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The Reduced Basis Method in Space and Time: Limits and Perspectives

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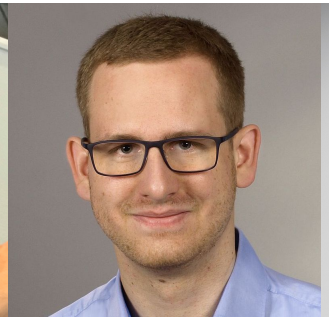
Thanks to my co-authors

Julia Brunken

Silke Glas

Constantin Greif


Julian Henning

Philipp Junk

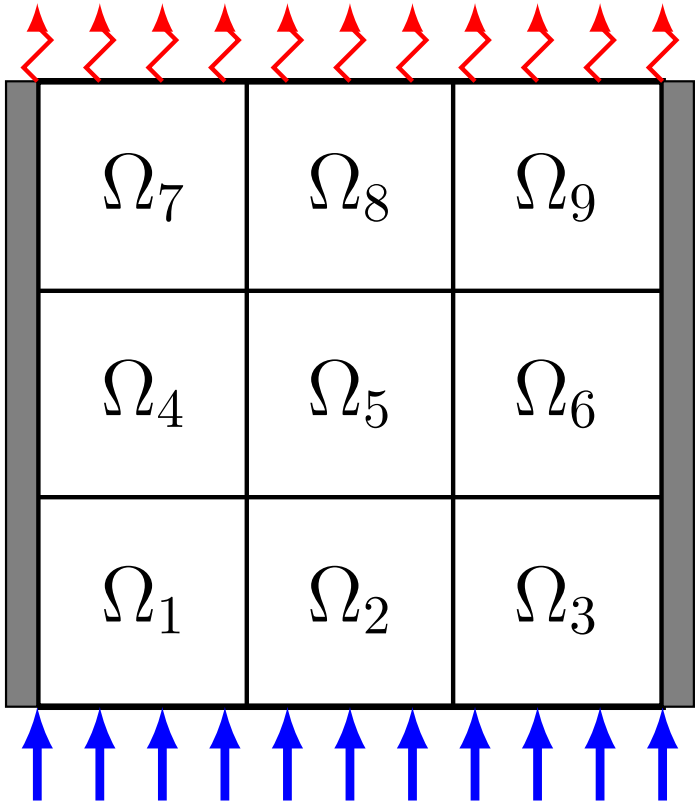
Davide Palitta

Tony Patera

Valeria Simoncini

Kathrin Smetana

The thermal block



- $\mathbb{R}^d \supset \Omega = \bigcup_{p=1}^{P} \Omega_p$

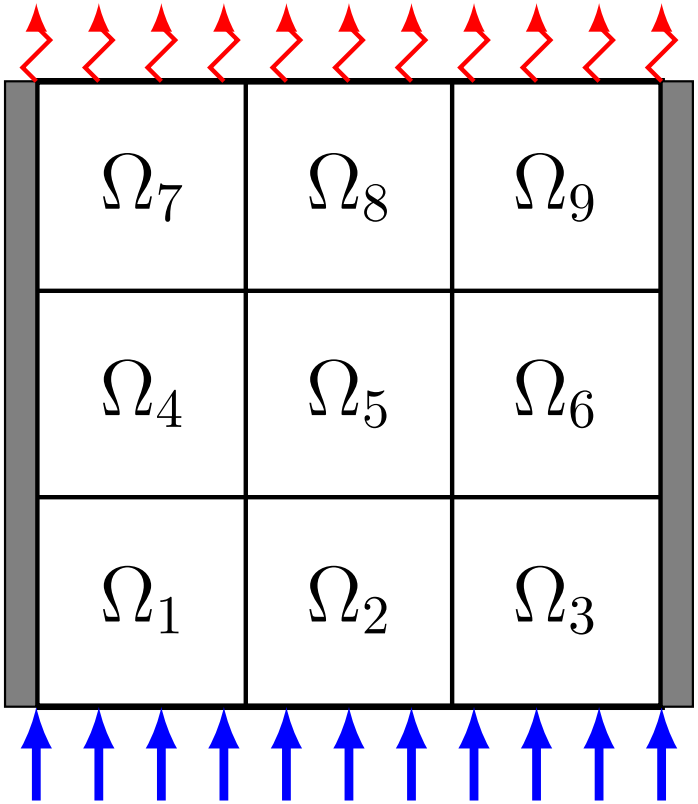
$$L_\mu u := -\sum_{p=1}^{P} \nabla \cdot (\mu_p \, \chi_{\Omega_p} \, \nabla u) = f,$$

$$\mu_p > 0, p = 1, ..., P,$$

$$u_{|\partial\Omega} = 0,$$

$f : \Omega \to \mathbb{R}$ external force

The thermal block



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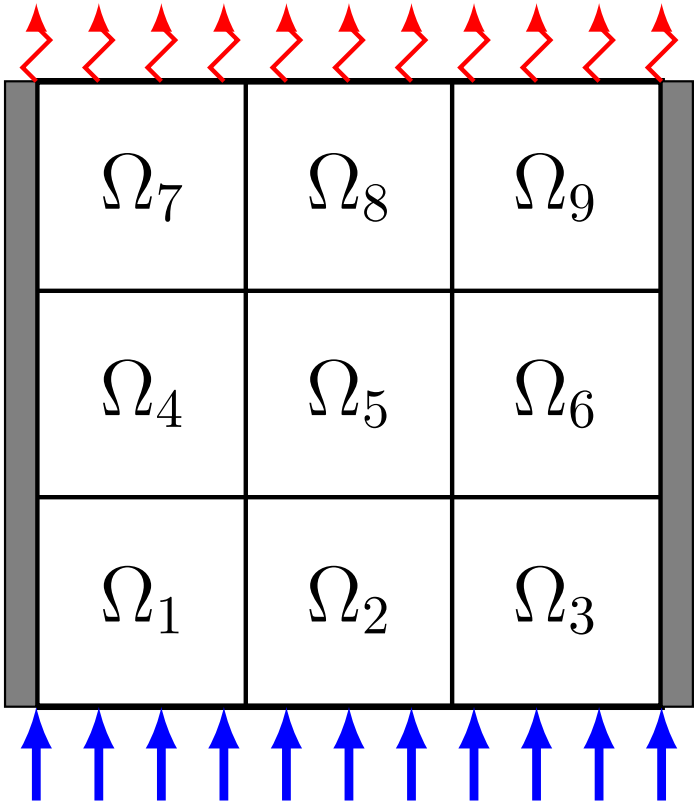

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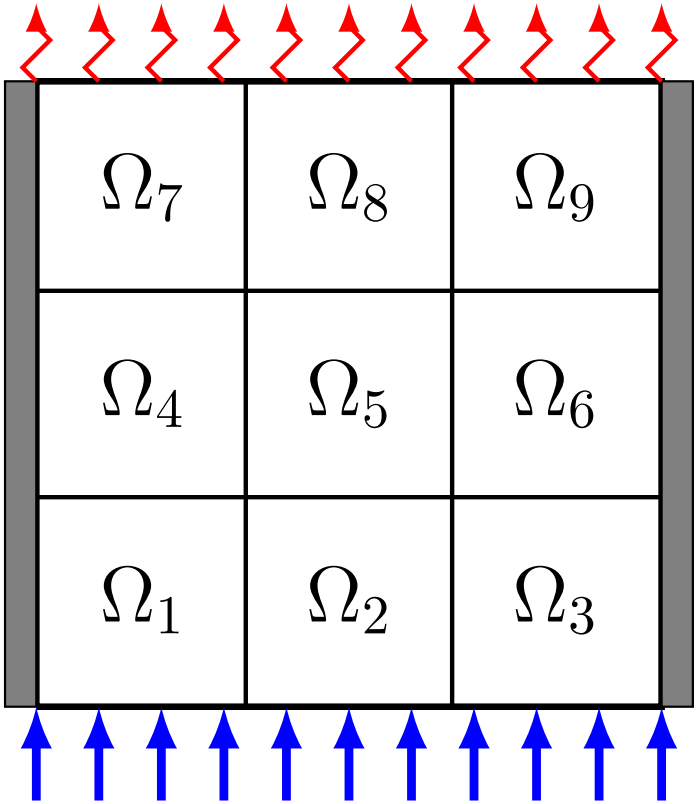

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- trial/ansatz spaces: $X = Y = H_0^1(\Omega)$
- solve for *many* parameters $\boldsymbol{\mu} = (\mu_1, ..., \mu_P)^T$

RBM in a nutshell

1) PPDE: $L_\mu u_\mu = f_\mu$ in X, $\mu \in \mathcal{P}$ $\rightsquigarrow$ $b_\mu(u, v) = f_\mu(v)$ $\forall v \in X$

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2) detailed discretization (e.g. FEM $\mathcal{N} = n_h$ "huge"): $X^\mathcal{N} \subset X$
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   - complexity $\mathcal{O}(\mathcal{N})$

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3) reduced space $X_N \subset X^\mathcal{N}$, $N \ll \mathcal{N}$ – offline
   - error estimate: $\|u_\mu^\mathcal{N} - u_\mu^N\| \leqslant \Delta_N(\mu)$
   - offline training: $\mathcal{P}_{\text{train}} \subset \mathcal{P}$ finite
   - select $\mu^{(1)}, \ldots, \mu^{(N)} \in \mathcal{P}$ by maximizing $\Delta_N(\mu)$, $\mu \in \mathcal{P}_{\text{train}}$

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   - determine "snapshots" $\xi^{(i)} := u^\mathcal{N}_{\mu^{(i)}}$, $i = 1, \ldots, N$
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   - $X_N := \operatorname{span}\{\xi^{(i)} : i = 1, \ldots, N\}$

4) online: $\mu \in \mathcal{P}$
   - compute u_μ^N — complexity $\mathcal{O}(N^3)$ independent of $\mathcal{N}$!

     "online efficient"
   - certification via $\Delta_N(\mu)$

Why does that work? – Separation of parameter & variables

- variational form: $u \in X := H_0^1(\Omega)$: $b(u, v; \mu) = (f, v) \; \forall v \in X$
- "affine decomposition": $b(u, v; \mu) = \sum_{p=1}^{P} \underbrace{\mu_p}_{=:\vartheta_p(\mu)} \underbrace{\int_{\Omega_p} \nabla u \cdot \nabla v \, dx}_{=:b_p(u,v)}$

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- stiffness matrix

$$\boldsymbol{B}_\mu^N = [b(\xi^{(i)}, \xi^{(j)}; \mu)]_{i,j=1,\dots,N} = \left[\sum_{p=1}^{P} \vartheta_p(\mu) \, b_p(\xi^{(i)}, \xi^{(j)}) \right]_{i,j=1,\dots,N}$$

$$= \sum_{p=1}^{P} \vartheta_p(\mu) \boldsymbol{B}_p$$

- $\boldsymbol{B}_p \in \mathbb{R}^{N \times N}$ (small)
- each entry requires $\mathcal{O}(\mathcal{N})$ computations (costly)
- precompute offline and store as $N \times N$ matrix

Why does that work? – Error estimation 1

- $\mu_\infty \geqslant \mu_p \geqslant \mu_0 > 0$ (otherwise not well-posed)
- the problem is coercive:

$$b(u,u;\mu) = \sum_{p=1}^{P} \mu_p \int_{\Omega_p} \nabla u \cdot \nabla u \, dx \geqslant \mu_0 \sum_{p=1}^{P} \int_{\Omega_p} \nabla u \cdot \nabla u \, dx$$

$$= \mu_0 \int_{\Omega} \nabla u \cdot \nabla u \, dx = \mu_0 |u|^2_{H^1(\Omega)} \geqslant C\mu_0 \|u\|^2_{H^1(\Omega)} \quad \Rightarrow \boxed{\alpha = C\mu_0}$$

$$b(u,v;\mu) \leqslant \mu_\infty \|u\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)}$$

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$$b(u,v;\mu) \leqslant \mu_\infty \|u\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)}$$

- error/residual-relation:

$$\alpha \|u_\mu - u_\mu^N\|_{H^1(\Omega)} \leqslant \frac{b(u_\mu - u_\mu^N, u_\mu - u_\mu^N; \mu)}{\|u_\mu - u_\mu^N\|_{H^1(\Omega)}}$$

$$\leqslant \sup_{v \in X} \frac{b(u_\mu - u_\mu^N, v; \mu)}{\|v\|_{H^1(\Omega)}} = \sup_{v \in X} \frac{(f,v) - b(u_\mu^N, v; \mu)}{\|v\|_{H^1(\Omega)}}$$

$$= \|r_\mu^N\|_{H^{-1}(\Omega)}$$

Why does that work? – Error estimation 2

- error/residual-relation:

$$\|u_\mu - u_\mu^N\|_{H^1(\Omega)} \leqslant \frac{1}{\alpha}\|r_\mu^N\|_{H^{-1}(\Omega)} =: \Delta_N(\mu)$$

- separation of parameter and variables

$$\|r_\mu^N\|^2_{H^{-1}(\Omega)} = \sum_{q=1}^{Q} \vartheta_q^r(\mu)\, R_q$$

$\rightsquigarrow$ $\Delta_N(\mu)$ can be computed online-efficient

Why does that work? – linear approximation

- benchmark: *Kolmogorov N-width*

$$d_N(\mathcal{P}) := \inf_{X_N \subset X,\ \dim(X_N)=N} \sup_{\mu \in \mathcal{P}} \inf_{v_N \in X_N} \|u_\mu^{\mathcal{N}} - v_N\|_X$$

- affine decomposition: $b(u, v; \mu) = \sum_{q=1}^{Q^b} \vartheta_q(\mu) b_q(u, v)$

Theorem (Buffa, Maday, Patrera, Prud'homme, Turinici, 2012; Ohlberger, Rave 2016)

Let $b(\cdot, \cdot; \mu)$ be bounded, coercive and affine decomposable, then

$$d_N(\mathcal{P}) \leqslant C \exp(-cN^{1/Q^b}) \tag{1}$$

Why does that work? – The greedy method I

Algorithm (Greedy)

1: choose $\mu^{(1)} \in \mathcal{P}_{\text{train}}$, compute $\xi^{(1)} := u^{\mathcal{N}}_{\mu^{(1)}}$
2: **for** n=1,... **do**
3: $\mu^{(n+1)} := \arg\max_{\mu \in \mathcal{P}_{\text{train}}} \Delta_N(\mu)$
4: $\xi^{(n+1)} := u^{\mathcal{N}}_{\mu^{(n+1)}}$
5: possibly (bi-)orthogonalize
6: If $\Delta_N(\mu^{(n+1)}) <$ tol STOP
7: **end for**

Why does that work? – The greedy method II

Theorem (Binev, Cohen, Dahmen, DeVore, Petrova, Wojtaszczyk 2011)

Let $0 < \gamma \leqslant 1$, $d_0(\mathcal{P}) \leqslant M$. Then

- if $d_N(\mathcal{P}) \leqslant M\, N^{-\alpha}$, $N > 0$, $\alpha > 0$, then

$$\max_{\mu \in \mathcal{P}} \|u_\mu^{\mathcal{N}} - u_\mu^N\|_X \leqslant C\, M\, N^{-\alpha}$$

  with $C := q^{1/2}(4q)^\alpha$, $q := \lceil 2^{\alpha+1}\gamma^{-1}\rceil^2$.

- if $d_N(\mathcal{P}) \leqslant M\, e^{-aN^\alpha}$, $N \geqslant 0$, $M, a, \alpha > 0$, then

$$\max_{\mu \in \mathcal{P}} \|u_\mu^{\mathcal{N}} - u_\mu^N\|_X \leqslant C\, M\, \exp(-cN^\beta)$$

  where $\beta := \frac{\alpha}{\alpha+1}$, $0 \leqslant \theta < 1$, $c := \min\{|\log\theta|, (4q)^{-\alpha}a\}$,
  $C := \max\{e^{cN_0^\beta}, q^{1/2}\}$, $q := \lceil 2\gamma^{-1}\theta^{-1}\rceil^2$, $N_0 := \lceil (8q)^{\alpha+1}\rceil$.

Where do we stand

The RBM works perfectly for

- linear, coercive problems
- affine decomposition

But what about...

- noncoercive problems
- time-depend
- transport
- wave
- Schrödinger
- ...

Variational formulations – non-corecive I

- PPDE: $L_\mu u_\mu = f_\mu$
  - $L_\mu \in \mathcal{L}(X, Y')$ isomorphism
  - X, Y Hilbert spaces
  - $\mu \in \mathcal{P} \subset \mathbb{R}^P$ compact parameter set
- variational form:

$$u_\mu \in X : \quad b(u_\mu, v; \mu) = f_\mu(v) \qquad \forall v \in Y \tag{2}$$

  - X: trial/ansatz space
  - Y test space
  - $b_\mu(\cdot, \cdot) \equiv b(\cdot, \cdot; \mu) : X \times Y \to \mathbb{R}$ bilinear form
  - $f_\mu(\cdot) : Y \to \mathbb{R}$ linear form ($f_\mu \in Y'$)

Variational formulations – non-corecive II

Example

(a) thermal block...

(b) parabolic: $\Omega \subset \mathbb{R}^d$, $I := (0,T)$, $\Omega_T := I \times \Omega$

$$L_\mu u := u_t - \mu \Delta u, \qquad u(0) = 0, u_{|\partial\Omega} = 0$$

– Time-stepping (POD-Greedy) $\rightsquigarrow$ growth over time ↯
– Consider space-time variational formulation:
  - integrate over space and time:

$$\int_I \int_\Omega (u_t(t,x) - \mu \Delta u(t,x))\, v(t,x)\, dx\, dt =$$

$$= \underbrace{\int_I \int_\Omega u_t(t,x)\, v(t,x)\, dx\, dt - \mu \int_I \int_\Omega \nabla u(t,x)) \cdot \nabla v(t,x)\, dx\, dt}_{=: b_\mu(u,v) \equiv b(u,v;\mu)}$$

$\rightsquigarrow$ trial and test space-time functions

Variational formulations – non-corecive III

- Let V be a function space on Ω with norm $\|\cdot\|_V$ (e.g. $H_0^1(\Omega)$, $|\cdot|_1$)
- Lebesgue-Bochner spaces:

$$L_2(I;V) := \left\{ v : I \to V : \|v\|^2_{L_2(I;V)} := \int_I \|v(t)\|_V^2 \, dt < \infty \right\}$$

$$H^1(I;V) := \{ v \in L_2(I;V) : v_t \equiv \dot{v} \in L_2(I;V) \}$$

$$H^1_{(0)}(I;V) := \{ v \in H^1(I;V) : v(0) = 0 \}$$

- $X := H^1_{(0)}(I;V') \cap L_2(I;V)$
- $Y := L_2(I;V)$ (i.e., $f \in L_2(I;V')$)

Variational formulations – non-corecive IV

(c) transport:

- $\Omega \subset \mathbb{R}^d$ or $\Omega = \mathbb{R}^d$
- $L_\mu u := u_t + \mu \nabla u$, $u(0) = u_0$
- weak form not obvious!

(d) wave equation:

- $\Omega \subset \mathbb{R}^d$ or $\Omega = \mathbb{R}^d$
- $L_\mu u := u_{tt} + \mu \Delta u$, $u(0) = u_0$, $u_t(0) = v_0$
- weak form not obvious!

Variational formulations – non-corecive V

Boundedness

In all cases, we can show:

$$\exists 0 < C < \infty : \qquad |b_\mu(u,v)| \leqslant C \, \|u\|_X \, \|v\|_Y$$

Theorem (Banach–Nečas)

- let $b_\mu(\cdot,\cdot)$ be bounded, $f_\mu \in Y'$, then

(2) admits a unique solution $u_\mu \in X$ s.t. $\|u_\mu\|_X \leqslant c \, \|f_\mu\|_{Y'}$ **if and only if**

$$(i) \qquad \exists \beta > 0 : \qquad \sup_{v \in Y} \frac{b_\mu(u,v)}{\|v\|_Y} \geqslant \beta \, \|u\|_X \quad \text{for all } u \in X$$

$$(ii) \qquad \text{for any } 0 \neq v \in Y \quad \exists u \in X : \quad b_\mu(u,v) \neq 0$$

Moreover $c = \beta^{-1}$.

Variational formulations – non-corecive VI

Corollary

- under conditions of Banach–Nečas–Thm.
- let $u^{\mathcal{N}}(\mu)$ be some approximation to $u(\mu)$

$$\begin{aligned}\|u(\mu) - u^{\mathcal{N}}(\mu)\|_X &\leqslant \frac{1}{\beta} \sup_{v \in Y} \frac{b_\mu(u_\mu - u_\mu^{\mathcal{N}}, v)}{\|v\|_Y} \\ &\leqslant \frac{1}{\beta} \sup_{v \in Y} \frac{f(v;\mu) - b_\mu(u_\mu^{\mathcal{N}}, v)}{\|v\|_Y} \\ &= \frac{1}{\beta} \|r^{\mathcal{N}}(\mu)\|_{Y'} \end{aligned} \tag{3}$$

Variational formulations – non-corecive VII

Example (continued)

(b) parabolic: $L_\mu = u_t + \mu A$
(ii) shown by Faedo-Galerkin approximation
(i) consider supremizer: $T_\mu : X \to Y$ defined by $(T_\mu u, v)_Y = b_\mu(u, v)$,

then ($A = -\Delta$)

$$b_\mu(u, v) = \langle u_t + \mu\, Au, v\rangle = \langle A^{-1}u_t + \mu\, u, Av\rangle$$
$$= (\underbrace{A^{-1}u_t + \mu\, u}_{=:T_\mu u}, v)_{L_2(I;V)} = (T_\mu\, u, v)_{L_2(I;V)} = (T_\mu u, v)_Y$$

which implies that $T_\mu u = A^{-1}u_t + \mu\, u$.
Then (...)

$$b_\mu(u, T_\mu u) = \|u\|_X\, \|T_\mu u\|_Y \qquad \rightsquigarrow \quad \beta = 1\,!$$

(c) transport: no idea yet

(d) wave equation: no idea yet

Petrov–Galerkin methods I

Form a discretization:

- trial: $X^{\mathcal{N}} \subset X$, $\dim X^{\mathcal{N}} = \mathcal{N} < \infty$ – large, but detailed
- test: $Y^{\mathcal{N}} \subset Y$ $\dim Y^{\mathcal{N}} = \mathcal{N} < \infty$ for simplicity

LBB condition

Definition

$X^{\mathcal{N}}$, $Y^{\mathcal{N}}$ satisfy the *LBB condition* if

$$\inf_{u^{\mathcal{N}} \in X^{\mathcal{N}}} \sup_{v^{\mathcal{N}} \in Y^{\mathcal{N}}} \frac{b_\mu(u^{\mathcal{N}}, v^{\mathcal{N}})}{\|u^{\mathcal{N}}\|_X \, \|v^{\mathcal{N}}\|_Y} \geqslant \beta > 0 \tag{4}$$

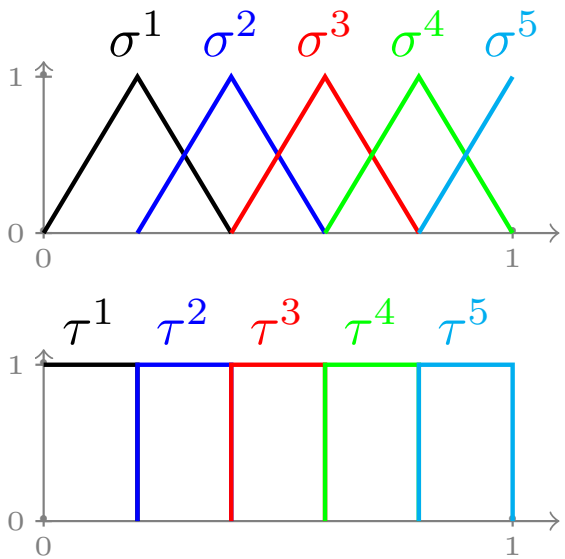
independent of $\mathcal{N} \to \infty$.

Petrov–Galerkin methods II

Example (continued)

(b) parabolic:

- $S_{\Delta t}$: piecewise linear finite elements in time
- $Q_{\Delta t}$: piecewise constant finite elements in time
- V_h: piecewise linear finite elements in space
- $X^{\mathcal{N}} = S_{\Delta t} \otimes V_h$
- $Y^{\mathcal{N}} = Q_{\Delta t} \otimes V_h$
- this yields Crank-Nicolson
- $\rightsquigarrow \beta = 1$ for heat eq.



(c) transport: still no idea yet

(d) wave equation: still no idea yet

Petrov–Galerkin methods III

Remark

(a) One may choose $Y^{\mathcal{N}} := T_\mu(X^{\mathcal{N}})$ – but there are other choices

(b) LBB ensures well-posedness of discrete problem

$$u_\mu^{\mathcal{N}} \in X^{\mathcal{N}} : \qquad b_\mu(u_\mu^{\mathcal{N}}, v^{\mathcal{N}}) = f_\mu(v^{\mathcal{N}}) \quad v^{\mathcal{N}} \in Y^{\mathcal{N}} \tag{5}$$

and $\|u_\mu^{\mathcal{N}}\|_X \leqslant \beta^{-1}\|f_\mu\|_{Y'}$

- $\Rightarrow$

$$\|u_\mu - u_\mu^{\mathcal{N}}\|_X \leqslant \beta^{-1}\|r_\mu^{\mathcal{N}}\|_{(Y^{\mathcal{N}})'}$$

Petrov–Galerkin methods IV

Theorem (Xu, Zikatanov, 2003)

- let $b_\mu(\cdot,\cdot)$ be bounded with constant $0 < C < \infty$
- let LBB hold with constant β

Then,

$$\|u_\mu - u_\mu^{\mathcal{N}}\|_X \leqslant \frac{C}{\beta} \inf_{v^{\mathcal{N}} \in X^{\mathcal{N}}} \|u_\mu - v^{\mathcal{N}}\|_X$$

- $\beta = C = 1 \Rightarrow$

$$\|u_\mu - u_\mu^{\mathcal{N}}\|_X = \frac{C}{\beta} \inf_{v^{\mathcal{N}} \in X^{\mathcal{N}}} \|u_\mu - v^{\mathcal{N}}\|_X = \|r_\mu^{\mathcal{N}}\|_{(Y^{\mathcal{N}})'}$$

Reduced Basis Method – revisited I

- use $X^{\mathcal{N}}$, $Y^{\mathcal{N}}$ as "truth" discretization
- first construct $X_N \subset X^{\mathcal{N}}$, $N = \dim X_N \ll \mathcal{N}$ (typical by greedy, see later)
- then construct corresponding Y_N (could be $Y_N(\mu)$)
- $\rightsquigarrow$ reduced problem

$$u_\mu^N \in X_N : \qquad b_\mu(u_\mu^N, v_N) = f_\mu(v_N) \quad v_N \in Y_N \tag{6}$$

- recall:

$$\boxed{\|u_\mu^{\mathcal{N}} - u_\mu^N\|_X \leqslant \frac{1}{\beta}\|r_\mu^N\|_{Y'} =: \Delta_N(\mu)}\,, \tag{7}$$

where

$$\|r_\mu^N\|_{Y'} = \sup_{v^{\mathcal{N}} \in Y^{\mathcal{N}}} \frac{f_\mu(v^{\mathcal{N}}) - b_\mu(u_\mu^N, v^{\mathcal{N}})}{\|v^{\mathcal{N}}\|_Y} \tag{8}$$

Reduced Basis Method – revisited II

- assume –as usual– "affine decomposition" (otherwise do EIM)

$$b_\mu(u,v) = \sum_{q=1}^{Q^b} \vartheta_q^b(\mu)\, b_q(u,v) \tag{9}$$

$$f_\mu(v) = \sum_{q=1}^{Q^f} \vartheta_q^f(\mu)\, f_q(v) \tag{10}$$

- determine $X_N :=$ span$\{u^{\mathcal{N}}_{\mu^{(1)}}, ..., u^{\mathcal{N}}_{\mu^{(N)}}\}$
  by *snapshots* $u^{\mathcal{N}}_{\mu^{(i)}}$ for $\mu^{(i)} \in S_N := \{\mu^{(1)}, ..., \mu^{(N)}\} \subset \mathcal{P}$
- using a *training set* $\mathcal{P}_{\text{train}} \subset \mathcal{P}$ of size $\mathcal{N}_{\text{train}}$
- construct test space $Y_N(\mu)$

Reduced Basis Method – revisited III

Remark

- The computation of $\Delta_N(\mu)$ is *online efficient*:
  - $\mathcal{O}(N^\bullet)$ independent of $\mathcal{N}$
  - use Riesz representation
  - β e.g. by Successive Constraint Method (SCM)
- Problem: "square root effect":

$$\|r_\mu^N\|_{Y'} = \|\hat{r}_\mu^N\|_Y = \sqrt{\dots}$$

  - Riesz representation: $(\hat{r}_\mu^N, y)_Y = r_\mu^N(y)\ \forall y$
  - Y is a Hilbert space:

$$\begin{aligned}\|\hat{r}_\mu^N\|_Y^2 &= (\hat{f}_\mu - \hat{B}_\mu \hat{u}_\mu^N, \hat{f}_\mu - \hat{B}_\mu \hat{u}_\mu^N)_Y \\ &= \|\hat{f}_\mu\|_Y^2 + \|\hat{B}_\mu \hat{u}_\mu^N\|_Y^2 - 2(\hat{f}_\mu, \hat{B}_\mu \hat{u}_\mu^N)_Y\end{aligned}$$

  - $\|r_\mu^N\|_{Y'} = \sqrt{\|\hat{r}_\mu^N\|_Y^2}$
- computation of u_μ^N is also online efficient

And the benchmark? I

Theorem (Ohlberger/Rave 2016 – slightly generalized)

Let $b(\cdot,\cdot;\mu)$ be bounded, inf-sup stable and affine decomposable, i.e.,

$$b(u,v;\mu) = \sum_{q=1}^{Q^b} \vartheta_q^b(\mu)\, b_q(u,v).$$

Let X_N, Y_N are LBB-stable, then

$$d_N(\mathcal{P}) \leqslant C \exp(-cN^{1/Q^b}) \tag{11}$$

And the benchmark? II

Theorem (Binev, Cohen, Dahmen, DeVore, Petrova, Wojtaszczyk 2011)

Let $0 < \gamma \leqslant 1$, $d_0(\mathcal{P}) \leqslant M$. Then

- if $d_N(\mathcal{P}) \leqslant M\, N^{-\alpha}$, $N > 0$, $\alpha > 0$, then

$$\max_{\mu \in \mathcal{P}} \|u_\mu^{\mathcal{N}} - u_\mu^N\|_X \leqslant C\, M\, N^{-\alpha}$$

  with $C := q^{1/2}(4q)^\alpha$, $q := \lceil 2^{\alpha+1}\gamma^{-1}\rceil^2$.

- if $d_N(\mathcal{P}) \leqslant M\, e^{-aN^\alpha}$, $N \geqslant 0$, $M, a, \alpha > 0$, then

$$\max_{\mu \in \mathcal{P}} \|u_\mu^{\mathcal{N}} - u_\mu^N\|_X \leqslant C\, M\, \exp(-cN^\beta)$$

  where $\beta := \frac{\alpha}{\alpha+1}$, $0 \leqslant \theta < 1$, $c := \min\{|\log\theta|, (4q)^{-\alpha}a\}$,
  $C := \max\{e^{cN_0^\beta}, q^{1/2}\}$, $q := \lceil 2\gamma^{-1}\theta^{-1}\rceil^2$, $N_0 := \lceil (8q)^{\alpha+1}\rceil$.

Where do we stand

The RBM works perfectly for

- linear, coercive problems
- affine decomposition
- parabolic problems (using space-time variational form)

But what about...

- transport
- wave
- Schrödinger
- ...

Beyond ’nice’ problems I

Theorem (Ohlberger, Rave, 2016)

For Example (c) – transport – with $\Omega = (0,1)$, $u(0,x;\mu) = 0$, $u(t,0;\mu) = 1$, it holds

$$d_N(\{u(t,\cdot;1) : t \in [0,1]\}) \geqslant \frac{1}{2} N^{-1/2}.$$

Beyond ’nice’ problems II

Theorem (Greif, U., 2019)

For Example (d) – wave – with $\Omega = \mathbb{R}$, $I = \mathbb{R}^+$, $v_0 = 0$ and,

$$u_0(x) := \begin{cases} 1 & x \leqslant 0, \\ -1 & x \geqslant 0, \end{cases}$$

it holds

$$\frac{1}{4} N^{-1/2} \leqslant d_N(\{u_\mu : \mu \in [0,1]\}) \leqslant \frac{1}{2}(N-1)^{-1/2}.$$

Remark Using POD-Greedy and energy-based estimators

for the wave equation yielded $N^{-7/2}$ in experiments.

Beyond ’nice’ problems III

Remark

Both cases admit easy solutions:

(c) transport:

$$u(t, x; \mu) = u_0(x - \mu t) \tag{12}$$

(d) wave (d’Alembert, for $v_0 = 0$):

$$u(t, x; \mu) = \frac{1}{2}\big[u_0(x + \mu t) + u_0(x - \mu t)\big] \tag{13}$$

Next targets:

1) well-posed variational formulations (even with $\beta = 1$)
2) develop efficient numerics
3) Ridge approximations

Ultra-weak formulations I

Reconsider Example (c) – transport

- $L_\mu u = u_t + \mu \nabla u$, $u(0) = 0$ (for simplicity)
- $u(t,x) = 0$, $x \in \Gamma_-$ $\quad \Gamma_\pm := \{x \in \partial\Gamma : 1 \cdot \vec{n} \lessgtr 0\}$
- integrate w.r.t. time & space and do integration by parts ($\Omega_I = I \times \Omega$):

$$(L_\mu u, v)_{L_2(\Omega_I)} = \int_I \int_\Omega L_\mu u(t,x)\, v(t,x)\, dx\, dt$$

$$= (u(T), v(T))_{L_2(\Omega)} - (u(0), v(0))_{L_2(\Omega)} - \int_I \int_\Omega u(t,x)\, v_t(t,x)\, dx\, dt$$

$$-\mu\, (u, \nabla v)_{L_2(\Omega_I)} + \mu \int_I \int_{\Gamma_+} u(s)\, v(s)\, ds\, dt$$

$$= (u, L_\mu^* v)_{L_2(\Omega_I)} \qquad \text{if } v(T) = 0, v(t)_{|\Gamma_+} = 0$$

- where $L_\mu^* v := -L_\mu v = -v_t - \mu \nabla v$

Ultra-weak formulations II

- set $C^1_{T,0} := \{v \in C^1(\Omega_I) : v(T) = 0, v(t)_{|\Gamma_+} = 0 \, \forall t \in I\}$
- $X := L_2(\Omega_I)$, $\Omega_I = I \times \Omega$
- $\|v\|_Y := \|L^*_\mu v\|_{L_2(\Omega_I)}$, $Y := \text{clos}_{\|\cdot\|_Y} C^1_{T,0}$

$$b_\mu(u, v) := (u, L^*_\mu v)_{L_2(\Omega_I)} \tag{14}$$

Lemma

The bilinear form $b_\mu(\cdot, \cdot)$ is bounded and inf-sup-stable with $C = \beta = 1$.

Ultra-weak formulations III

Discretization???

- double greedy (Dahmen, Schwab, Welper)
- alternative (Brunken, Smetana, U.):
  - choose test first: $Y^{\mathcal{N}} \subset Y$, $\dim Y^{\mathcal{N}} = \mathcal{N} < \infty$
  - then, set $X^{\mathcal{N}} := L_\mu^* Y^{\mathcal{N}}$

$$\rightsquigarrow \inf_{u^{\mathcal{N}} \in X^{\mathcal{N}}} \sup_{v^{\mathcal{N}} \in Y^{\mathcal{N}}} \frac{b_\mu(u^{\mathcal{N}}, v^{\mathcal{N}})}{\|u^{\mathcal{N}}\|_X \, \|v^{\mathcal{N}}\|_Y} = 1$$

- example:
  $Y^{\mathcal{N}} = S_{\Delta t, T} \otimes V_{h,\Gamma_+} \subset C^0_{T,0} = \{v \in C^0(\Omega_I) : v(T) = 0, v(t)_{|\Gamma_+} = 0 \, \forall t \in I\}$
  - $S_{\Delta t, T}$: piecewise linear finite elements σ^k with $\sigma^k(T) = 0$
  - V_{h,Γ_+}: piecewise linear finite elements ϕ_i with $\phi_i|_{\Gamma_+} = 0$

Ultra-weak formulations IV

Some issues

- stiffness matrix

$$(B^{\mathcal{N}})_{(k,i),(\ell,j)} = \left(L_\mu^*(\sigma^k \otimes \phi_i), L_\mu^*(\sigma^\ell \otimes \phi_j)\right)_{L_2(\Omega_I)}$$

  leads to

$$B^{\mathcal{N}} = A_{\Delta t} \otimes M_h + \mu(N_{\Delta t} \otimes N_h^T + N_{\Delta t}^T \otimes N_h) + \mu^2 M_{\Delta t} \otimes A_h$$

  - A_*: stiffness matrix
  - M_*: mass matrix
  - N_*: nonsymmetric matrix $(\dot{\sigma}, \tau)$
- inf-sup $= 1$, but $\kappa(B^{\mathcal{N}})$ may be large
- we need efficient numerical solvers (see below)

Ultra-weak formulations V

Reduced Basis Method

- error estimator

$$\Delta_N(\mu) := \|r_\mu^N\|_{(Y^\mathcal{N})'} = \sup_{v^\mathcal{N} \in Y^\mathcal{N}} \frac{f_\mu(v^\mathcal{N}) - (u_\mu^N, L_\mu^* v^\mathcal{N})_{L_2(\Omega_I)}}{\|L_\mu^* v^\mathcal{N}\|_{L_2(\Omega_I)}}$$

- can be computed online efficient
  - since f_μ is affine decomposable
  - if L_μ^* is affine decomposable
  - via Riesz representation
  - square root effect
- Greedy
  - determine $\xi^{(n)} = u_{\mu^{(n)}}^\mathcal{N}$ as before
  - note, that $\xi^{(n)} = L_{\mu^{(n)}}^* \eta^{(n)}$ with $\eta^{(n)} \in Y_N$
  - either build Y_N by $\eta^{(n)}$
  - or use supremizers (also online for new μ)

Ultra-weak formulations VI

Example (d) – wave

- $L_\mu u = u_{tt} - \mu \Delta u$, for simplicity $u(0) = u_t(0) = 0$, $u_{|\partial\Omega} = 0$
- $L_\mu^* = L_\mu$, but with adjoint terminal conditions $u(T) = u_t(T) = 0$
- $C^2_{T,0} := \{v \in C^2(\Omega_I) : v(T) = v_t(T) = 0, v_{|\partial\Omega} = 0\}$
- $X = L_2(\Omega_)$
- $Y = \text{clos}_{\|\cdot\|_Y} C^2_{T,0}$, $\|v\|_Y := \|L_\mu^* v\|_{L_2(\Omega_I)}$
- again $\beta = C = 1$
- $Y \cong H^2(\Omega_I) \cap H^1_0(\Omega_I)$
- same issues as before (Henning, Palitta, Simoncini, U.)

Ultra-weak formulations VII

Remark – Natural regularity

For transport and wave, we have

$$u_0 \in L_2 \text{ and not more } \Rightarrow \quad u(t) \in L_2 \ \forall t \text{ and not more!}$$

$\rightsquigarrow$ ultra-weak seems to be “the right” ansatz for low regularity!

Some numerics I

Example 2: Parabolic

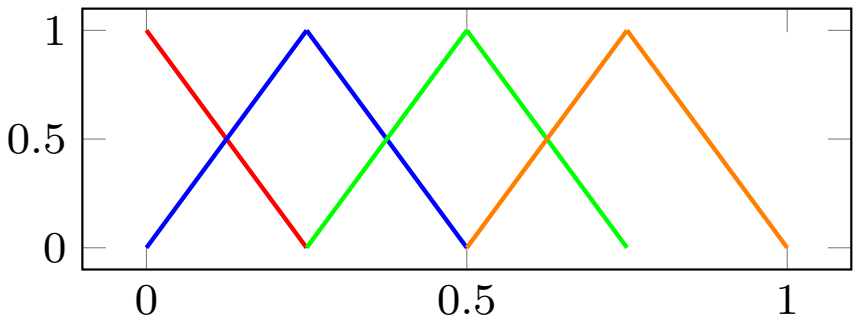
		RKSM				LR-FGMRES+RKSM				CN	
N_h	N_t	Its	μmem	rank(U_δ)	Time (s)	Its	μmem	rank(U_δ)	Time (s)	Direct	Iterative
41300	300	13	14	9	25.96	4	74	10	82.89	123.43	59.10
	500	13	14	9	30.46	4	75	11	83.93	143.71	78.01
	700	13	14	9	28.17	4	86	11	89.99	153.38	93.03
347361	300	14	15	9	820.17	4	78	9	2319.67	14705.10	792.42
	500	14	15	9	828.34	4	80	9	2384.39	15215.47	1041.47
	700	14	15	7	826.93	4	97	9	2327.76	15917.52	1212.57

- RKSM: Rational Krylov Space Method
- LR-FGMRES-RKSM: Low-Rank preconditioned GMRES
- CN: Crank Nicolson

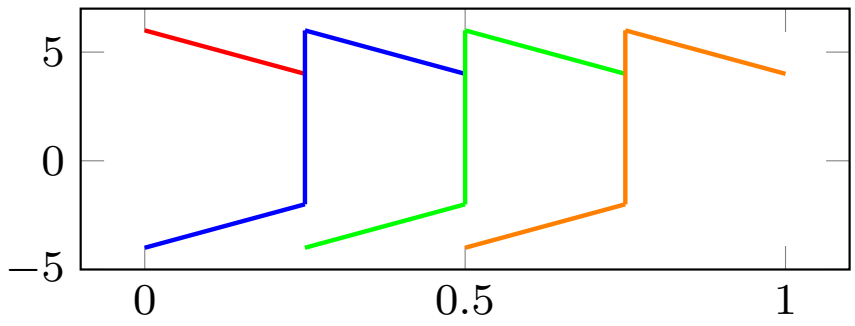
Some numerics II

Example 3: Transport

Basis of $\mathcal{Y}^h$

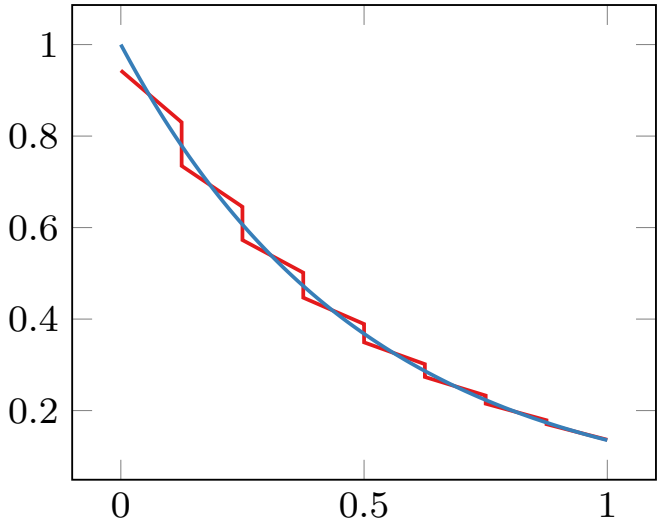


Basis of $\mathcal{X}^h = B^*\mathcal{Y}^h$



Rate of convergence

$1/h$	Linear FE		Quadratic FE	
	L_2-error	rate	L_2-error	rate
4	0.03311	—	0.00247	—
8	0.01664	0.99274	0.00062	1.98932
16	0.00833	0.99817	0.00016	1.99729
32	0.00417	0.99954	3.896e-05	1.99932
64	0.00208	0.99989	9.741e-06	1.99983
128	0.00104	0.99997	2.435e-06	1.99996
256	0.00052	0.99999	6.088e-07	1.99999



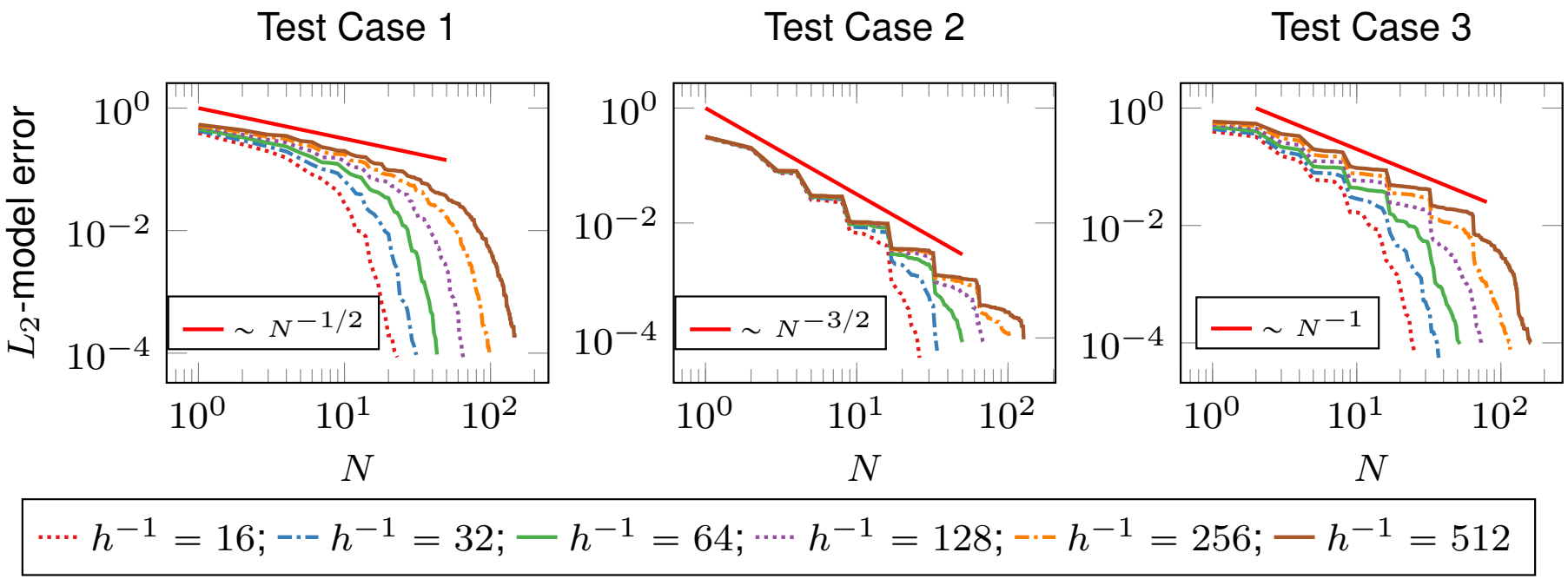
Some numerics III

Model Reduction -1-

	Test Case 1	Test Case 2	Test Case 3
$\vec{b}_\mu$	$(\mu, 1)^T$	$(\cos\mu, \sin\mu)^T$	$(\cos\mu, \sin\mu)^T$
$\mathcal{P}$	$[0.01, 1]$	$[0.2, \frac{\pi}{2} - 0.2]$	$[0.2, \frac{\pi}{2} - 0.2]$
c	$\equiv 0$	$\equiv 1$	$\equiv 1$
f	$\equiv 0$	$\equiv 1$	$\begin{cases} 0.5, & x < y \\ 1, & x \geqslant y \end{cases}$
g	$\begin{cases} 1, & x = 0 \\ 0, & y = 0 \end{cases}$	$\equiv 0$	$\begin{cases} 1 - y, & x \leqslant 0.5 \\ 0, & x \geqslant 0.5 \end{cases}$

Some numerics IV

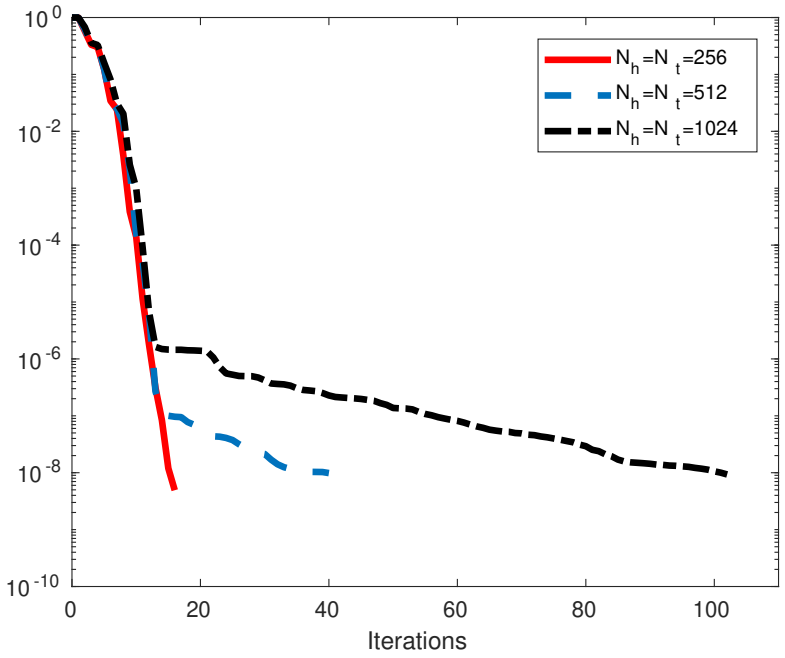
Model Reduction -2-



Some numerics V

Example 4: wave 1d

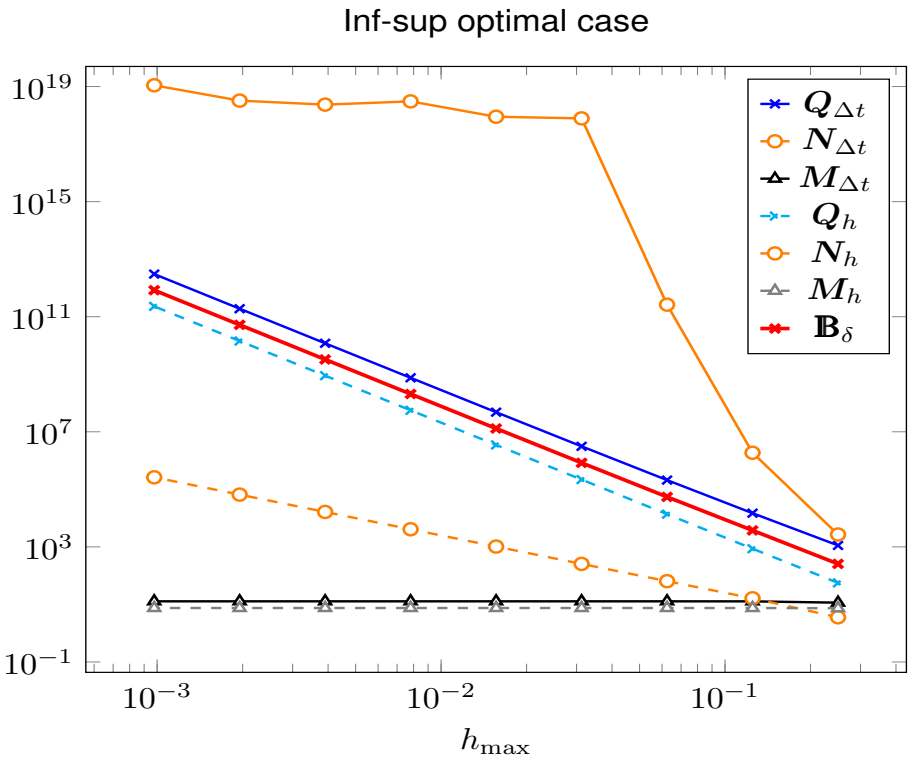
		GMRES+LYAP			backslash
N_h	N_t	Its.	rank(U_δ)	Time (s)	Time (s)
256	256	16	13	0.21	1.17
	512	36	35	1.51	2.39
	1024	81	74	20.97	12.61
512	256	26	31	0.61	2.30
	512	40	43	2.64	5.09
	1024	81	74	20.97	12.61
1024	256	50	59	3.55	4.82
	512	68	72	10.12	11.13
	1024	102	92	54.15	24.28

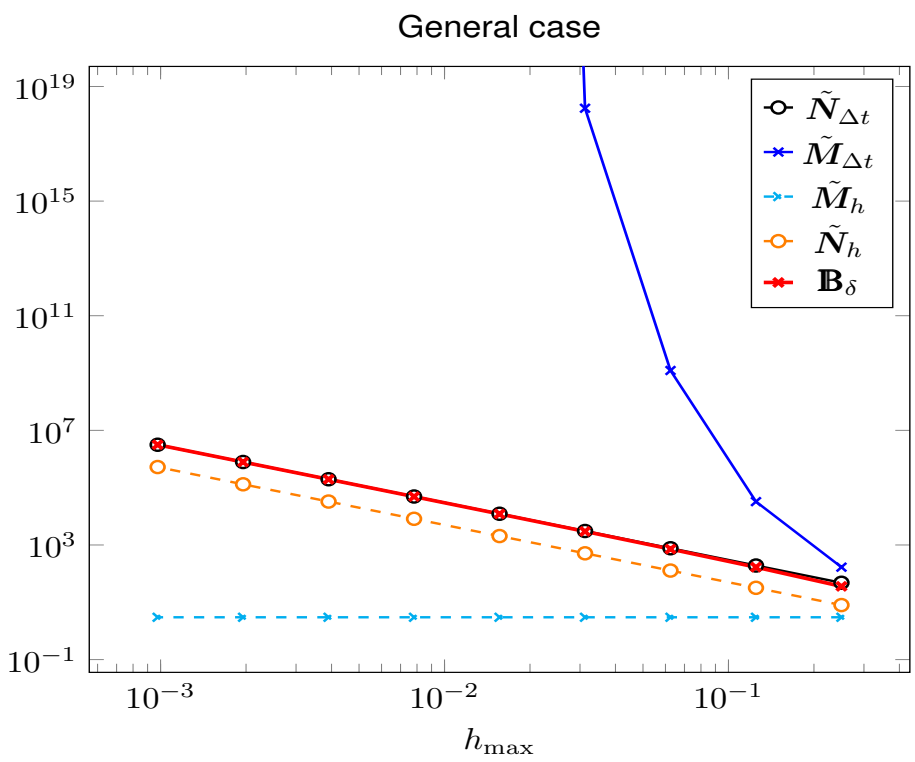


- LYAP: Generalized Lyapunov (i.e., Sylvester) equation solver

Some numerics VI

Condition numbers





$$\mathbb{B}_\delta = \tilde{\boldsymbol{N}}_{\Delta t} \otimes \tilde{\boldsymbol{M}}_h + \tilde{\boldsymbol{M}}_{\Delta t} \otimes \tilde{\boldsymbol{N}}_h, \qquad \text{“general” case,} \tag{15}$$

$$\mathbb{B}_\delta = \boldsymbol{Q}_{\Delta t} \otimes \boldsymbol{M}_h + \boldsymbol{N}_{\Delta t} \otimes \boldsymbol{N}_h^\top + \boldsymbol{N}_{\Delta t}^\top \otimes \boldsymbol{N}_h + \boldsymbol{M}_{\Delta t} \otimes \boldsymbol{Q}_h, \text{“optimal”} \tag{16}$$

Some numerics VII

Example 4: wave 3d

	Case 1	Case 2
$u_0(r)$	$(1 - \frac{5}{\sqrt{2}} r) \cdot \mathbb{1}_{r<\sqrt{2}/5}$	$\mathbb{1}_{r<\sqrt{2}/5}$
u	$\in C(\bar{I} \times \bar{\Omega}) \backslash C^1(I \times \Omega)$	$\notin C(\bar{I} \times \bar{\Omega})$

Case 1: Continuous, but not continuously differentiable: $c = 1$

Refinement		2	3	4	5
Unknowns	Time	4	8	16	32
	Space	64	515	4,096	32,768
Time stepping	Wall time [s]	$1.87 \cdot 10^{-2}$	$2.00 \cdot 10^{-2}$	$6.82 \cdot 10^{-1}$	$8.85 \cdot 10^{0}$
	L_2 error	$4.27 \cdot 10^{-1}$	$7.10 \cdot 10^{-2}$	$2.85 \cdot 10^{-2}$	$1.20 \cdot 10^{-2}$
Space-Time	L_2 error	$5.31 \cdot 10^{-2}$	$4.48 \cdot 10^{-2}$	$3.45 \cdot 10^{-2}$	$2.50 \cdot 10^{-2}$
PCG ($\mathbb{K}_\delta^\top \mathbb{M}_\delta^{-1} \mathbb{K}_\delta$)	Wall time [s]	$9.59 \cdot 10^{-2}$	$9.73 \cdot 10^{-1}$	$2.17 \cdot 10^{1}$	$1.07 \cdot 10^{3}$
	# Iterations	9	7	7	6
PCG (Sylvester)	Wall time [s]	$3.01 \cdot 10^{-3}$	$3.85 \cdot 10^{-2}$	$1.55 \cdot 10^{0}$	$8.57 \cdot 10^{1}$
	# Iterations	9	9	13	17
Galerkin	Wall time [s]	$2.24 \cdot 10^{-1}$	$6.21 \cdot 10^{-1}$	$1.20 \cdot 10^{0}$	$1.61 \cdot 10^{1}$
	# Iterations	2	6	15	24

Some numerics VIII

Case 1: Continuous, but not continuously differentiable: various c

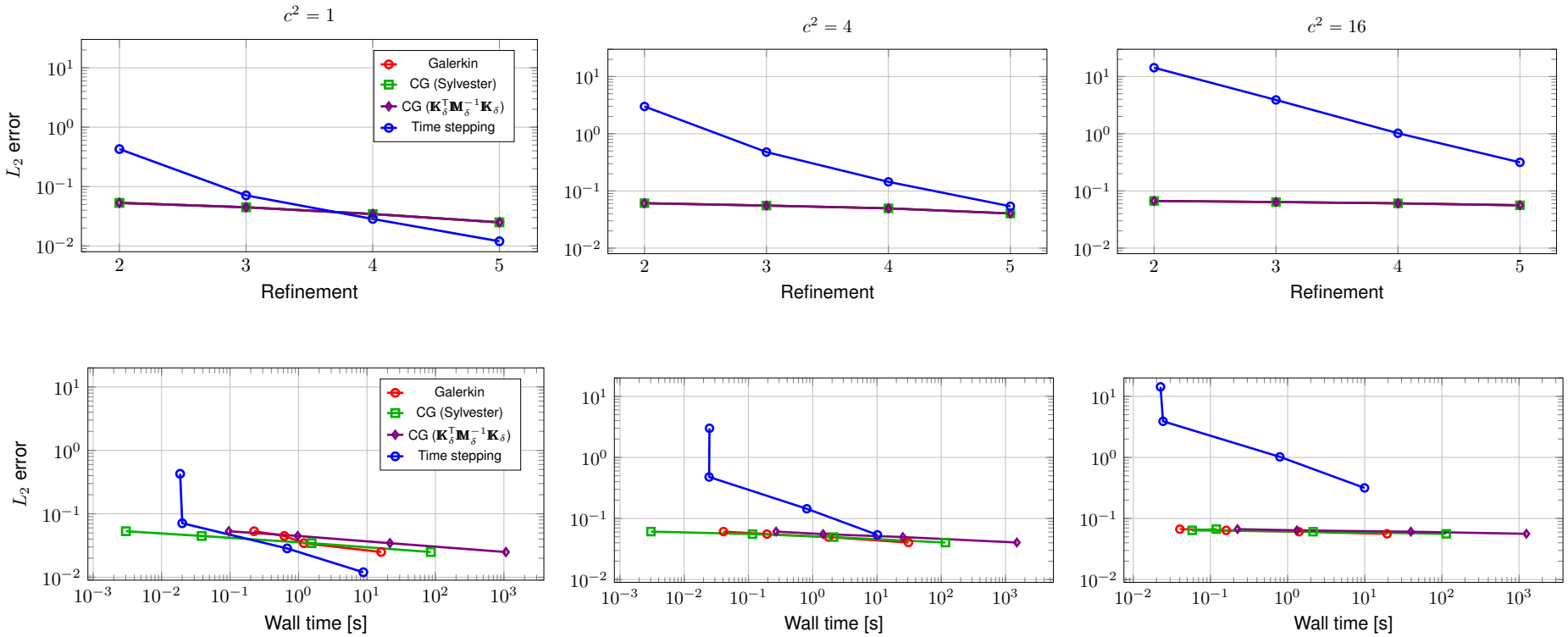


Figure: Case 1: Continuous solution, $c^2 = 1, 4, 16$ (left, center, right).

Some numerics IX

Case 2: Discontinuous

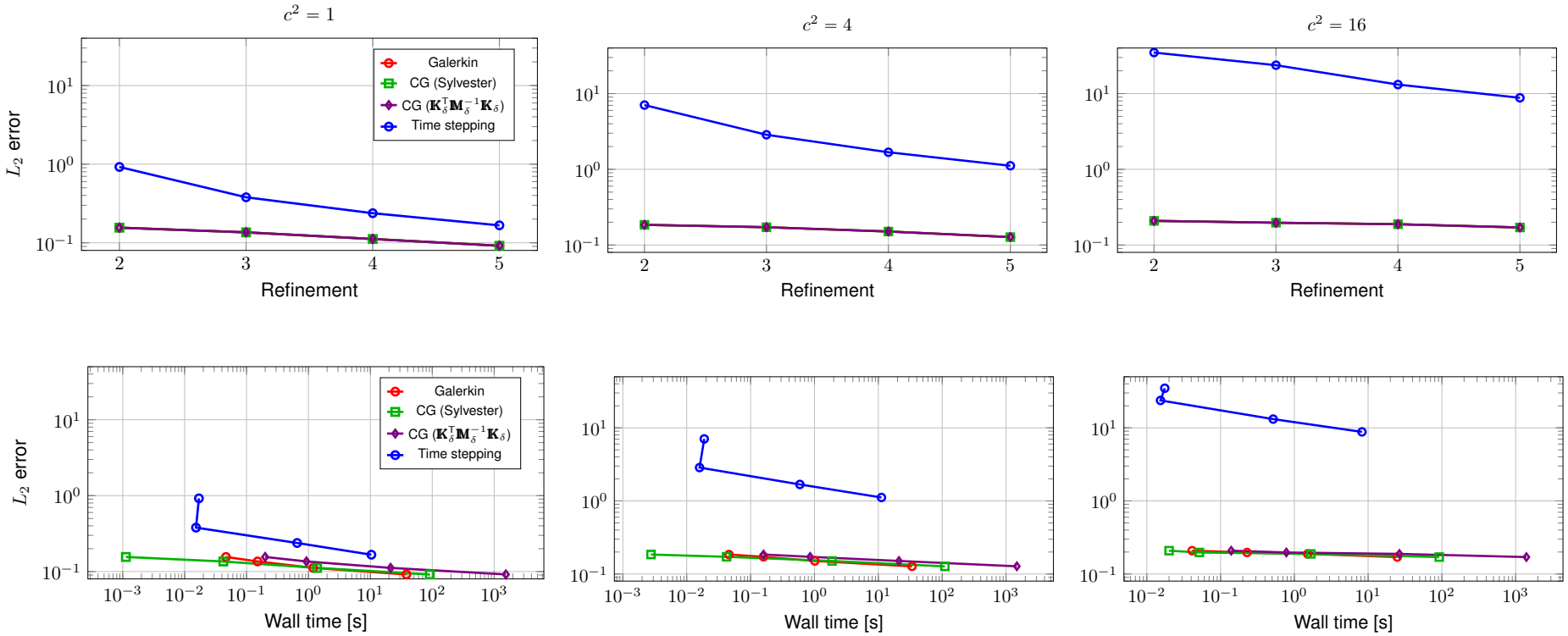


Figure: Case 2: Discontinuous solution, $c^2 = 1, 4, 16$ (left, center, right).

Ridge function approximations I

Example – again

(c) 1d: $u_t(t,x) + \mu u_x(t,x)$, $u(0,x) = u_0(x)$

$$u(t,x;\mu) = u_0(x - \mu t)$$

(d) 1d: $u_{tt(}t,x) - \mu u_{xx}(t,x)$, $u(0,x) = u_0(x)$, $u_t(0,x) = 0$

$$u(t,x;\mu) = \frac{1}{2}\big[u_0(x + \mu t) + u_0(x - \mu t)\big]$$

Ridge function approximations II

Definition – Ridge function

Let $a \in \mathbb{R}^d$, $b \in \mathbb{R}$ and $v : \mathbb{R} \to \mathbb{R}$. Then,

$$w : \Omega \to \mathbb{R}, \qquad w(x) := v(a^\top x + b) \tag{17}$$

is called *ridge function* with *profile* v, *direction* a and *offset* b.

Ridge function approximations III

Definition – Linear/Ridge expansion

Let $M, N \in \mathbb{N}$ and

- $X_N := \mathrm{span}(\Phi_N) \subset L_2(\Omega)$, $\Phi_N := \{\varphi_1, ..., \varphi_N\}$
- $\mathcal{V}_M := \{v_1, ..., v_M\} \subset L_2(\Omega)$ set of profiles

$$U_{N,M} := \left\{ u_\delta(x) = \sum_{i=1}^{N} \alpha_i \, \varphi_i(x) + \sum_{j=1}^{M} c_j \, v_j(a_j^\top x + b_j), \;\; \alpha_i, b_j, c_j \in \mathbb{R}, \; a_j \in \mathbb{R}^d \right\} \tag{18}$$

Some $u_\delta \in U_{N,M}$ is called *Linear/Ridge approximation*

Ridge function approximations IV

Example – again

(c) $u_\mu(t,x) = u_0 x + \mu t) = c_1\, v_1(a_1^T(t,x) + b_1)$, i.e.,

- $c_1 = 1$
- $v_1 = u_0$
- $a_1^T = (-\mu, 1)$
- $b_1 = 0$

d) $u_\mu(t,x) = \frac{1}{2}[u_0(x-\mu t) + u_0(x+\mu t)]$

- $c_1 = c_2 = \frac{1}{2}$
- $v_1 = v_2 = u_0$
- $a_1^T = (-\mu, 1)$, $a_2^T = (\mu, 1)$
- $b_1 = b_2 = 0$

General: dof for $U_{N,M}$: $\alpha_1, ..., \alpha_N \in \mathbb{R}$, $a_1, ..., a_M \in \mathbb{R}^d$, $b_1, ..., b_M \in \mathbb{R}$,

$c_1, ..., c_M \in \mathbb{R}$

$\rightsquigarrow$ total number: $N + M(d+2)$

Ridge function approximations V

Linear/Ridge optimization

Idea:

- given $u \in L_2(\Omega)$, determine

$$u_\delta^* = \arg\min\{\|u - u_\delta\|_0 : u_\delta \in U_{N,M}\} \tag{19}$$

- given $\mu \in \mathcal{P}$, determine

$$u_\delta^*(\mu) = \arg\min\{\|f_\mu - L_\mu u_\delta\|_0 : u_\delta \in U_{N,M}\} \tag{20}$$

Ridge function approximations VI

Lemma

Let $u \in L_2(\Omega)$, Φ_N, $\mathcal{V}_M$ are given.
Set $A := [(\varphi_i, \varphi_j)]_{i,j}$, $B := [\varphi_i, v_j(a_j^T \cdot + b_j)]_{i,j}$,

$C := [v_j(a_j^T \cdot + b_j), v_{j'}(a_{j'}^T \cdot + b_{j'})]_{j,j'}$.
Then, α and c are given by

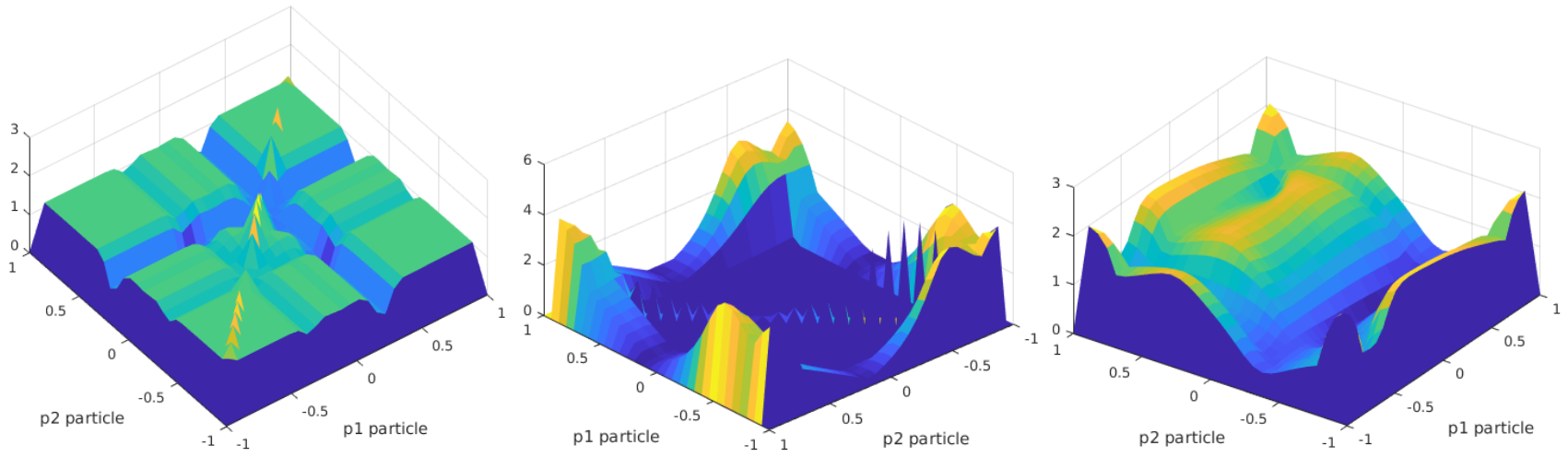
$$\begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \begin{pmatrix} \alpha \\ c \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

$\rightsquigarrow$ (19) reduces to an optimization problem in $\mathbb{R}^{(d+1)M}$

Ridge function approximations VII

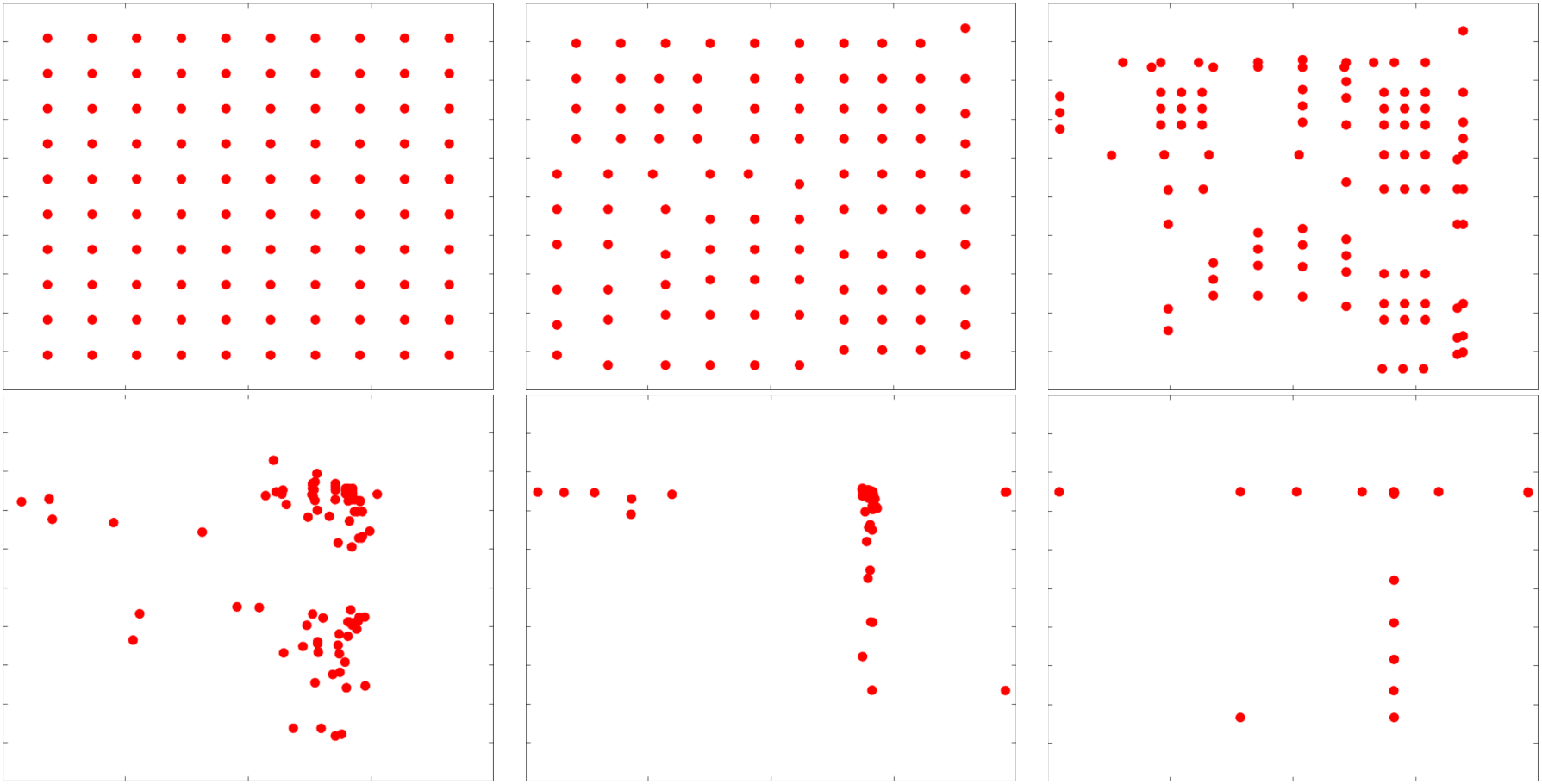
Optimization problem

Case	$u(x_1, x_2)$	$v_1(\xi)$	$v_2(\xi)$
1	$1.6\,\cos(10x_1 + \frac{10}{3}x_2) + 0.8\,\cos(10x_1 - 5x_2)$	$\cos(10\xi)$	$\cos(10\xi)$
2	$\cos(x_1 + 2x_2) + \cos(x_1 - 0.5\,x_2)$	$\cos(\xi)$	$\cos(\xi)$
3	$5\,\lvert x_1 - \frac{1}{2}x_2 - \frac{1}{2}\rvert + 0.6\,(x_1 + \frac{1}{3}x_2)^2$	$\lvert\xi - \frac{1}{2}\rvert$	ξ^2



Ridge function approximations VIII

A particle-grid algorithm



Ridge function approximations IX

A particle grid algorithm

- associate directions/offsets to *particles*
- in dimension $(d+1)M$
- map to $(-1,1)^{(d+1)M}$
- arrange in a grid
- use particle swarm methodology on that grid

Ridge function approximations X

Case	PPDE	parameter μ	no. iterat. K	L_2-error
1	Thermal block	$(0.1, 10, 1, 0.6)$	1	$5.1019e-15$
1	Thermal block	$(10, 2, 0.1, 0.5)$	1	$1.4446e-14$
1	Thermal block	$(0.4, 2, 0.3, 5)$	1	$6.0861e-15$
2	Transport	$1/4$	12	$7.1348e-05$
2	Transport	$1/4$	66	$4.6205e-16$
2	Transport	1	19	$3.0119e-05$
2	Transport	1	70	$9.3829e-17$
2	Transport	4	24	$6.1985e-05$
2	Transport	4	67	0
3	Wave	$1/4$	20	$7.6682e-05$
3	Wave	$1/4$	83	$8.9850e-16$
3	Wave	1	21	$8.2400e-05$
3	Wave	1	86	$3.1765e-16$
3	Wave	4	28	$4.3012e-05$
3	Wave	4	83	$8.9850e-16$

Ridge function approximations XI

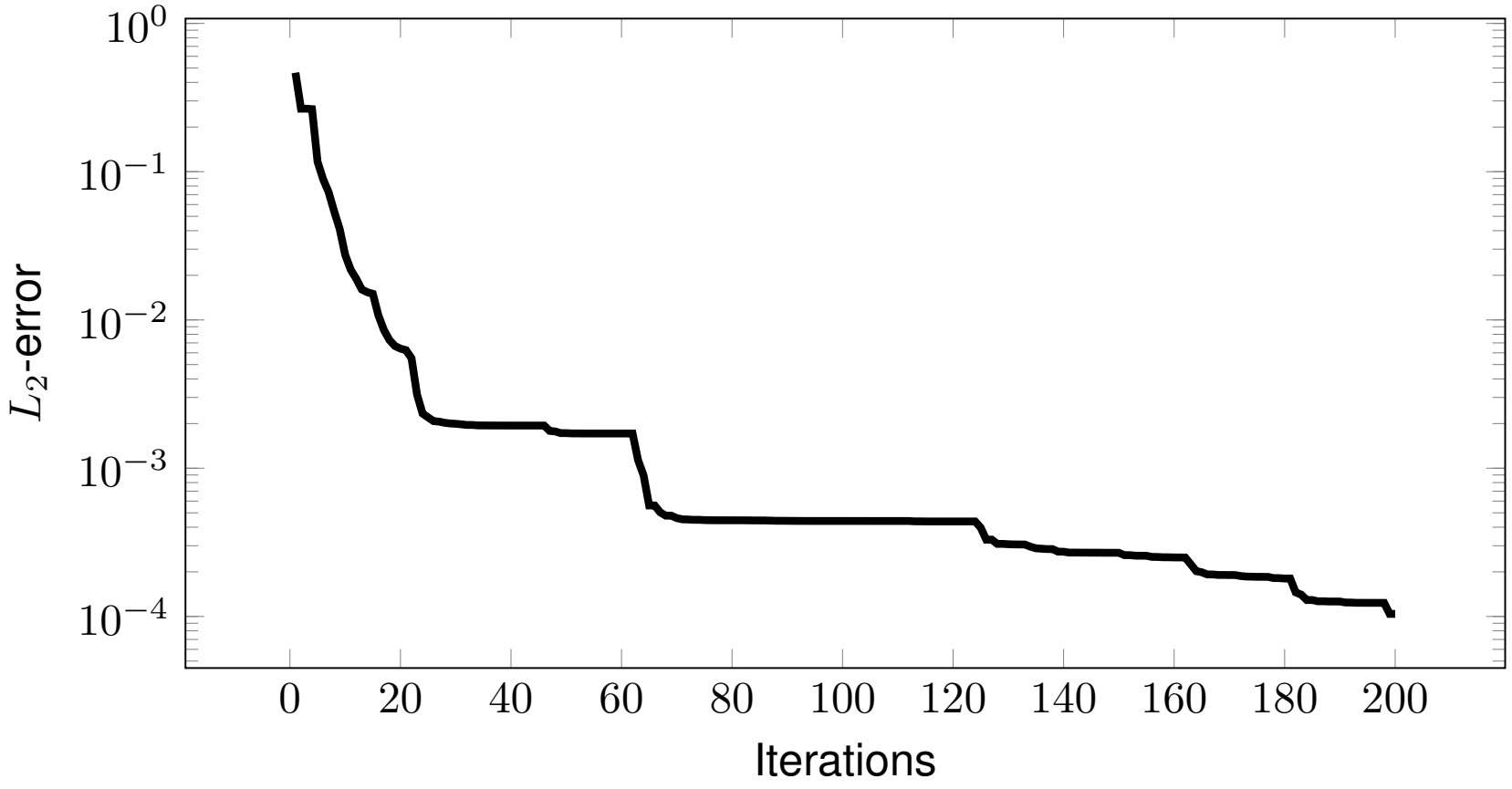


Figure: 3d planar wave.

Summary

The Reduced Basis Method – a short introduction

- The thermal block
- RBM in a nutshell
- Why does that work?

Beyond coercivity – inf-sup-stable problems

- Variational formulations
- Petrov–Galerkin methods
- The RBM revisited
- And the benchmark?

Beyond “nice” problems – transport and wave equation

- The Kolmogorov N-width
- Ultra-weak formulations
- Some numerics
- Ridge function approximations