The Reduced Basis Method: Basic Ideas, Applications and Implementation Aspects

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1 Overview over the Reduced Basis Method
   - Fields of Application and Aim

2 Reduced Basis Method for Linear Evolution Problems
   - Problem and Discretization
   - Numerical Scheme
   - Reduced Basis Method
   - Offline/Online-Decomposition
   - Selection of the Reduced Basis Functions

3 Implementation Aspects
   - Implementation concept
   - Numerical results

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Summary

Aim: Separate solution of parametrized partial differential equations into offline and online phase where

- **Offline phase:** slow, high-dimensional function spaces, FV, FE
- **Online phase:** quick, low-dimensional function spaces

\[ \{ U_{\mu}^k | \mu \in \mathcal{P}, 0 \leq k \leq K \} \]
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\[ \mathcal{W}_H \]

\[ \{ U^k_H(\mu) | \mu \in \mathcal{P}, 0 \leq k \leq K \} \]

\[ \mathcal{W}_N \]
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- online simulation
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Problem and Discretization

Parametrized Linear Evolution Equation

Let $\mu \in \mathcal{P} \subset \mathbb{R}^p$, $t \in [0, T]$. Where are then looking for $u(\cdot, t; \mu) \in \mathcal{W} \subset L^2(\Omega)$, s.t.

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

with given initial data and boundary conditions.
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Discretization

- Time discretization: $0 < t^0 < \cdots < t^K = T$
- Approximate $\mathcal{W}$ by $H$-dimensional space $\mathcal{W}_H \subset L^2(\Omega)$
- Assumption: explicit discretization of spatial operator: 
  $\mathcal{L}_E^k(\mu) = \mathcal{L}_E(\mu, t^k) : \mathcal{W}_H \rightarrow \mathcal{W}_H$
- We are looking for $u^k_H(\mu) \in \mathcal{W}_H$ for all $t^k$. 
Example: Finite Volume Scheme

Using the time discretization we get:

\[
\frac{1}{\Delta t^k} \left( u^{k+1}(\mu) - u^k(\mu) \right) + \mathcal{L}_E(\mu, t^k)[u^k(\mu)] = 0,
\]
Example: Finite Volume Scheme

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\]

where \( \mathcal{L}_E^k(\mu)[u] = \mathcal{L}_E^k(\mu)[u] + b^k(\mu) \) and \( b^k \) comprises the boundary values.
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\[
\frac{1}{\Delta t^k} \left( u^{k+1}(\mu) - u^k(\mu) \right) + \mathcal{L}_E(\mu, t^k)[u^k(\mu)] = 0,
\]

where \( \mathcal{L}_E^k(\mu)[u] = \overline{\mathcal{L}}_E^k(\mu)[u] + b^k(\mu) \) and \( b^k \) comprises the boundary values.

Now let

\[
\mathcal{L}_E^k(\mu)[u] := u - \Delta t^k \overline{\mathcal{L}}_E^k(\mu)[u],
\]

we then get the scheme

\[
\begin{align*}
    u^0 &:= P[u_0(\cdot; \mu)] \\
    u^{k+1} &= \mathcal{L}_E^k(\mu)[u^k] + \Delta t^k b^k(\mu).
\end{align*}
\]
Let $S \subset \mathcal{P}$ be a finite sample of parameters.

Let $\mathcal{W}_N \subset \text{span}\{u_H(\cdot, t_n^k; \mu_n) \mid (\mu_n, t_n^k) \in S \times \{t^k\}_{k=0}^K\}$, the reduced basis space. ($\mathcal{W}_N \subset \mathcal{W}_H$ $N$-dimensional)

Let $\Phi_N := \{\varphi_n\}_{n=1}^N$ be an orthonormalized basis of $\mathcal{W}_N$, the reduced basis.
The Reduced Basis Space

1. Let $S \subset P$ be a finite sample of parameters.
2. Let $\mathcal{W}_N \subset \text{span} \left\{ u_H(\cdot, t_n^k; \mu_n) \mid (\mu_n, t_n^k) \in S \times \{t^k\}_{k=0}^K \right\}$, the reduced basis space. ($\mathcal{W}_N \subset \mathcal{W}_H$ $N$-dimensional)
3. Let $\Phi_N := \{\varphi_n\}_{n=1}^N$ be an orthonormalized basis of $\mathcal{W}_N$, the reduced basis.

Dimension Reduction

Galerkin-project the problem onto the reduced space: Look for $\{u^k_N(\mu)\}_{k=0}^K$, such that for all $\varphi \in \mathcal{W}_N$, $k = 0, \ldots, K - 1$ holds

$$\int_\Omega \left( u^0_N - P[u_0(\cdot; \mu)] \right) \varphi = 0$$

$$\int_\Omega \left( u^{k+1}_N - L_E[u^k_N] - \Delta t^k b^k \right) \varphi = 0.$$
RB Approximation Scheme

Expanding the solution as $u_N^k(\mu) = \sum_{i=0}^{N} a_i^k \varphi_i$, where $a^k = (a_i^k)_{i=1}^{N} \in \mathbb{R}^N$, we get the RB-approximation scheme

$$a_0^n := \int_{\Omega} P[u_0(\mu)] \varphi_n$$

$$a^{k+1} = L_k^E(\mu) a^k + \Delta t^k b^k(\mu),$$
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\begin{align*}
a^0_n &:= \int_{\Omega} P[u_0(\mu)]\varphi_n \\
a^{k+1} &:= L^k_E(\mu)a^k + \Delta t^k b^k(\mu),
\end{align*}
\]

where

\[
\begin{align*}
(L^k_E(\mu))_{mn} &:= \int_{\Omega} \varphi_m L^k_E(\mu)[\varphi_n] \\
(b^k)_n &:= \int_{\Omega} b^k(\mu)\varphi_n.
\end{align*}
\]
Expanding the solution as $u_N^k(\mu) = \sum_{i=0}^{N} a_i^k \varphi_i$, where $a^k = (a_i^k)_{i=1}^{N} \in \mathbb{R}^N$, we get the RB-approximation scheme

$$a_0^n := \int_{\Omega} P[u_0(\mu)] \varphi_n$$

$$a^{k+1} = L_E^k(\mu) a^k + \Delta t^k b^k(\mu),$$

where

$$(L_E^k(\mu))_{mn} := \int_{\Omega} \varphi_m L_E^k(\mu)[\varphi_n]$$

$$(b^k)_n := \int_{\Omega} b^k(\mu) \varphi_n.$$
Affine Parameter Dependence

Assumption: Operators can be written as a linear combination of \textit{parameter dependent} and \textit{parameter independent} parts:

\[
L_E^k(\mu)[u] = \sum_{q=0}^{Q_{L_E}} L_{E}^{k,q}[u] \cdot \sigma_{E}^{q}(\mu)
\]

\[
b^{k}(x, \mu) = \sum_{q=0}^{Q_{b}} b^{k,q}(x) \cdot \sigma_{b}^{q}(\mu)
\]

\[
P[u_0(\mu)] = \sum_{q=0}^{Q_{P}} P^{q}[u_0] \cdot \sigma_{P}^{q}(\mu)
\]
Affine Parameter Dependence

Assumption: Operators can be written as a linear combination of parameter dependent and parameter independent parts:

\[
L^k_E(\mu)[u] = \sum_{q=0}^{Q_L} L^k_q[U] \cdot \sigma^q_E(\mu) \quad \rightarrow \quad L^k_E(\mu) = \sum_{q=0}^{Q_L} L^k_q \sigma^q_E(\mu)
\]

\[
b^k(x, \mu) = \sum_{q=0}^{Q_B} b^k_q(x) \cdot \sigma^q_B(\mu) \quad \rightarrow \quad b^k = \sum_{q=0}^{Q_B} b^k_q \sigma^q_B(\mu)
\]

\[
P[u_0(\mu)] = \sum_{q=0}^{Q_P} P^q[u_0] \cdot \sigma^q_P(\mu)
\]
Affine Parameter Dependence

Assumption: Operators can be written as a linear combination of parameter dependent and parameter independent parts:

\[ L^k_E(\mu)[u] = \sum_{q=0}^{Q_{L_E}} L^{k,q}_E[u] \cdot \sigma^q_E(\mu) \rightarrow L^k_E(\mu) = \sum_{q=0}^{Q_{L_E}} L^{k,q}_E \sigma^q_E(\mu) \]

\[ b^k(x,\mu) = \sum_{q=0}^{Q_b} b^{k,q}(x) \cdot \sigma^q_b(\mu) \rightarrow b^k = \sum_{q=0}^{Q_b} b^{k,q} \sigma^q_b(\mu) \]

\[ P[u_0(\mu)] = \sum_{q=0}^{Q_P} P^q[u_0] \cdot \sigma^q_P(\mu) \]

where

\[ (L^{k,q}_E)_{mn} = \int_\Omega \varphi_m L^{k,q}_E[\varphi_n] \]

\[ (b^{k,q})_n = \int_\Omega b^{k,q} \varphi_n. \]
Affine Parameter Dependence

Assumption: Operators can be written as a linear combination of parameter dependent and parameter independent parts:

\[ L_E^k(\mu)[u] = \sum_{q=0}^{Q_{LE}} L_{E}^{k,q}[u] \cdot \sigma_{E}^{q}(\mu) \quad \Rightarrow \quad L_E^k(\mu) = \sum_{q=0}^{Q_{LE}} L_{E}^{k,q} \sigma_{E}^{q}(\mu) \]

\[ b^k(x, \mu) = \sum_{q=0}^{Q_{b}} b^{k,q}(x) \cdot \sigma_{b}^{q}(\mu) \quad \Rightarrow \quad b^k = \sum_{q=0}^{Q_{b}} b^{k,q} \sigma_{b}^{q}(\mu) \]

\[ P[u_0(\mu)] = \sum_{q=0}^{Q_{P}} P^q[u_0] \cdot \sigma_{P}^{q}(\mu) \]

where

\[ (L_{E}^{k,q})_{mn} = \int_{\Omega} \varphi_m L_{E}^{k,q} \varphi_n \]

\[ (b^{k,q})_{n} = \int_{\Omega} b^{k,q} \varphi_n. \]

\[ \Rightarrow \text{ Enables an efficient offline/online-decomposition.} \]
Example: POD-Greedy

Need rigorous and efficient a posteriori error bound: \( \| u^k_H(\mu) - u^k_N(\mu) \| \leq \Delta^k_N(\mu) \). Then proceed as follows:

1. Add a first function to the reduced space (\( P^k[u_0] \) for all \( k \), e.g.).
2. Find the \( \mu^* \in S \subset P, k^* \in K \) that maximize the error in the current reduced space (Greedy):
   \[ \Delta^{k^*}_N(\mu^*) = \max_{\mu \in S, 0 \leq k \leq K} \Delta^k_N(\mu). \]
3. Perform the detailed simulation for this \( (\mu^*, k^*) \).
4. From the whole trajectory \( \{ u^k_H(\mu^*) \}_{k=0}^K \), choose a new base function using principal component analysis (PCA).
5. Repeat steps 2-4 until a desired accuracy is reached.
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4. Outlook
Idea: Separate low- and high-dimensional computations.

Wanted:

- Easy-to-use interface for low dimensional computations and control of the reduced basis generation $\Rightarrow RBmatlab^a$
- Rapid and easily adaptable solver for all high dimensional computations $\Rightarrow DUNE^b$
- Communication over network, s.t. the two phases can be distributed to different machines.

\[^a\text{http://www.morepas.org}\]
\[^b\text{http://www.dune-project.org}\]
Implementation Aspects

- Implementation concept
  - high dim computation
    - communication of low dim data
  - low dim computation
    - Control structures
      - direct parameter function usage
      - model
    - Visualization
    - Reconstruction

Offline data
- reduced basis space
- grid
- high dim operators

Solvers
- dune
- comsol
- others

Network
- Server
- Client

RBmatlab
- Reduced simulation
- Visualization control
- Reduced basis generation
  - greedy

Error estimators

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### Implementation Aspects

#### Numerical results

<table>
<thead>
<tr>
<th>Scenario</th>
<th>One High-dim. Solution</th>
<th>Generation of Reduced Basis</th>
<th>Generation of Online Matrices</th>
<th>Reduced Simulation</th>
<th>Reconstruction</th>
<th>Number of Grid Cells</th>
<th>Mean $L^\infty$-$L^2$-Error $^1$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>2D Transport (25 base functions)</strong></td>
<td>11s</td>
<td>8m 23s</td>
<td>6,69s</td>
<td>0,11s</td>
<td>0,33s</td>
<td>1024</td>
<td>1,42E-03</td>
</tr>
<tr>
<td><strong>2D Transport (50 base functions)</strong></td>
<td>11s</td>
<td>37m 30s</td>
<td>21s</td>
<td>0,15s</td>
<td>0,42s</td>
<td>1024</td>
<td>4,64E-04</td>
</tr>
<tr>
<td><strong>3D Transport (50 base functions)</strong></td>
<td>15m 44s</td>
<td>43h 37m</td>
<td>77m 39s</td>
<td>0,15s</td>
<td>26s</td>
<td>32768</td>
<td>9,11E-04</td>
</tr>
</tbody>
</table>

$^1$ Error between full and reduced simulation, tested with 250 randomized $\mu$-Values

**Figure:** Numerical results for a transport problem in 2D and 3D with non-divergence-free velocity.

**Figure:** Transport with velocity $\nu = (0.8, -2 \cdot y^2 + 2 \cdot y + \frac{1}{2}, -0.8)^T$
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Future work

- Implementation of different fluxes and implicit operators.
- GUI, visualization using GRAPE\textsuperscript{a}.
- Parallelization of the offline phase.
- Empirical interpolation of discrete operators for operators with non-affine parameter dependence and non-linear operators.
- Advanced application of the RB method to homogenization\textsuperscript{b} and corresponding implementation.

\textsuperscript{a}http://numod.ins.uni-bonn.de/grape/

\textsuperscript{b}Based on [Boyaval, 2008]
References

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_reduced-basis approach for homogenization beyond the periodic setting._  

[DUNE] Website.  
_DUNE - distributed and unified numerics environment._  
http://www.dune-project.org

[DUNE-RB] Website.  
RBmatlab.  
http://www.morepas.org
Thank you for your attention!