RBM for linear evolution equations and inverse problems

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Joint work with Bernard Haasdonk and Bastian von Harrach

RBM summer school 2013
Kopp, Germany, August 20-23, 2013.

RBM for linear evolution equations

Motivation

- Parabolic parametrized partial differential equation of the form

$$\partial_t u(\mathbf{x}, t; \mu) + \mathcal{L}u(\mathbf{x}, t; \mu) = f, \tag{1a}$$

$$u(\mathbf{x}, 0; \mu) = u_0, \tag{1b}$$

- Solution of (1) for many different parameters in a small amount of time (i.e. design optimization, optimal control, online-simulation, financial markets)
- Computation of a detailed solution (i.e. FEM, FV, FD) is rather expensive

$\rightsquigarrow$ **model order reduction**

The detailed (semi-discretized) evolution problem

Let $X \subset Y := L^2(\Omega)$ be a Hilbert space and $\mu \in \mathcal{P} \subset \mathbb{R}^p$. We want the solution sequence $u = \left(u^k\right)_{k=0}^{M} \in (X)^{M+1}$ of the **detailed evolution scheme**

$$u^0 = P_X(u_0) \tag{2a}$$

$$\mathfrak{L}^I(\mu, t^k)u^{k+1} = \mathfrak{L}^E(\mu, t^k)u^k + b(\mu, t^k) \tag{2b}$$

$$s^k(\mu) = l(u^k, \mu), \tag{2c}$$

with $\mathfrak{L}^I, \mathfrak{L}^E \in L(X)$, $P_X : Y \to X$ the continuous projection, $l : X \times \mathcal{P} \to \mathbb{R}$ a linear and continuous functional, $u_0 \in Y$ the initial values and $b \in X$ the inhomogeniety, so that

$$u^k(x;\mu) \approx u(x, t^k; \mu),\ k = 0, \ldots, M.$$

The reduced (semi-discretized) evolution problem

Let a problem (2) be given. Let $X_N \subset X$ be a reduced basis space, $\mu \in \mathcal{P}$. We want the solution sequence $u_N = \left(u_N^k\right)_{k=0}^M \in (X_N)^{M+1}$ of the **reduced evolution scheme**

$$u_N^0 = P_{X_N}(P_X(u_0)) \tag{3a}$$

$$\mathfrak{L}_N^I(\mu, t^k)u_N^{k+1} = \mathfrak{L}_N^E(\mu, t^k)u_N^k + b_N(\mu, t^k) \tag{3b}$$

$$s_N^k(\mu) = l(u_N^k, \mu), \tag{3c}$$

with $P_{X_N} : X \to X_N$ the orthogonal projection related to the scalar product $\langle \cdot, \cdot \rangle_X$ and with the operators

$$\mathfrak{L}_N^I := P_{X_N} \circ \mathfrak{L}^I$$

$$\mathfrak{L}_N^E := P_{X_N} \circ \mathfrak{L}^E$$

$$b_N := P_{X_N}(b).$$

A-posteriori error estimator

Definition of the residual

$$R^k := \frac{1}{\Delta t}\left(\mathfrak{L}^E u_N^{k-1} - \mathfrak{L}^I u_N^k + b\right) \in X$$

Let u and u_N be solutions of (2) and (3), then the error $e^k := \|u^k - u_N^k\|_X$ is bounded by

$$\|u^k - u_N^k\|_X \leq \Delta_N(\mu, t^k)$$

with

$$\Delta_N(\mu, t^k) := \sum_{i=1}^{k} \left(\frac{\gamma^E}{\alpha^I}\right)^{k-i} \frac{\Delta t}{\alpha^I} \|R^i\|_X + \left(\frac{\gamma^E}{\alpha^I}\right)^{k} \|e^0\|.$$

Offline/online decomposition?

$\rightsquigarrow$ is possible!

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Regarding the reduced space X_N

- $u^{k+1}(\mu)$ depends on $u^k(\mu)$
- $u^M(\mu) \in X_N$ not sufficiet for $u_N^M(\mu) = u^M(\mu)$. Whole trajectory has to be well approximated

Idea of the POD-Greedy-procedure

$$X_N := \underset{\substack{Y \subset X \\ \dim Y = N}}{\arg\min} \max_{\mu \in P_{train}} \frac{1}{M+1} \sum_{k=0}^{M} \|u^k(\mu) - P_Y u^k(\mu)\|^2$$

POD-Greedy-procedure

Let $P_{train} \subset \mathcal{P}$ be finite, $\varepsilon_{tol} > 0$, $\Delta(\mu, X_N)$ a suitable error indicator, $\Phi_{N_0} \subset X$ initial RB an ONB with $N_0 := |\Phi_{N_0}|$:

- **input**: Φ_{N_0}, N_0
- $N := N_0$, $\Phi_N := \Phi_{N_0}$, $X_N := \mathrm{span}\{\Phi_N\}$
- **while** $\max\limits_{\mu \in P_{train}} \Delta(\mu, X_N) > \varepsilon_{tol}$ **compute**
  - $\mu_{N+1} := \arg\max\limits_{\mu \in P_{train}} \Delta(\mu, X_N)$
  - $\{u^k(\mu_{N+1})\}_{k=0}^{M}$
  - $e_{N+1}^k := u^k(\mu_{N+1}) - P_{X_N} u^k(\mu_{N+1}),\ k = 0, \ldots, M$
  - $\varphi_{N+1} := \arg\min\limits_{\substack{\varphi \in X \\ \|\varphi\| = 1}} \sum_{k=0}^{M} \|e_{N+1}^k - \langle \varphi, e_{N+1}^k \rangle \varphi\|^2$
  - $\Phi_{N+1} := \Phi_N \cup \{\varphi_{N+1}\}$, $X_{N+1} := \mathrm{span}\{\Phi_{N+1}\}$, $N := N + 1$

Evolution scheme in space-time (via PG)

Let X be a Hilbert space (HS) and $X_N \subset X$ be a RB-space. Then $\tilde{X} := (X)^{M+1}$ is a HS with $\tilde{X}_N := (X_N)^{M+1} \subset \tilde{X}$ the corresponding RB-space. We define

$$a(u, v; \mu) := \sum_{k=0}^{M-1} \langle \mathfrak{L}^I(\mu, t^k) u^{k+1} - \mathfrak{L}^E(\mu, t^k) u^k, v^{k+1} \rangle_X + \langle u^0, v^0 \rangle_X$$

$$f(v; \mu) := \sum_{k=0}^{M-1} \langle b(\mu, t^k), v^{k+1} \rangle_X + \langle P_X u_0(\mu), v^0 \rangle_X .$$

If a and f are continuous

$$(2) \iff \text{find } u(\mu) \in \tilde{X} : a(u(\mu), v; \mu) = f(v; \mu), \quad v \in \tilde{X}$$

$$(3) \iff \text{find } u_N(\mu) \in \tilde{X}_N : a(u_N(\mu), v; \mu) = f(v; \mu), \quad v \in \tilde{X}_N$$

Definition: primal/dual detailed model

Let $\tilde{X}$ be a HS, $\mathcal{P} \subset \mathbb{R}^p$, a a suitable bilinearform and $f, \tilde{l}$ suitable linearforms. We define the primal detailed solution $u^{pr}(\mu) \in \tilde{X}$ through

$$a(u^{pr}(\mu), v; \mu) = f(v; \mu), \qquad \forall v \in \tilde{X} \tag{4}$$

and the dual detailed solution $u^{du}(\mu) \in \tilde{X}$ through

$$a(v, u^{du}(\mu); \mu) = -\tilde{l}(v; \mu), \qquad \forall v \in \tilde{X}. \tag{5}$$

The output is defined through

$$s(\mu) = \tilde{l}(u^{pr}(\mu); \mu). \tag{6}$$

Definition: primal/dual reduced model

Let $X_N^{pr}, X_N^{du} \subset X$ be two RB-spaces. Then $\tilde{X}_N^{pr} := \left(X_N^{pr}\right)^{M+1}$, $\tilde{X}_N^{du} := \left(X_N^{du}\right)^{M+1}$ are two RB-spaces with dimension $N^{pr}, N^{du} \in \mathbb{N}$. Given $\mu \in \mathcal{P}$ we define the primal reduced solution $u_N^{pr}(\mu) \in \tilde{X}_N^{pr}$ through

$$a(u_N^{pr}(\mu), v; \mu) = f(v; \mu), \qquad \forall v \in \tilde{X}_N^{pr}, \tag{7}$$

the dual reduced solution $u_N^{du}(\mu) \in \tilde{X}_N^{du}$ through

$$a(v, u_N^{du}(\mu); \mu) = -\tilde{l}(v; \mu), \qquad \forall v \in \tilde{X}_N^{du}, \tag{8}$$

and the improved reduced output $s_N^*(\mu) \in \mathbb{R}$ through

$$s_N^*(\mu) = \tilde{l}(u_N^{pr}(\mu)) - r^{pr}(u_N^{du}(\mu); \mu). \tag{9}$$

Further steps I

Using the space-time BLF and linearform in (5) and assuming $\tilde{l}(u;\mu) = l(u^M;\mu)$ yields the **dual detailed evolution scheme**

$$u^{du,M} = -\left(\mathfrak{L}^{du,I}(\mu, t^k)\right)^{-1} v_l \tag{10a}$$

$$\mathfrak{L}^{du,I}(\mu, t^k)u^{du,k} = \mathfrak{L}^{du,E}(\mu, t^k)u^{du,k+1}, \; k = 1, \dots, M-1 \tag{10b}$$

$$u^{du,0} = \mathfrak{L}^{du,E}(\mu, t^k)u^{du,1} \tag{10c}$$

with $\mathfrak{L}^{du,I} = \left(\mathfrak{L}^I\right)^\dagger$, $\mathfrak{L}^{du,E} = \left(\mathfrak{L}^E\right)^\dagger$ and v_l the riesz-representant of l.

Further steps II

The same can be done for the reduced case in (8) yielding the **dual reduced evolution scheme**

$$u_N^{du,M} = -\left(\mathfrak{L}_N^{du,I}(\mu, t^k)\right)^{-1} v_{N,I} \tag{11a}$$

$$\mathfrak{L}_N^{du,I}(\mu, t^k) u_N^{du,k} = \mathfrak{L}_N^{du,E}(\mu, t^k) u_N^{du,k+1}, \; k = 1, \dots, M-1 \tag{11b}$$

$$u_N^{du,0} = \mathfrak{L}_N^{du,E}(\mu, t^k) u_N^{du,1} \tag{11c}$$

with the dual residual

$$R^{du,k} := \frac{1}{\Delta t} \begin{cases} -\mathfrak{L}^{du,I} u_N^{du,k} + \mathfrak{L}^{du,E} u_N^{du,k+1}, & k = 1, \dots, M-1 \\ -u_N^{du,0} + \mathfrak{L}^{du,E} u_N^{du,1}, & k = 0 \end{cases} .$$

Further steps III

The typical error estimators hold:

$$\|e^{pr}(\mu)\| \leq \Delta_N^{pr,*}(\mu) := \frac{\|v_r^{pr}(\mu)\|}{\tilde{\alpha}_{LB}(\mu)}$$

$$\|e^{du}(\mu)\| \leq \Delta_N^{du,*}(\mu) := \frac{\|v_r^{du}(\mu)\|}{\tilde{\alpha}_{LB}(\mu)}$$

$$|s(\mu) - s_N^*(\mu)| \leq \Delta_N^{s,*}(\mu) := \frac{\|v_r^{pr}\| \, \|v_r^{du}\|}{\tilde{\alpha}_{LB}(\mu)}$$

Offline/online-decompositions for $s_N^*(\mu)$, $\Delta_N^{pr,*}$ and $\Delta_N^{du,*}$ possible.

Application - The Black-Scholes-Equation

Pricing of a vanilla European put option, i.e. searching the solution $P(S_1, S_2, t, \mu)$ of the parametrized parabolic PDE

$$\frac{\partial P}{\partial t} - \frac{1}{2}\sum_{k,l=1}^{2} \Xi(k,l) S_k S_l \frac{\partial^2 P}{\partial S_k \partial S_l} - \sum_{k=1}^{2} r S_k \frac{\partial P}{\partial S_k} + rP = 0$$

with the parameter matrix

$$\Xi = \begin{pmatrix} \sigma_1^2 & \frac{2\rho}{1+\rho^2}\sigma_1\sigma_2 \\ \frac{2\rho}{1+\rho^2}\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

and the parameter vector $\mu = (r,\, \rho,\, \sigma_1,\, \sigma_2)$.

Numerical results - error estimator

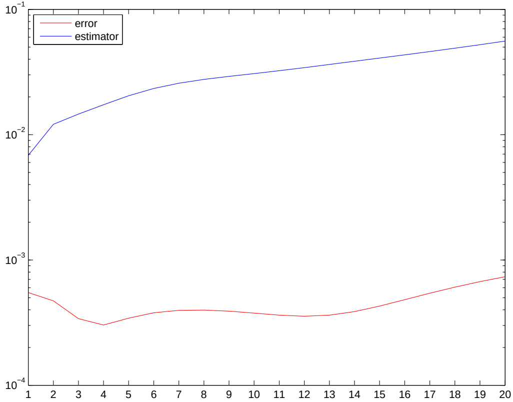

Figure: Sequences of the error $e^k := \|u^k - u_N^k\|_X$ (red) and the error estimator $\Delta_N(\mu, t^k)$ (blue) over the time steps t^k for a reduced basis with 200 basis vectors and $\mu = (0.05, 0.4, 2, 0.5)$.

Numerical results - dual problem improvements

functional l	$\frac{1}{\lvert G_0 \rvert} \sum_{x_{ij} \in G_0} P_{i,j}^k$	$\frac{1}{\lvert G_0 \rvert} \sum_{x_{ij} \in G_0} \frac{P_{i+1,j}^k - P_{i-1,j}^k}{2h_1}$
$s^{20}(\mu)$	13.8331045579815	-0.248507988692125
$s_N^{20}(\mu)$	13.8324367556314	-0.248461984173756
$s_N^*(\mu)$	13.8324367558403	-0.248461984698320
Δ_N^s	$2.975 \cdot 10^4$	$2.661 \cdot 10^4$
$\Delta_N^{s,*}$	0.062	0.018

Table: Table including detailed output $s^{20}(\mu)$, reduced output $s_N^{20}(\mu)$, reduced improved output $s_N^*(\mu)$ and the difference between the output error estimator Δ_N^s and improved output error estimator $\Delta_N^{s,*}$ for various output functionals and $\mu = (0.05, 0.4, 2, 0.5)$.

Conclusion

- Presented a complete reduced basis method for linear evolution equations
- Extended the method with a dual problem resulting in an improved reduced output and improved output error estimator (shown by numerical results)
- Implementet in RBmatlab

RBM for inverse problems

Model problem

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

$$\operatorname{div}(\sigma \nabla u) = 1, \quad \text{in } \Omega, \tag{12}$$

with $\sigma \in L_+^\infty(\Omega)$, $\Omega = [0,1]^2$.

Forward problem

$F : \mathcal{D}(F) = L_+^\infty \subset L^2(\Omega) \to H_0^1(\Omega)$ the non-linear forward-operator maps a parameter $\sigma \in L_+^\infty(\Omega)$ to a solution u of (12):

$$F(\sigma) = u.$$

Inverse problem

For a given $u \in H_0^1(\Omega)$ find the corresponding $\sigma \in L_+^\infty(\Omega) \subset L^2(\Omega)$ with $F(\sigma) = u$.

How to tackle inverse problems

General motivation

- Inverse problem is ill-posed (i.e. F^{-1} is discontinuous)
- Only noisy data u^δ with $\|u - u^\delta\|_{H^1} < \delta$ given
- $\Rightarrow F^{-1}(u^\delta) \nrightarrow F^{-1}(u)$ for $\delta \to 0$
- Replace F^{-1} by continuous approximations R_α
  Aim: $R_{\alpha(\delta,u^\delta)} u^\delta \to F^{-1}(u)$ for $\delta \to 0$

[1] see A.Rieder: Keine Probleme mit Inversen Problemen

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Other approach[1]

- To numerically solve the inverse problem consider $\sigma_{n+1}^\delta = \sigma_n^\delta + s_n^\delta$ with a starting value $\sigma_0^\delta \in \mathcal{D}(F)$
- Try to approximate $s_n^e := \sigma^+ - \sigma_n^\delta$ with s_n^δ, where σ^+ is a solution

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REGINN(REGularisation based on INexact Newtoniteration)

REGINN$(\sigma, \tau, \{t_i\}, \{\Theta_n\})$

$n := 0,\ \sigma_0^\delta := \sigma;$

while $\|F(\sigma_n^\delta) - u^\delta\|_{H^1} > \tau\delta$ do

$\{ \quad i = 0;$

repeat

$i := i + 1;$

$s_{n,i} := \left(F'(\sigma_n^\delta)^* F'(\sigma_n^\delta) + t_i I\right)^{-1} F'(\sigma_n^\delta)^* (u^\delta - F(\sigma_n^\delta));$

until $\|F'(\sigma_n^\delta) s_{n,i} + F(\sigma_n^\delta) - u^\delta\|_{H^1} < \Theta_n \|F(\sigma_n^\delta) - u^\delta\|_{H^1};$

$\sigma_{n+1}^\delta := \sigma_n^\delta + s_{n,i};$

$n := n + 1;$

$\};$

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$\sigma_{n+1}^\delta := \sigma_n^\delta + s_{n,i}$;

$n := n + 1$;

};

$\sigma := \sigma_n^\delta$;

Outlook

- First numerical results
  - Comparison REGINN with RB vs. without RB
  - Model problem too simple?
  - More sophisticated algorithm/RB-space construction?
- How to treat a continuous parameter $\sigma \in L^\infty_+$ theoretically and numerically

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Thanks for your attention!