require full computation of the operator:
  - Solution: Restriction to „localized operators“, i.e. small domain of dependence, e.g. FV-discretizations
  - Online-Phase:

local reconstruction of u_N^k from coefficients $\mathbf{a}^k$

local evaluation $\mathcal{L}_h(\boldsymbol{\mu}, t^k)[u_N^k](x_m)$



  - Requires Offline: numerical subgrid, local representation of Φ_N

RB-Method for Nonlinear Schemes

- Thm: A-Posteriori L²-Error Estimator (explicit linear case)
  - Assumption: $Id - \Delta t \mathcal{L}_h^E(\boldsymbol{\mu}, t^k)$ has Lipschitzconstant C_E

    initial data $P_h[u_0(\boldsymbol{\mu})] \in \mathcal{X}_N$

    and $\mathcal{L}_h^E(\boldsymbol{\mu}, t^k)[u_N^k] \in \mathcal{X}_{M+1}$
  - Then for all times the following estimate holds

$$\boxed{\left\| u_N^k(\boldsymbol{\mu}) - u_h^k(\boldsymbol{\mu}) \right\|_{L^2(\Omega)} \leq \Delta_{N,M}^k(\boldsymbol{\mu})}$$

  - The bound is effectively computable by

$$\Delta_{N,M}^k(\boldsymbol{\mu}) := \sum_{k'=0}^{k-1} \Delta t C_E^{k-1-k'} \left(|\theta_{M+1}^{k'}(\boldsymbol{\mu})| \, \|q_{M+1}\|_{L^2} + \left\| R^{k'}(\boldsymbol{\mu}) \right\|_{L^2} \right)$$

    with EI error estimator

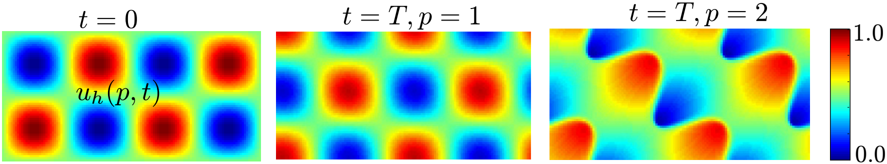
$$\theta_{M+1}^{k'}(\boldsymbol{\mu}) := \mathcal{L}_h^E(\boldsymbol{\mu}, t^{k'})[u_N^{k'}](x_{M+1}) - \mathcal{I}_M[\mathcal{L}_h^E(\boldsymbol{\mu}, t^{k'})[u_N^{k'}]](x_{M+1}).$$

- Implicit, nonlinear case: [DHO10], cont. time DEIM [WSH13]

Nonlinear Conservation Laws

- Convection, explicit FV Discretization (HO08b)

$$\partial_t u(\boldsymbol{\mu}) + \nabla \cdot (\mathbf{v} u(\boldsymbol{\mu})^p) = 0 \text{ in } \Omega \times [0, T]$$



- RB scheme: Empirical Interpolation + Collateral RB

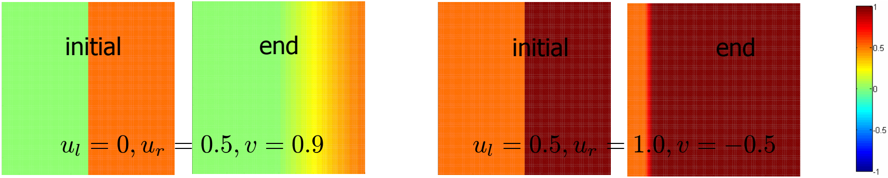
Approximation	Dimension	Mean Runtime [s]
detailed	$H = 7200$	10.69
reduced	$N = 20, M = 30$	0.45
reduced	$N = 40, M = 60$	0.60
reduced	$N = 70, M = 105$	0.84
reduced	$N = 100, M = 150$	1.06

Nonlinear Conservation Laws

- Nonlinear 2D Burgers equation

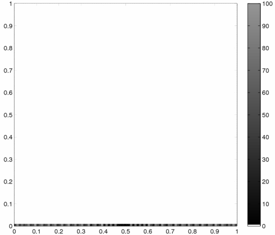
$$\partial_t u(\boldsymbol{\mu}) + \nabla \cdot ((v,0)^T u(\boldsymbol{\mu})^2) = 0 \text{ in } \Omega \times [0,T]$$
$$u(\cdot,0;\boldsymbol{\mu}) = u_0(\boldsymbol{\mu}) \text{ in } \Omega$$

  - Left & right: Dirichlet values u_l, u_r
  - Top & bottom: noflow Neumann conditions
- Discretization:
  - Cartesian Grid, Explicit FV, Engquist-Osher flux
- RB Parameter variation: $\boldsymbol{\mu} = (u_l, u_r, v) \in [-1,1]^3$



Nonlinear Conservation Laws

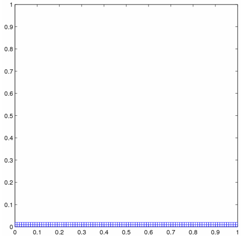
- Empirical Interpolation:
  - L_{train} : 3x3x3 complete time trajectories
  - $M = 100$ interpolation points:



Dimension redundancy
of problem is detected
2D => 1D

  - Subgrid for online phase:

small subset of
detailed grid (200/10000)



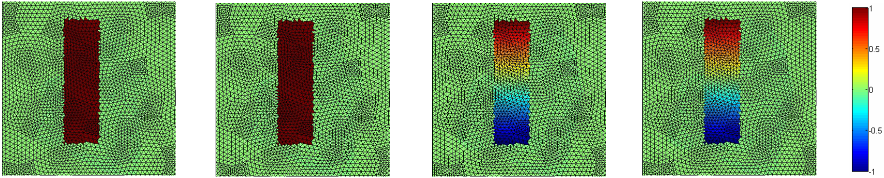
Nonlinear Conservation Laws

- Nonlinear 2D Burgers equation

$$\partial_t u(\boldsymbol{\mu}) + \nabla \cdot (\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu})^2) = 0 \text{ in } \Omega \times [0,T]$$
$$u(\cdot, 0; \boldsymbol{\mu}) = u_0(\boldsymbol{\mu}) \text{ in } \Omega$$
$$(\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu})^2) \cdot \mathbf{n} = 0 \text{ in } \Gamma_{\text{neu}} \times [0,T]$$

- Explicit FV discretization: Engquist-Osher flux
- RB-Parameter variation: $\boldsymbol{\mu} = (\phi, c_{\text{low}}) \in [-\frac{\pi}{4}, 0] \times [-1, 1]$

$\phi = 0, c_{low} = 1$ $\quad$ $\phi = -\frac{\pi}{4}, c_{low} = 1$ $\quad$ $\phi = 0, c_{low} = -1$ $\quad$ $\phi = -\frac{\pi}{4}, c_{low} = -1$

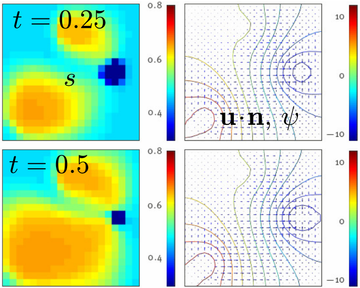


TPF in Porous Media (Drohmann&al. 2012)

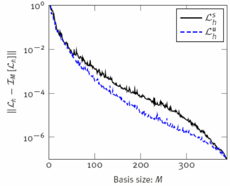
- Global Pressure Formulation

$$\partial_t s + \nabla \cdot (f(s)\mathbf{u} - v(s)\nabla s) = q_1$$
$$\nabla(M(s)\nabla\psi) = q_1 + q_2$$
$$\mathbf{u} = -M(s)\nabla\psi$$

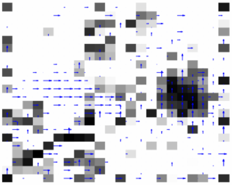
- Implicit FV-Discr. (Michel 2004)
- RB & EI of Nonlinear Operators



Interpolation error



Interpolation DOFs



Runtimes and Accuracies

Detailed simulation time: $\approx$ **52 s**

Table: Error and timings of reduced simulations with different basis sizes.

$(N_s, N_{\mathbf{u}}, N_\psi)$	$(M_s, M_{\mathbf{u}})$	$\|s_h - s_{\text{red}}\|$	$\|\psi_h - \psi_{\text{red}}\|$	time
(28,72,34)	(387,386)	$6.2 \cdot 10^{-5}$	$4.11 \cdot 10^{-4}$	30.15
(28,72,34)	(75,75)	$1.03 \cdot 10^{-4}$	$2.11 \cdot 10^{-3}$	21.56
(28,72,34)	(75,125)	$7.59 \cdot 10^{-5}$	$8.69 \cdot 10^{-4}$	20.61
(23,58,28)	(75,125)	$2.47 \cdot 10^{-4}$	$2.55 \cdot 10^{-3}$	18.24

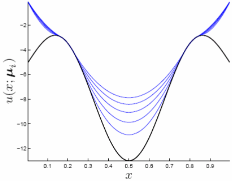
RB for Variational Inequalities (HSW12)

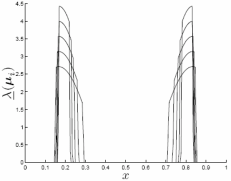
- RB for Variational Inequalities
  - Parametrized saddle point problems

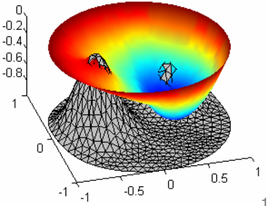
$$a(u, v; \boldsymbol{\mu}) + b(v, \lambda) = f(v; \boldsymbol{\mu}), \quad v \in X$$
$$b(u, \eta - \lambda) \leq g(\eta - \lambda; \boldsymbol{\mu}), \quad \eta \in M$$

  - RB Scheme: Parametrized QP
  - Analysis: Stability, L-Continuity, Error Bounds
  - Applications: Contact Mechanics Option Pricing

$$\partial_t P - \frac{1}{2}\sigma^2 s^2 \partial_{ss}^2 P - (r-q)s\partial_s P + rP \geq 0$$
$$P - \psi \geq 0$$
$$\left(\partial_t P - \frac{1}{2}\sigma^2 s^2 \partial_{ss}^2 P - (r-q)s\partial_s P + rP\right) \cdot (P - \psi) = 0$$







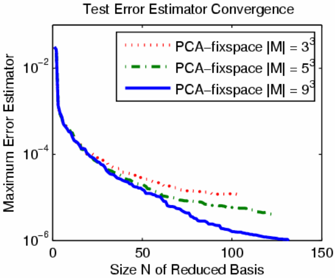
Offline Adaptivity: Train Set Refinement

Haasdonk, B. & Ohlberger, M.: P. Díez and K. Runesson (Eds.), Basis Construction for Reduced Basis Methods By Adaptive Parameter Grids, Proc. International Conference on Adaptive Modeling and Simulation, ADMOS 2007, CIMNE, Barcelona, 2007, 116-119.

Haasdonk, B.; Dihlmann, M. & Ohlberger, M.: A Training Set and Multiple Basis Generation Approach for Parametrized Model Reduction Based on Adaptive Grids in Parameter Space, Mathematical and Computer Modelling of Dynamical Systems, 2011, 17, 423-442.

Offline Adaptivity: Train Set

- Problems of (POD-)Greedy
  - Tends to overfit for small training sets
  - Infeasible for overly large training sets
  - Infeasible in absence of error estimators
- Remedy
  - Automatic training set adaptation
  - Related:
    - multistage greedy [Se08]
    - train set randomization [HSZ13]
    - Optimization in greedy loop [UVZ14]

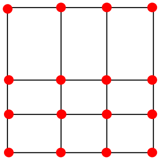


Offline Adaptivity: Train Set

- Solution Part I: Greedy Search + Early Stopping
  - Choose M_{train} as gridpoints of parameter mesh
  - Early stopping of Greedy procedure if overfitting detected
  - Overfitting control by ratio of training/validation error

ESGREEDY$(\Phi_0, M_{train}, \varepsilon_{tol}, \boxed{M_{val}, \rho_{tol}})$

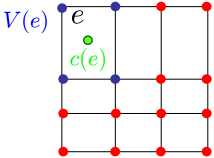
$\Phi := \Phi_0$
repeat
  $\boldsymbol{\mu}^* := \arg\max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
  if $\Delta(\boldsymbol{\mu}^*) > \varepsilon_{tol}$
   then
    $\varphi :=$ ONBASISEXT$(u_H(\boldsymbol{\mu}^*), \Phi)$
    $\Phi := \Phi \cup \{\varphi\}$
  $\varepsilon := \max_{\boldsymbol{\mu} \in M_{train}} \Delta(\boldsymbol{\mu}, \Phi)$
  $\boxed{\rho := \max_{\boldsymbol{\mu} \in M_{val}} \Delta(\boldsymbol{\mu}, \Phi)/\varepsilon}$
 until $\varepsilon \leq \varepsilon_{tol}$ **or** $\boxed{\rho \geq \rho_{tol}}$
return Φ, ε



$M_{train} \subset \mathcal{P}$

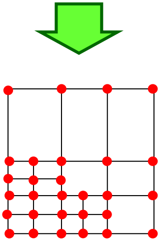
Offline Adaptivity: Train Set

- Solution Part II: Adaptive Training Set Extension
  - Compute element error indicators



$$\eta(e) := \left(\max_{\boldsymbol{\mu} \in V(e) \cup \{c(e)\}} \Delta(\boldsymbol{\mu}, \Phi_N) \right) + \gamma s(e)$$

  - Mark & refine fraction $\Theta \in (0, 1]$ of elements



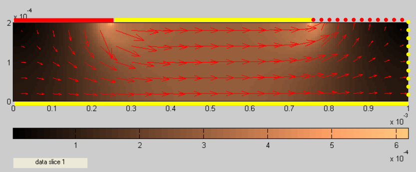
```
RBADAPTIVE(Φ_0, M_0, ε_tol, M_val, ρ_tol)
Φ := Φ_0, M := M_0
repeat
        M_train := V(M)
        [Φ, ε] := ESGREEDY(Φ, M_train, ε_tol, M_val, ρ_tol)
        if ε > ε_tol
          then
                η = ELEMENTINDICATORS(M, Φ, ε)
                M := MARK(M, η)
                M := REFINE(M)
    until ε ≤ ε_tol
return Φ
```

Offline Adaptivity: Train Set

- Evolution Equation: Scalar Advection-Diffusion

$$\partial_t u(\boldsymbol{\mu}) + \nabla \cdot (\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu}) - d(\boldsymbol{\mu}) \nabla u(\boldsymbol{\mu})) = 0 \text{ in } \Omega \times [0, T]$$
$$u(\boldsymbol{\mu}, 0) = u_0(\boldsymbol{\mu}) \text{ in } \Omega$$
$$u(\boldsymbol{\mu}) = b_{\text{dir}}(\boldsymbol{\mu}) \text{ in } \Gamma_{\text{dir}} \times [0, T]$$
$$(\mathbf{v}(\boldsymbol{\mu}) u(\boldsymbol{\mu}) - d(\boldsymbol{\mu}) \nabla u(\boldsymbol{\mu})) \cdot \mathbf{n} = b_{\text{neu}}(u; \boldsymbol{\mu}) \text{ in } \Gamma_{\text{neu}} \times [0, T]$$

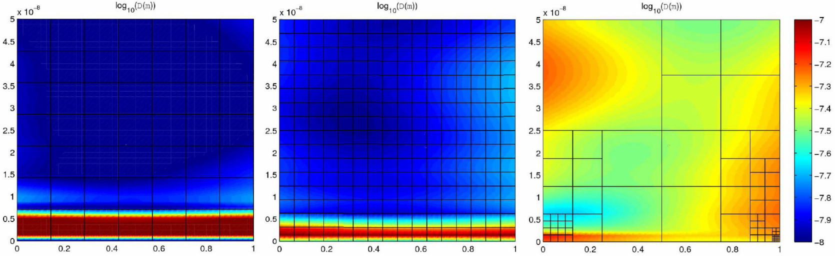
- Geometry and Data
  - „Gas diffusion layer"
  - Velocity field precomputed
  - Diffusivity: k
  - Initial data: $u_0 = c_{\text{init}} \sin(\omega_x x)$
  - Neuman-boundary: $\boxed{\text{noflow,}}$ $\boxed{\text{outflow}}$
  - Dirichlet-boundary: $b_{\text{dir}} = \beta \chi_{\boxed{\Gamma_1}} + (1 - \beta) \chi_{\boxed{\Gamma_2}}$
  - Parameter $\boldsymbol{\mu} = (c_{\text{init}}, \beta, k) \in [0, 1] \times [0, 1] \times [0, 5 \cdot 10^{-8}]$



Offline Adaptivity: Train Set

- Qualitative Results in 2D Parameter Domain
  - Parameter domain $\boldsymbol{\mu} = (\beta, k) \in [0,1] \times [0, 5 \cdot 10^{-8}]$
  - Basis size $N = 130$, random validation set $|M_{val}| = 10, \rho_{tol} = 1.0$
  - Resulting error (estimator) : plot of $\log \Delta(\boldsymbol{\mu}, \Phi_N)$

uniform-fixed | uniform-refined | adaptive-refined, $\Theta = 0.05$

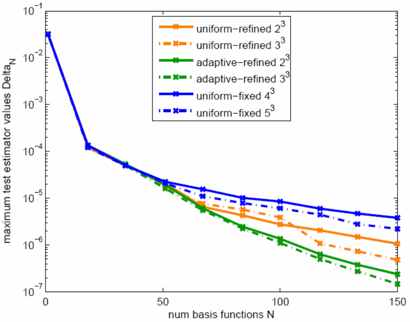


  - Overfitting in uniform-fixed grid (standard greedy search)
  - Improved uniform error distribution by adaptive approach

Offline Adaptivity: Train Set

- Quantitative Results in 3D Parameter Domain

max. test error decrease



- Full 3D parameter domain

  $\boldsymbol{\mu} = (c_{\text{init}}, \beta, k)$

  $\mathcal{P} := [0,1] \times [0,1] \times [0, 5 \cdot 10^{-8}]$

- Random test set

  $|M_{test}| = 1000$

- Maximum test error

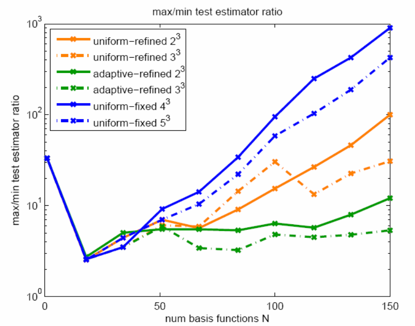
$$\max_{\boldsymbol{\mu} \in M_{test}} \Delta(\boldsymbol{\mu}, \Phi_N)$$

- Flattening of test error curve in uniform-fixed approach
- Improved convergence for adaptive approach

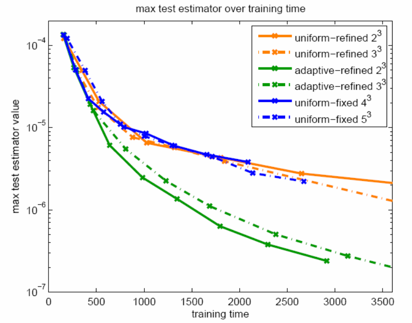
Offline Adaptivity: Train Set

- Quantitative Results in 3D Parameter Domain

ratio of max./min. test error



max. test error over train time



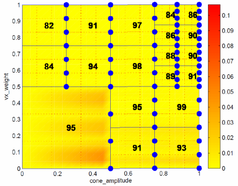
- Improved equal distribution of test error
- Considerable gain in computation time for fixed accuracy

Offline Adaptivity: P-partition

Haasdonk, B.; Dihlmann, M. & Ohlberger, M.: A Training Set and Multiple Basis Generation Approach for Parametrized Model Reduction Based on Adaptive Grids in Parameter Space, Mathematical and Computer Modelling of Dynamical Systems, 2011, 17, 423-442.

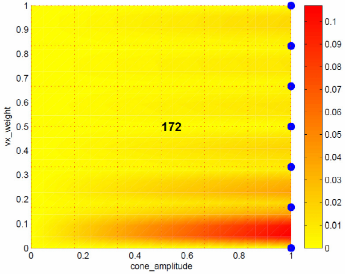
Offline Adaptivity: P-Partition

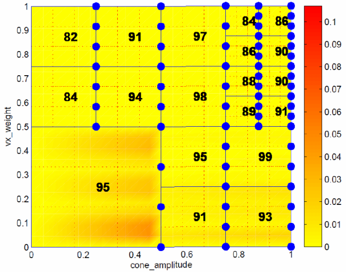
- (POD-)Greedy in Case of Large Solution Variety:
  - Large basis required for good accuracy
  - ROM may be inpractically large (small, but dense matrices!)
  - No simultaneous prescription of accuracy and online runtime
- Idea: Parameter Domain Partitioning
  - Decompose Parameter domain in Subdomains
  - Single (POD-)Greedy basis per Subdomain
  - Online: Select corresponding submodel
- Adaptive Parameter-Domain Partition
  - hp-RB [EPR09,EKP11]: bisection
  - P-partition [HDO11,ES11]: structured
  - Implicit partitioning [Wieland'13]



Offline Adaptivity: P-Partition

- Adaptive P-Partition [HDO11]
  - Goal: bases with desired accuracy & online runtime: ϵ_{tol}, N_{max}
  - (adaptive POD)-Greedy Basis per parameter-subdomain.
  - If not $(\epsilon_{extrapol} \leq \epsilon_{tol}) \wedge (N \leq N_{max})$ then refine subdomain
  - Early Stopping Greedy by error decay extrapolation



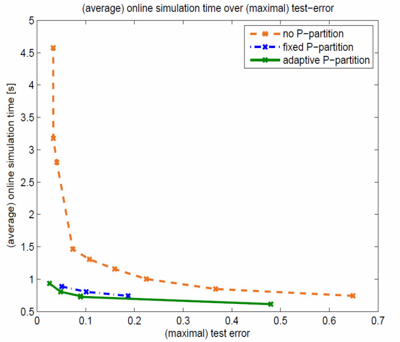


Increased offline cost, improved online time vs. accuracy

Offline Adaptivity: P-Partition

- Verification of Online Efficiency:
  - Considerably reduced online computation time with equal accuracy
  - Further orders of magnitude improvement by combination with adaptive training set extension

online time / test-error



Offline Adaptivity: T-partition

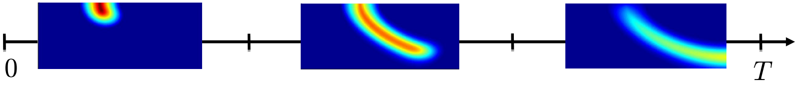
Ref: Dihlmann, M.; Drohmann, M. & Haasdonk, B.: Model Reduction of Parametrized Evolution Problems using the Reduced basis Method with Adaptive Time-Partitioning, Proc. of ADMOS 2011.

Offline Adaptivity: T-Partition

- Time-dependent problems
  - High solution variety over time, large RB required
  - „final" snapshots may be very different from „initial" snapshots
- Idea
  - Time as prior knowledge, is simple & robust scalar „feature extraction"
  - Partitioning of time-axis in subintervals
  - RB-space by POD-Greedy per subinterval
  - Rigorous treatment of basis change in scheme and error-estimators
  - Adaptive Partitioning, Early stopping greedy
- Related
  - T-partitioning for EIM [DOH11]
  - Local bases [AZF12]
  - Implicit Partitioning EIM [Wi13]
  - Localized DEIM [PBWB13]

Offline Adaptivity: T-Partition

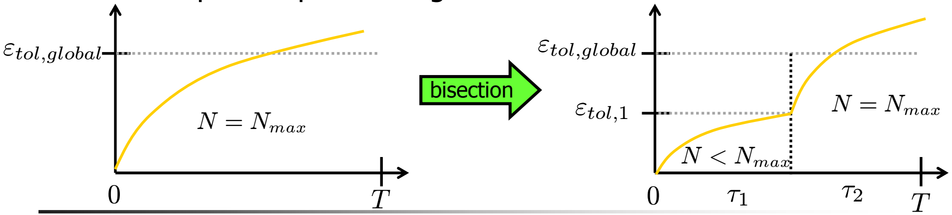
- POD-Greedy with Adaptive T-Partitioning [DDH11]
  - Individual POD-Greedy spaces X_{N_i} on time-subintervals



  - Extension of RB-Scheme and error estimators

$$\left\langle u^{k(i)}_{N_{i-i}} - u^{k(i)}_{N_i}, \varphi_{n,i} \right\rangle = 0 \qquad \Delta^k_N(\boldsymbol{\mu}) := \sum_{n=1}^{k} C_E^{k-n} (\Delta t \, \|R^n_h(\boldsymbol{\mu})\| + \|\tilde{R}^n(\boldsymbol{\mu})\|)$$

  - Adaptive T-partitioning:



Offline Adaptivity: T-Partition

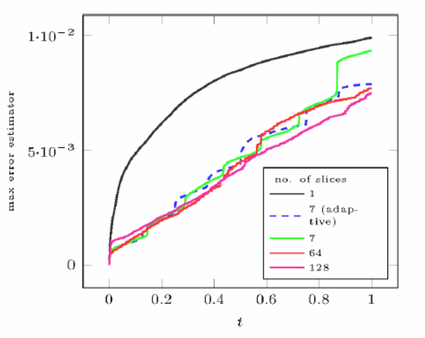
- Experiments:
  - Advection problem (1-parameter)
    - FV-Discretization: 4096 DOFs
    - Explicit Euler time integration: 512 time steps
  - Adaptive reduced basis settings:
    - $\varepsilon_{tol,global} = 0.01, N_{max} = 45$
  - Testing the reduced model by performing reduced simulations for 20 randomly chosen parameters

adaptation	Υ	ø-dim(RB)	max. error	offline time[h]
-	1	84.00	$9.87 \cdot 10^{-3}$	0.84
yes	7	33.63	$7.85 \cdot 10^{-3}$	2.10
no	7	34.31	$9.32 \cdot 10^{-3}$	0.70
no	64	24.61	$6.28 \cdot 10^{-3}$	5.08
no	128	23.43	$7.36 \cdot 10^{-3}$	12.13

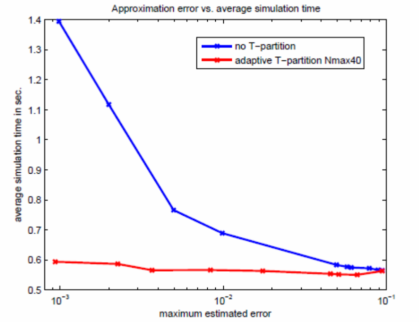
Offline Adaptivity: T-Partition

- Exemplary Results:

test error estimator over time



online runtime vs. accuracy



- Error estimator approximating linear „target curve“
- Simultaneous prescription of online-runtime and accuracy!

Online Adaptivity: Basis Adaptation

Ref: Haasdonk, B. & Ohlberger, M.: Space-Adaptive Reduced Basis Simulation for Time-Dependent Problems, Proc. MATHMOD 2009, 6th Vienna International Conference on Mathematical Modelling, 2009.

Kaulmann, S. & Haasdonk, B.: Online Greedy Reduced Basis Construction Using Dictionaries. In In Moitinho de Almeida, José Paulo Baptista and Diez, Pedro and Tiago, Carlos and Parés, Núria (Eds.), VI International Conference on Adaptive Modeling and Simulation (ADMOS 2013), 2013, 365-376

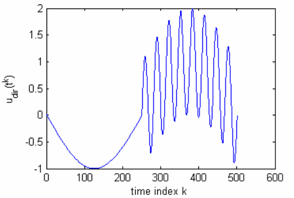
Online Adaptivity: N Adaptation

- Usually: Fixed Basis Size in Time
  - Model either too precise (costly) or too coarse (but rapid)
  - Identical basis size may be inappropriate for different parameters
  - Suboptimal in view of „minimal computational cost for desired accuracy“
- Idea: N-adaptation over time
  - Automatic adaptation of basis size over time
  - Guarantee prescribed error threshold
  - Dimension choice by growth of a-posteriori error estimator
  - Note: No projection error by basis change!

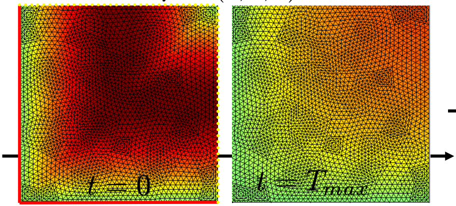
Online Adaptivity: N Adaptation

- Geometry and Data
  - Domain $\Omega = [0,1]^2, t \in [0,2]$
  - Dirichlet values: amplitudes c_1, c_2
  - Initial values: sinusoidal, amplitude c_1
  - Velocity: $\mathbf{v} = (1,1)^T$
  - Diffusivity: d
  - Neumann-boundary: outflow
  - Parameter $\boldsymbol{\mu} = (c_1, c_2, d) \in [0,1]^3$
- Examples of Solution Variety

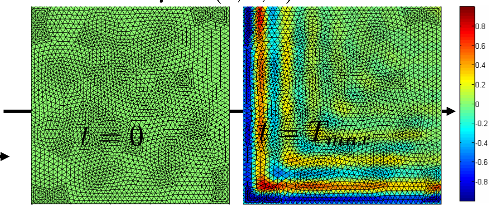
$$u_{dir}(t, \boldsymbol{\mu}) = c_1 \sin(-\pi t)\chi_{[0,1)}(t) + c_2 \sin(-16\pi t + \pi)\chi_{[1,2)}(t)$$



$\boldsymbol{\mu} = (1,0,1)^T$

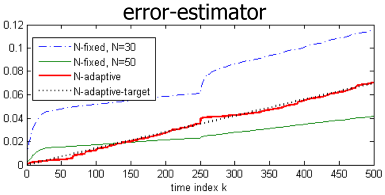


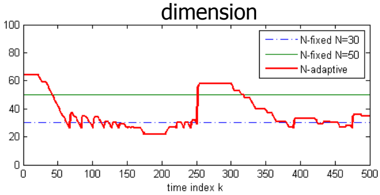
$\boldsymbol{\mu} = (0,1,0)^T$



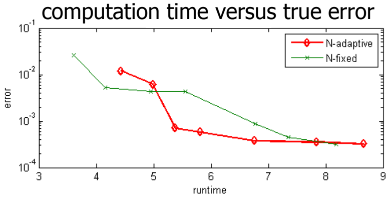
Online Adaptivity: N Adaptation

- Results: $\boldsymbol{\mu} = (1, 1, 1)^T$





⇨ Attaching to target, detecting varying model difficulty over time

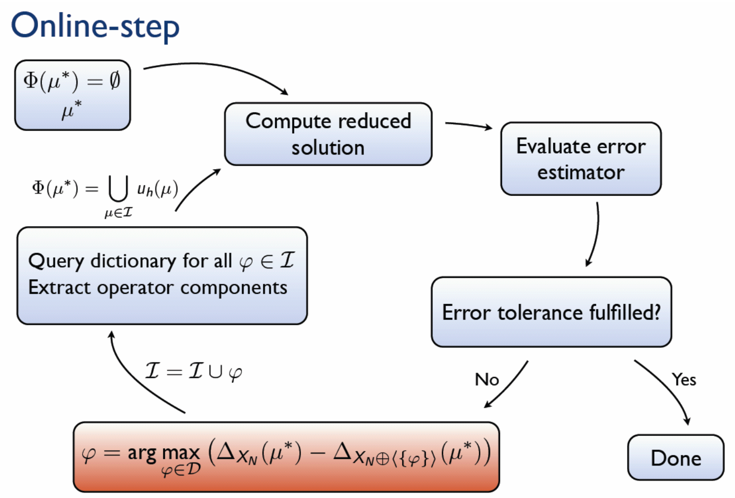


⇨ N-adaptive computationally faster than N-fixed for high accuracies

Online Adaptivity: Greedy

- Extensions:
  - Nearest Neighbour in Parameter Space for Local Basis Generation [Stamm&Maday'13]
  - Online Greedy [KH13]
    - Dictionary D of Snapshots
    - Online Greedy Basis Generation by iteratively extending basis by dictionary element that realizes maximum error estimator decrease
    - Efficient „Simultaneous" computation of all extended RB solutions and error bounds
    - Online Orthonormalization of Basis

Online Adaptivity: Greedy



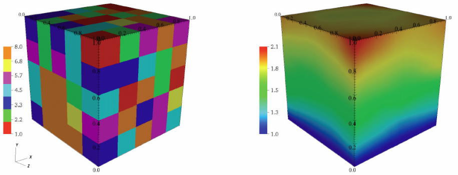
Online Adaptivity: Greedy

Experiments: 3D Thermal Block

- For $\boldsymbol{\mu} \in \mathcal{P} = (0, 10]^8$ solve

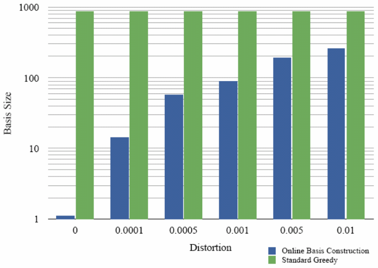
$$-\nabla \cdot (\lambda(\mathbf{x}; \boldsymbol{\mu}) \nabla u(\mathbf{x})) = 1 \quad \text{in } \Omega = [0, 1]^3$$

- $\lambda(\mathbf{x}; \boldsymbol{\mu}) = \sum_{i=1}^{8} (\boldsymbol{\mu})_i \cdot \chi_i(\mathbf{x})$,
- Dirichlet-zero on bottom, Neumann-zero on all other boundaries



- Greedy basis constructed using $|\mathcal{S}_G| = 1000$ and tolerance 10^{-5}
- Dictionary constructed using $\mathcal{S}_\mathcal{D} \supset \mathcal{S}_G$, $|\mathcal{S}_\mathcal{D}| = 2000$

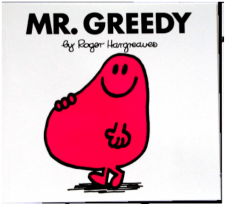
	Duration	Storage
Standard Greedy	> 9h	575 MB
Dictionary Method	~ 1h	1.1 GB



Summary and Conclusion

Summary and Conclusion

- RB for Linear Coercive Problems
  - Compliant case: analysis, error-control, basis-generation, offline/online procedure, software, experiments
  - Extension to non-compliant case by primal-dual approach
- RB for Polynomial Nonlinearities
  - Tensor approach enables efficiency by offline-online decomposition
  - A-posteriori well-posedness and error statements
- RB for Parametric Time-dependent PDEs
  - Empirical Interpolation for Nonlinearities
  - Basis generation: POD-Greedy procedure + Convergence Rates
  - Inequality Constraints can be included



Age: 2+

Summary and Conclusion

- Adaptivity in Basis Generation
  - Offline: Train set refinement allows equidistribution of model error and offline runtime improvement
  - Offline: Adaptive partitioning approaches: simultaneous accuracy and online-runtime control
  - Online: Parameter/time-dependent small bases assembly promising for "nonlinear approximation"
- Extensions not Addressed Here
  - Noncoercive (inf-sup stable) problems, (Navier)-Stokes
  - Geometry param., domain decomposition, multiphysics
  - Optimization, optimal control, feedback
  - Multiscale problems, stochastic problems
  - True error certificates

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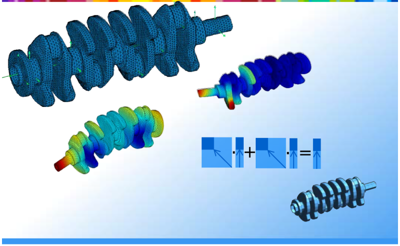

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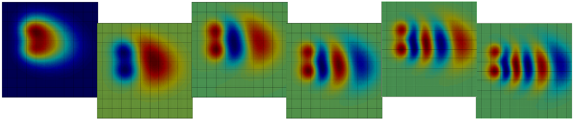
Thank you!



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