Reduced Basis Methods for PDEs with High-Dimensional Parameter Spaces

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Parametrized PDEs and Reduced Basis Methods

\[ D \subset \mathbb{R}^p : \text{parameter domain, } \mu = (\mu_1, \cdots, \mu_p) \in D : \text{parameter values} \]

\[ X: \text{suited functional space; } X^{fe}: \text{suited finite element space} \]

### Parametrized Variational Problems

For any \( \mu \in D \), evaluate \( s(\mu) = \ell(u(\mu), \mu) \) where \( u(\mu) \in X \) is the solution of:

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

for some parameter dependent bilinear and linear forms \( a \) and \( f \)

### Parametrized FE Problems

For any \( \mu \in D \), evaluate \( s^{fe}(\mu) = \ell(u^{fe}(\mu), \mu) \) where \( u^{fe}(\mu) \in X^{fe} \) is the solution of:

\[
a(u^{fe}(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X^{fe}.
\]

\[ S_N = \{\mu^1, \cdots, \mu^N\} \subset D: \text{a selection of parameter values in } D \]

\[ X_N^{rb} = \text{span}\{u^{fe}(\mu^1), \cdots, u^{fe}(\mu^N)\}: \text{reduced basis space} \]

RBM: Given a \( \mu \), \( u^{fe}(\mu) \) can be approximated by \( X_N^{rb} \) with big enough \( N \)

### Reduced Basis Problems

For any \( \mu \in D \), evaluate \( s^{rb}(\mu) = \ell(u^{rb}(\mu), \mu) \) where \( u^{rb}(\mu) \in X^{rb} \) is the solution of:

\[
a(u^{rb}(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X^{rb}.
\]
Offline and Online Stages of RBM

Offline Stage:
- $S_N = \{\mu^1, \cdots, \mu^N\}$, a selection of samples in parameter space $D$
- $X_{rb}^N = \{u^{fe}(\mu^1), \cdots, u^{fe}(\mu^N)\}$, bases corresponding to $S_N$
- Error Estimator for a $\mu \in D$: $\eta(\mu, X_{rb}^N)$ (workload independent of dof of FE)

| Input: A fine train set $\Xi_{\text{train}} \subset D$, a tolerance $tol > 0$ |
| Output: $S_N$ and $X_{rb}^N$ |

| Initialization: $S_1, X_{rb}^1$ |
| while $\max_{\mu \in \Xi} \eta(\mu; X_{rb}^N) > tol$ do |
| For all $\mu \in \Xi_{\text{train}}$, compute $\eta(\mu; X_{rb}^N)$; // huge cost |
| Choose $\mu^{N+1} = \arg\max_{\mu \in \Xi_{\text{train}}} \eta(\mu; X_{rb}^N)$; |
| Update $S_N, X_{rb}^N$ |
| end while |

Online Stage:
Under an affine assumption of the bilinear and linear forms, matrices and vectors can be precomputed. For any $\mu \in D$, evaluate $s_{rb}(\mu) = \ell(u_{rb}(\mu), \mu)$ where $u_{rb}(\mu) \in X_{rb}^N = \{u^{fe}(\mu^1), \cdots, u^{fe}(\mu^N)\}$, is the solution of:

$$a(u_{rb}(\mu), v; \mu) = f(v; \mu), \quad \forall v \in X^{rb}.$$ 

A problem of size $N$ (independent of the size of the finite element space $X^{fe}$) needs to be solved.
Problems Faced with High Dimensional Parameter Space

Offline stage:
- Almost impossible to have a fine enough train set for problems with a high number of parameters
- Huge offline computational cost due to the size of $\Xi_{\text{train}}$
- Quality of RB is only guaranteed on the initial train set $\Xi_{\text{train}} \subset D$

Methods to cure:
- Build the basis by adaptive train sets with reasonable size, but verify the RB by a fine enough subset of $D$.
- Accelerated greedy algorithms.

Online stage:
- The Online stage is complicated if there are many parameters
- The resultant RB space may have many basis functions.

Methods to cure:
- Use ANOVA expansion to freeze very unimportant parameters. An RB-ANOVA-RB algorithm.
- ANOVA based hp RBM (Use ANOVA sensitivity analysis to do anisotropic domain decomposition of the parameter domain)
Hierarchical: $S_N \subset S_M$, $X^r_N \subset X^r_M$ if $1 \leq N \leq M$

- error $\rightarrow 0$ as number of RBs $\rightarrow \infty$,
- It’s natural to assume a Saturation Assumption holds:

$$\eta(\mu; X^r_M) \leq C_{sa}\eta(\mu; X^r_N)$$ for some $C_{sa} > 0$, $\forall 0 < N < M$.

Modification of the original Greedy Algorithm:

- Create an error profile $\eta_{\text{saved}}(\mu)$ for all $\mu \in \Xi$.
- In the loop for the maximum, compare $C_{sa}\eta_{\text{saved}}(\mu)$ with current temp max.
  - If $C_{sa}\eta_{\text{saved}}(\mu) < \text{current temp max}$, then this particular $\mu$ will never be a max in this round of searching! Thus the computation of the error estimator can be skipped!
  - Else, do the regular error estimation and update $\eta_{\text{saved}}(\mu)$.
\[
\begin{aligned}
-\nabla \cdot (\alpha \nabla u) &= 0 \quad \text{in} \quad \Omega = (0, 1)^2, \\
u &= 0 \quad \text{on} \quad \Gamma_{\text{top}} = \{x \in (0, 1), y = 1\}, \\
\alpha \nabla u \cdot n &= 0 \quad \text{on} \quad \Gamma_{\text{side}} = \{x = 0 \text{ and } x = 1, y \in (0, 1)\}, \\
\alpha \nabla u \cdot n &= 1 \quad \text{on} \quad \Gamma_{\text{base}} = \{x \in (0, 1), y = 0\},
\end{aligned}
\]

3 subdomains: \( R_1 = (0, 0.5) \times (0.5, 1), \) \( R_2 = (0.5, 1) \times (0, 0.5), \) and \( R_3 = (0, 1)^2 \setminus (R_1 \cup R_2). \) The diffusion constant \( \alpha \) is set to be

\[
\alpha = \begin{cases} 
\alpha_i &= 100^2 \mu_i^{-1}, & x \in R_i, \ i = 1, 2, \\
\alpha_3 &= 1, & x \in R_3,
\end{cases}
\]

where \( \mu = (\mu_1, \mu_2) \in [0, 1]^2. \) The domain of \( \alpha_i, \ i = 1, 2 \) is set to \([1/100, 100], \) \( \Xi: 10'000 \) points.
Adaptively Enriching Greedy Algorithm for Problems with a High Number of Parameters

- Generate RB based on a relatively coarse train set, do a "Safety Check"/Validation step with a large number of random parameters to guarantee the quality of the RB.
- Choose an acceptable size of the train set, generate an initial train set randomly.
- After each round of searching, remove those points whose errors $\leq \epsilon$ from train set.
- Enrich the train set by random parameters to keep the size of train set a constant.
- Saturation Assumption Based Technique can be applied.

$$AEGA = \text{a fixed train set size} + \text{remove points whose errors are less than tol}$$
$$+ \text{enrich new points to keep the size of the train set}$$
$$+ \text{saturation assumption based technique} + \text{a final safety check/validation step}$$

Can be applied to EIM and SCM.
Adaptively Enriching Greedy Algorithm for Problems with a High Number of Parameters

\[
\begin{cases}
-\nabla \cdot (\alpha \nabla u) &= 0 \quad \text{in} \quad \Omega = (0,1)^2, \\
u &= 0 \quad \text{on} \quad \Gamma_{\text{top}} = \{x \in (0,1), y = 1\}, \\
\alpha \nabla u \cdot \mathbf{n} &= 0 \quad \text{on} \quad \Gamma_{\text{side}} = \{x = 0 \text{ and } x = 1, y \in (0,1)\}, \\
\alpha \nabla u \cdot \mathbf{n} &= 1 \quad \text{on} \quad \Gamma_{\text{base}} = \{x \in (0,1), y = 0\},
\end{cases}
\]

Let \( \Omega_k = (\frac{i-1}{4}, \frac{i}{4}) \times (\frac{j-1}{4}, \frac{j}{4}) \), for \( i, j \in \{1, 2, 3, 4\}, k = 4(i - 1) + j \).

\[
\alpha = \begin{cases}
\alpha_i &= 5^{2\mu_i - 1} \quad x \in R_i, \quad i = 1, 2, \cdots, 15, \\
\alpha_{16} &= 1 \quad x \in R_{16}.
\end{cases}
\]

where \( \mu = [\mu_1, \mu_2, \cdots, \mu_{15}] \in [0,1]^{15} \). Notice the domain of \( \alpha_i, i = 1, 2, \cdots, 15 \) is \([1/5, 5] \).
Percentage of work (effected at each step N) w.r.t. the fixed size of train set M at each step N, and of the number of points remained in the train set (at each step N)
ANOVA Sensitivity Analysis

$D = [0, 1]^p$, $P = \{1, \cdots, p\}$, $t \subset P$ be any subset of the coordinates indices, $A^{\mid t\mid}$ be the $t$-dimensional unit hypercube

**ANOVA (ANalysis Of VAriation)**

$$s(\alpha) = s_0 + \sum_{t\in P} s_t(\alpha_t)$$

or

$$s(\alpha) = s_0 + \sum_i s_i(\alpha_i) + \sum_{ij} s_{ij}(\alpha_i, \alpha_j) + \cdots + s_{12 \cdots p}(\alpha_1, \ldots, \alpha_p)$$

where the term is defined recursively by $s_t(\alpha_t) = \int_{A^{p-\mid t\mid}} s(\alpha) d\mu(\alpha_{P\setminus t}) - \sum_{W\subset t} s_W(\alpha_W) - s_0$

with $s_0 = \int_{A^P} s(\alpha) d\mu(\alpha)$.

Let the variance $V_t(s)$ and the total variance $V(s)$ be

$$V_t(s) = \int_{A^P} (s_t(\alpha_t))^2 d\alpha \quad \text{and} \quad V(s) = \sum_{\mid t\mid > 0} V_t(u)$$

The ratios

$$S_{i_1 \cdots , i_d} = V_{i_1 \cdots , i_d} / V;$$

are called global sensitivity indices.
Reduced Basis Method based ANOVA Sensitivity Analysis

ANOVA is expansive!
- For a functional $s$ based on a parameter-dependent PDE problem,
- The numerical integration used in ANOVA needs evaluations of $s$ for different parameters for many times.
- Each evaluation needs to solve the PDE.

Reduced Basis Method provides a cheap evaluation of the functional $s$.
- Build RB space for the parameter-dependent pde problem using the improved greedy algorithm.
- Numerical quadrature in ANOVA can be cheaply computed via RB.
- Do sensitivity analysis and other analysis by ANOVA.
3 step RB-ANOVA-RB method

- Build RB for the full parametric problem with high tol (not so accurate but cheap)
- ANOVA sensitivity analysis to $s(\mu)$ to identify important parameters.
- Freeze those very unimportant parameters. Build new RB for those important parameters.

Acoustic horn problem example (8 parameters)

Figure: The domain of the horn problem.

Figure: Boundaries of the domain.
\[ \begin{aligned}
\Delta u + 4u &= 0 \quad \text{in} \quad \Omega, \\
(2i + \frac{1}{25})u + \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \Gamma_{\text{out}}, \\
2iu + \frac{\partial u}{\partial n} &= 4i \quad \text{on} \quad \Gamma_{\text{in}}, \\
i\mu_j u + \frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \Gamma_j, j = 1, \cdots, 8, \\
\frac{\partial u}{\partial n} &= 0 \quad \text{on} \quad \text{other boundaries.}
\end{aligned} \] (1.1)

with parameters \( \mu = (\mu_1, \mu_2, \cdots, \mu_8) \in [0, 1]^8 \). We choose the output of interest as

\[ s(\mu) = \ell(u) = \text{real}\left( \int_{\Gamma_{\text{in}}} uds \right). \] (1.2)

1. Full RB with \( tol = 0.001 \)
2. ANOVA Sensitivity Analysis: \( S_3 = 0.4321, S_5 = 0.4314, \) and \( S_{35} = 0.1256, \) and \( D = 3.08 \times 10^{-4} \). Thus \( S_3 + S_5 + S_{35} = 0.9891 \).
3. Only parameters \( \mu_3 \) and \( \mu_5 \) are important. Build new RB for the 2-parameter problem.
ANOVA-based hp RBM

A recursive offline procedure to do parameter domain decomposition (h-part) and build RB locally in those subdomains with less than prescribed basis size (p-part) ([Eftang, Patera] for RBM, [Eftang, Stamm] for EIM)

For many parameter problems, we cannot afford decompose the parameter domain to $2^p$-subdomains, we have to only decompose in the important parameter direction. We use ANOVA to determine the importance.

```
1: function (T(D), S(T(D)), X^{rb}(T(D))) = AhpRB (S_{N_0}, D, X^{rb}_{N_0}, D, N_{max}, tol, s)
2: (X^{rb}_{N,D}, S_{N,D}, conv) = AEGA (S_{N_0}, D, X^{rb}_{N_0}, D, N_{max}, tol);
3: if conv then
4:   T(D) = {D}, S(T(D)) = {S_{N,D}}, X^{rb}(T(D)) = {X^{rb}_{N,D}};
5: else
6:   sens = ANOVA (s, D);
7:   (sensd, K) = MARK (sens);
8:   (\{D_k\}_{k=1}^{2^K}, \{S_{N_k,D_k}\}_{k=1}^{2^K}, \{X^{rb}_{N_k,D_k}\}_{k=1}^{2^K}) = REFINE (D, S_{N,D}, X^{rb}_{N,D}, sensd, K);
9:   for k = 1 to 2^K do
10:      (T(D_k), S(T(D_k)), Y^{rb}(T(D_k))) = AhpRB (X^{rb}_{N_k,D_k}, X^{rb}_{N_k,D_k}, D_k, N_{max}, tol, s);
11:   end for
12: (T(D), S(T(D)), X^{rb}(T(D)) =
13:   COMBINE (\{T(D_k)\}_{k=1}^{2^K}, \{S(T(D_k))\}_{k=1}^{2^K}, \{X^{rb}(T(D_k))\}_{k=1}^{2^K});

Algorithm 1: Recursive definition of the main function AhpRB (ANOVA-hp-Reduced Basis)
```
Since it very hard to illustrate the domain decomposition in high-dimensional space, we first consider the thermal block equation (8) with two parameters to demonstrate the algorithm. Let \( R_1 = (0, 0.5)^2, \ R_2 = (0.5, 1)^2, \) and \( R_3 = (1, 1)^2 \setminus (R_1 \cup R_2) \). The diffusion constant \( \alpha \) is assumed to be

\[
\alpha = \begin{cases} 
\alpha_k = 10^{2\mu_i^{-1}}, & x \in R_k, \ k = 1, 2, \\
\alpha_k = 1, & x \in R_k, \ k = 3. 
\end{cases}
\]

The tolerance is set to be \( 10^{-5} \) and \( N_{max} \) is set to be 7. We set \( K_{max} = 1 \), implying that only one component is split. During the final stage, subdomain \( D_{10} \) needs 6 bases to converge, and all others need 7 bases.

**Figure:** Tree structure of the subdomains

**Figure:** First level of domain decomposition.
Figure: Second level of domain decomposition.

Figure: Third level of domain decomposition.
Conclusions

To reduce both the offline and online computational costs for RBM with high-dimensional parameters

- New greedy algorithms to reduce the offline computational cost.
- The 3 step RB-ANOVA-RB to reduce the size of parameters.
- ANOVA-based hp RBM to do sensitivity based parameter domain decomposition (h-adaptation).