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A REDUCED BASIS METHOD FOR PARAMETER OPTIMIZATION OF MULTISCALE PROBLEMS

MARIO OHLBERGER * AND MICHAEL SCHAEFER*

Abstract. Many natural or technical processes can be described by parameterized partial differential equations (P^2DEs) that include different length-scales. Typical applications include parameter studies or optimal control where the model has to be solved for a huge variety of different parameters resulting in enormous computational times for classical discretization techniques. The reduced basis method was introduced to overcome this problem. The aim of this contribution is to extend the reduced basis methodology to optimization problems that are constrained by a parameterized multiscale problem. We introduce the methodoly in detail and give numerical experiments that demonstrate the efficiency of the model reduction approach in multiscale optimization problems.

Key words. reduced basis method, multiscale modelling, homogenization, optimization

1. Introduction. Reduced basis methods (RBM) [11] are model order reduction techniques originally developed for parameterized partial differential equations. Main fields of application are the *real-time context* where the solution for a given parameter configuration has to be calculated quasi instantaneous, and the *multi-query context* where the problem has to be solved repeatedly for different parameters. Examples are parameter studies, inverse problems or optimal control.

Although developed already in the 1980's, major progress in RBM has been made during the last decade where the methodology was accomplished with rigorous a posteriori error analysis that is used both, in the construction process of the reduced models, and for computing error bounds for the reduced model with respect to an underlying traditional high dimensional finite element, finite volume or finite difference approximation. Starting with elliptic equations [11], the methodology was extended to parabolic [5] and general evolution equations [6]. All these works dealt with linear equations and assumed an affine parameter dependence that allows an efficient offline/online decomposition of the resulting reduced schemes. Over the last years new techniques were introduced to handle more general problems, namely the empirical interpolation [1] for non-affine data functions and the empirical operator interpolation [3] for general nonaffine, nonlinear differential operators. Latest results include the treatment of nonlinear, instationary systems [2, 4] and variational inequalities [7].

Applications of the RBM to optimization problems have been studied in [10]. The aim of this paper is to extend the ideas presented there to the following multiscale optimization setting:

$$\left.\begin{array}{rl} \text{Find} & \mu^* = \arg\min J(u(\mu),\mu) \\ \text{subject to} & C_j(u(\mu),\mu) \leq 0 \quad \forall j = 1,\dots,N, \\ & \mu \in \mathcal{P} \end{array}\right\} \tag{1.1}$$

with a compact *parameter set* $\mathcal{P} \subset \boldsymbol{R}^P$. In (1.1), the *state variable* $u(\mu) = u^\varepsilon(\mu)$ is

*Institute for Computational and Applied Mathematics, University of Muenster, Einsteinstrasse 62, 48149 Muenster, Germany ({mario.ohlberger,michael.schaefer}@uni-muenster.de).

solution of the following (parameterized) multiscale problem:

$$\left.\begin{aligned} -\nabla \cdot (A^\varepsilon(x;\mu)\nabla u^\varepsilon(x;\mu)) &= f(x;\mu) \quad (x \in \Omega) \\ u^\varepsilon(x;\mu) &= 0 \qquad\quad (x \in \partial\Omega) \end{aligned}\right\} \tag{1.2}$$

Here, $\Omega \subset \boldsymbol{R}^d$ is a bouded domain, and the diffusion tensor is assumed to be rapidly oscillating: $A^\varepsilon(\cdot;\mu) = \left(a_{ij}^\varepsilon(\cdot;\mu)\right)_{i,j=1}^d$, where $a_{ij}^\varepsilon(\cdot;\mu) := a_{ij}(\cdot/\varepsilon;\mu)$ for Y-periodic functions $a_{ij}(\cdot;\mu) \in L^\infty(Y)$ with the *reference cell* $Y := (0,1)^d$. To have a more compact notation, we will also use the abbreviation $u^\varepsilon(\mu) := u^\varepsilon(\cdot;\mu)$. Analogue expressions will be used for all functions depending on space and parameter.

There is a huge variety of numerical algorithms to solve general optimization problems such as (1.1), see for example [13]. Since neccessary and sufficient conditions for local optima include derivatives of first and second order of the involved functions, most algorithms make use of these quantities. In this regard it is clear that we will not only need RB approximations for the state variable $u^\varepsilon(\mu)$ itself, but also for the derivatives with respect to the parameter μ.

The rest of this paper is organized as follows: In Section 2 we will shortly recall results from homogenization theory that will allow us to replace $u^\varepsilon(\mu)$ by its macroscopic approximation $u^0(\mu)$. Section 3 is devoted to the definition and discussion of a reduced basis multiscale approximation of (1.1). Finally, in Section 4 we present numerical experiments that demonstrate the applicability and efficiency of our model reduction approach for multiscale optimization problems.

2. Homogenization. The length-scale ε in problem (1.2) is typically very small, i.e. $\varepsilon \ll |\Omega|$. Thus, an approximation of the optimization problem with classical discretization techniques is extremely expensive, since the underlying grids must resolve the fine scale ε. The idea of *homogenization* is to study properties of a sequence u^ε in the limit $\varepsilon \to 0$. The main homogenization result for our approach is the following theorem (cf. [12]) which gives an explicit description of the limit u^0:

THEOREM 2.1. *Let $\mu \in \mathcal{P}$ be fix and $u^\varepsilon(\mu)$ the solution of (1.2). If $A^\varepsilon(\mu)$ is continuous and uniformly elliptic, and $f(\mu) \in H^{-1}(\Omega)$, then*

1. *$u^\varepsilon(\mu) \to u^0(\mu)$ weakly in $H_0^1(\Omega)$ and*
2. *$A^\varepsilon(\mu)\nabla u^\varepsilon(\mu) \to A^0(\mu)\nabla u^0(\mu)$ weakly in $\left(L^2(\Omega)\right)^d$.*

Here, $A^0(\mu) \in \boldsymbol{R}^{d\times d}$ is a constant matrix, and the limit $u^0(\mu) \in H_0^1(\Omega)$ solves the homogenized problem

$$\left.\begin{aligned} -\nabla \cdot \left(A^0(\mu)\nabla u^0(\mu)\right) &= f(\mu) \quad \text{in } \Omega \\ u^0(\mu) &= 0 \qquad \text{on } \partial\Omega \end{aligned}\right\} \tag{2.1}$$

An explicit expression for the *effective tensor* $A^0(\mu)$ can also be derived. To that end we introduce the *cell problems*

$$\left.\begin{aligned} -\nabla \cdot \left(A^t(y;\mu)\nabla\chi^k(y;\mu)\right) &= -\nabla \cdot \left(A^t(y;\mu)e_k\right) \quad \text{in } Y \\ \chi^k(y;\mu) &\text{ is } Y\text{-periodic} \\ \int_Y \chi^k(y;\mu)\,\mathrm{d}y &= 0 \end{aligned}\right\} \tag{2.2}$$

with $\boldsymbol{e}_k \in \boldsymbol{R}^d$ being the k-th canonical basis vector. Then, $A^0(\mu) = (a^0_{ij}(\mu))^d_{i,j=1}$ satisfies

$$a^0_{ij}(\mu) = \int_Y A^t(y;\mu)\left(\boldsymbol{e}_i - \nabla\chi^i(y;\mu)\right)\cdot\left(\boldsymbol{e}_j - \nabla\chi^j(y;\mu)\right)\,\mathrm{d}y. \tag{2.3}$$

2.1. Weak formulation. Instead of (2.1) and (2.2) we work with corresponding weak formulations. Let $C^\infty_\#(Y)$ be the subspace of Y-periodic functions of $C^\infty(\boldsymbol{R}^d)$. We define the space $H^1_\#(Y)$ as the closure of $C^\infty_\#(Y)$ w.r.t. the $H^1(Y)$-Norm. With the (bi-)linear forms

$$\begin{aligned}
\mathcal{A}_Y(u,v;\mu) &:= \int_Y A^t(\mu)\nabla u\cdot\nabla v\,\mathrm{d}y,\\
\mathcal{F}_{Y,k}(v;\mu) &:= \int_Y A^t(\mu)\boldsymbol{e}_k\cdot\nabla v\,\mathrm{d}y,\\
\mathcal{A}(u,v;\mu) &:= \int_\Omega A^0(\mu)\nabla u\cdot\nabla v\,\mathrm{d}x,\\
\mathcal{F}(v;\mu) &:= \int_\Omega f(\mu)\varphi\,\mathrm{d}x,
\end{aligned}$$

the weak solutions $\chi^k(\mu) \in H^1_\#(Y)$ of (2.2) and $u^0(\mu) \in H^1_0(\Omega)$ of (2.1) are then given by

$$\mathcal{A}_Y(\chi^k(\mu),\psi;\mu) = \mathcal{F}_{Y,k}(\psi;\mu) \qquad \forall\,\psi \in H^1_\#(Y), \tag{2.4}$$

$$\mathcal{A}(u^0(\mu),\varphi;\mu) = \mathcal{F}(\varphi;\mu) \qquad \forall\,\varphi \in H^1_0(\Omega). \tag{2.5}$$

Finally, the effective tensor $A^0(\mu)$ can be written as (cf. (2.3))

$$a^0_{ij}(\mu) = \mathcal{A}_Y(y_i - \chi^i(\mu), y_j - \chi^j(\mu)). \tag{2.6}$$

3. Reduced Basis Method. As a first step towards model reduction we replace all occurances of the fine-scale solution u^ε by its homogenized limit u^0. In order to derive a reduced scheme for (1.1) we need reduced basis approximations for $u^0(\mu)$ and its parameter derivatives. Since the weak formulation (2.5) includes the effective tensor $A^0(\mu)$ we will also need RB approximations of the cell problems $\chi^k(\mu)$, cf. equation (2.6).

The structure of this section is as follows: In 3.1, the reduced approximations for all neccessary quantities (including parameter derivatives) are introduced, while in 3.2 we discuss a possible offline-online splitting of the computational load for all involved quantities. Finally, Subsection 3.3 puts all the pieces together and concludes with a reduced scheme for the optimization problem (1.1).

3.1. RB approximations. For the (finite) *sample sets* $\mathcal{S}, \mathcal{S}^k_Y \subset \mathcal{P}$ we define the *reduced basis spaces*

$$\begin{aligned}
\mathcal{W}^k_{N,Y} &:= \operatorname{span}\left\{\chi^k(\mu) \mid \mu \in \mathcal{S}^k_Y\right\} = \operatorname{span}\left\{\psi^k_1,\ldots,\psi^k_{N_Y(k)}\right\},\\
\mathcal{W}_N &:= \operatorname{span}\left\{u^0(\mu) \mid \mu \in \mathcal{S}\right\} = \operatorname{span}\left\{\varphi_1,\ldots,\varphi_N\right\},
\end{aligned}$$

with $\chi^k(\mu)$, $u^0(\mu)$ as in (2.4), (2.5). Besides, $N := \dim(\mathcal{W}_N)$, $N_Y(k) := \dim(\mathcal{W}^k_{N,Y})$ and $\{\psi^k_j\}^{N_Y(k)}_{j=1}$, $\{\varphi_j\}^N_{j=1}$ are orthonormal bases.[1]

[1] In actual simulations the basis functions have of course to be replaced by discrete approximations (via FEM, FV or other) of reasonably high dimension. This fact will be ignored in the further presentation.

The RB approximation $\chi_N^k(\mu) \in \mathcal{W}_{N,Y}^k$ is now defined as the Galerkin projection of (2.1) onto $\mathcal{W}_{N,Y}^k$:

$$\mathcal{A}_Y(\chi_N^k(\mu), \psi; \mu) = \mathcal{F}_{Y,k}(\psi; \mu) \qquad \forall\, \psi \in \mathcal{W}_{N,Y}^k \tag{3.1}$$

With coefficient vectors $\boldsymbol{\alpha}^k(\mu) \in \boldsymbol{R}^{N_Y(k)}$ we have the basis representations $\chi_N^k(\mu) = \sum_{i=1}^{N_Y(k)} \boldsymbol{\alpha}_i^k(\mu)\psi_i^k$. In a natural way we choose for the RB approximation of $A^0(\mu)$: $A_N^0(\mu) = (a_{N,i,j}(\mu))_{i,j=1}^d$ with

$$a_{N,i,j}(\mu) := \mathcal{A}_Y(y_i - \chi_N^i(\mu), y_j - \chi_N^j(\mu); \mu). \tag{3.2}$$

The defining equation for $u^0(\mu)$ contains the tensor $A^0(\mu)$ which is not available in classical reduced simulations. To get the RB approximation for $u_N^0(\mu)$ we thus replace $A^0(\mu)$ by $A_N^0(\mu)$: With a new bilinear form

$$\mathcal{A}_N(u, v; \mu) := \int_\Omega A_N^0(\mu)\nabla u \cdot \nabla v \, \mathrm{d}x,$$

we choose $u_N^0 \in \mathcal{W}_N$ as solution of

$$\mathcal{A}_N(u_N^0(\mu), \varphi; \mu) = \mathcal{F}(\varphi; \mu) \qquad \forall\, \varphi \in \mathcal{W}_N. \tag{3.3}$$

The corresponding basis representation will be denoted by $u_N^0(\mu) = \sum_{i=1}^N \boldsymbol{\beta}_i(\mu)\varphi_i$.

3.1.1. Parameter derivatives. As stated in the introduction, derivatives of $u_N^0(\mu)$ with respect to parameters are neccessary for the optimization procedure. To compute such derivatives, we differentiate the defining equation (3.3) with respect to μ_i. Thus, we get the following weak formulation for $\partial_{\mu_i} u_N^0(\mu)$:

$$\mathcal{A}_N(\partial_{\mu_i} u_N^0(\mu), \varphi; \mu) = \partial_{\mu_i}\mathcal{F}(\varphi; \mu) - \partial_{\mu_i}\mathcal{A}_N(u_N^0(\mu), \varphi; \mu) \qquad \forall \varphi \in \mathcal{W}_N. \tag{3.4}$$

A closer look at the third term reveals that since $\mathcal{A}_N$ includes the effective tensor $A_N^0(\mu)$, we must provide parameter derivatives of it. The proof of corollary 3.2 below shows that to this end it is sufficient to have the corresponding derivatives of the cell problems. These are defined in the same manner as those for the $u_N^0(\mu)$, i.e. by deriving the defining equation (3.1) which results in

$$\mathcal{A}_Y(\partial_{\mu_i}\chi_N^k(\mu), \psi; \mu) = \partial_{\mu_i}\mathcal{F}_{Y,k}(\psi; \mu) - \partial_{\mu_i}\mathcal{A}_Y(\chi_N^k(\mu), \psi; \mu) \quad \forall \psi \in \mathcal{W}_{N,Y}^k. \tag{3.5}$$

Higher order derivatives can be specified by further differentiation of (3.5).

3.2. Offline-online splitting. In the previous section we defined RB approximations for $u^0(\mu)$ and the corresponding cell problems. The calculation of these approximations still involves the integration of high-dimensional data, namely the basis functions φ_i. To overcome this problem we make the following assumption: The diffusion tensor $A(x; \mu)$ and the source term $f(x; \mu)$ in (1.2) allow *affine parameter decompositions*, i.e. for $Q_A, Q_f \in \boldsymbol{N}$ and functions $\sigma_A^q, \sigma_f^q : \mathcal{P} \to \boldsymbol{R}$, $A^q : \boldsymbol{R}^d \to \boldsymbol{R}^{d\times d}$, $f^q : \boldsymbol{R}^d \to \boldsymbol{R}$ it holds

$$A(x; \mu) = \sum_{q=1}^{Q_A} \sigma_A^q(\mu)A^q(x),$$

$$f(x; \mu) = \sum_{q=1}^{Q_f} \sigma_f^q(\mu)f^q(x),$$

both for all $x \in \boldsymbol{R}^d$, and $\mu \in \mathcal{P}$. Note that σ_A^q, σ_f^q depend on the parameter but not on the spatial variable, while A^q, f^q are parameter independent. As can be easily seen, this implies affine decompositions for the bilinear form $\mathcal{A}_Y$ and right hand side $\mathcal{F}_Y^k$ in (2.4) as well as for $\mathcal{F}$ in (2.5). We will denote these decompositions as $\mathcal{A}_Y(u,v;\mu) = \sum_{q=1}^{Q_{A_Y}} \sigma_{\mathcal{A}_Y}^q(\mu)\mathcal{A}_Y^q(u,v)$, $\mathcal{F}_Y^k(v;\mu) = \sum_{q=1}^{Q_{\mathcal{F}_Y^k}} \sigma_{\mathcal{F}_Y^k}^q(\mu)\mathcal{F}_Y^{k,q}(v)$ and $\mathcal{F}(v) = \sum_{q=1}^{Q_{\mathcal{F}}} \sigma_{\mathcal{F}}^q(\mu)\mathcal{F}^q(v)$.

PROPOSITION 3.1. *For $k = 1, \ldots, d$, the coefficient vector $\boldsymbol{\alpha}^k(\mu)$ of $\chi_N^k(\mu)$ is the solution of*

$$\left[\sum_{q=1}^{Q_A} \sigma_A^q(\mu)\boldsymbol{\mathcal{A}}_Y^{k,q}\right]\boldsymbol{\alpha}^k(\mu) = \sum_{q=1}^{Q_A} \sigma_A^q(\mu)\boldsymbol{\mathcal{F}}_Y^{k,q} \tag{3.6}$$

with

$$\boldsymbol{\mathcal{A}}_Y^{k,q} = \{\mathcal{A}_Y^q(\psi_i^k, \psi_j^k)\}_{i,j=1}^{N_Y(k)}, \qquad \boldsymbol{\mathcal{F}}_Y^{k,q} = \{\mathcal{F}_Y^{k,q}(\psi_i)\}_{i=1}^{N_Y(k)}.$$

Proof. The proof is straight forward. It uses the basis representation of $\chi_N^k(\mu)$, the affine decompositions of $\mathcal{A}_Y$ and $\mathcal{F}_Y^k$, and the fact that in (3.1) it is sufficient to test with the basis functions ψ_j^k. □

COROLLARY 3.2. *The RB approximation $A_N^0(\mu)$ of the effective tensor allows an offline-online splitting of the form*

$$A_N^0(\mu) = \sum_{q=1}^{Q_{A_N^0}} \sigma_{A_N^0}^q(\mu)\boldsymbol{A}_N^{0,q} \tag{3.7}$$

with constant matrices $\boldsymbol{A}_N^{0,q} \in \boldsymbol{R}^{d\times d}$.

Proof. The definition of $A_N^0(\mu)$ (cf. (3.2)) and the affine decomposition of $\mathcal{A}_Y$ yield

$$\begin{aligned}\left[A_N^0(\mu)\right]_{ij} &= \mathcal{A}_Y(y_i - \chi_N^i(\mu), y_j - \chi_N^j(\mu)) \\ &= \sum_{q=1}^{Q_A} \sigma_A^q(\mu)\Big(\mathcal{A}_Y^q(y_i, y_j) - \mathcal{A}_Y^q(y_i, \chi_N^j(\mu)) \\ &\qquad - \mathcal{A}_Y^q(\chi_N^i(\mu), y_j) + \mathcal{A}_Y^q(\chi_N^i(\mu), \chi_N^j(\mu))\Big).\end{aligned}$$

Using the basis representations of $\chi_N^i(\mu)$ and $\chi_N^j(\mu)$ we end up with

$$\mathcal{A}_Y^q(y_i, \chi_N^j(\mu)) = \sum_{k=1}^{N_Y(j)} \boldsymbol{\alpha}_k^j(\mu) \underbrace{\mathcal{A}_Y^q(y_i, \psi_k^j)}_{=:\left(\boldsymbol{C}^{q,i,j}\right)_k}$$

$$\mathcal{A}_Y^q(\chi_N^i(\mu), y_j) = \sum_{k=1}^{N_Y(i)} \boldsymbol{\alpha}_k^i(\mu) \underbrace{\mathcal{A}_Y^q(\psi_k^i, y_j)}_{=:\left(\boldsymbol{D}^{q,i,j}\right)_k}$$

$$\mathcal{A}_Y^q(\chi_N^i(\mu), \chi_N^j(\mu)) = \sum_{k=1}^{N_Y(i)} \sum_{l=1}^{N_Y(j)} \boldsymbol{\alpha}_k^i(\mu)\boldsymbol{\alpha}_l^j(\mu) \underbrace{\mathcal{A}_Y^q(\psi_k^i, \psi_l^j)}_{=:\left(\boldsymbol{E}^{q,i,j}\right)_{kl}}.$$

Together with $\boldsymbol{B}^q_{ij} := \mathcal{A}^q_Y(y_i, y_j)$ this implies the following splitting:

$$\left(A^0_N(\mu)\right)_{ij} = \sum_{q=1}^{Q_A} \sigma^q_A(\mu) \left(\boldsymbol{B}^q_{ij} - \boldsymbol{\alpha}^j(\mu) \cdot \boldsymbol{C}^{q,i,j} - \boldsymbol{\alpha}^i(\mu) \cdot \boldsymbol{D}^{q,i,j} + \boldsymbol{\alpha}^i(\mu) \cdot \boldsymbol{E}^{q,i,j} \boldsymbol{\alpha}^j(\mu)\right).$$

It is clear that this expression can be cast in the asserted form. □

Notice that the above corollary directly yields an affine decomposition for the bilinear form $\mathcal{A}_N$ which we denote $\mathcal{A}_N(u, v; \mu) = \sum_{q=1}^{Q_{\mathcal{A}_N}} \sigma^q_{\mathcal{A}_N}(\mu) \boldsymbol{\mathcal{A}}^q_N(u, v)$.

COROLLARY 3.3. *The coefficient vector $\boldsymbol{\beta}(\mu)$ of $u^0_N(\mu)$ is the solution of*

$$\left[\sum_{q=1}^{Q_{A^0_N}} \sigma^q_{A^0_N}(\mu) \boldsymbol{\mathcal{A}}^q_N\right] \boldsymbol{\beta}(\mu) = \sum_{q=1}^{Q_f} \sigma^q_f(\mu) \boldsymbol{\mathcal{F}}^q \tag{3.8}$$

with

$$\boldsymbol{\mathcal{A}}^q_N = \{\mathcal{A}^q_N(\varphi_i, \varphi_j)\}^N_{i,j=1}, \qquad \boldsymbol{\mathcal{F}}^q = \{\mathcal{F}^q(\varphi_i)\}^N_{i=1}.$$

3.2.1. Reduced basis method for derivatives with respect to parameters. We start with the offline-online splitting for the cell problems. The same arguments as in the proof of Proposition 3.1 can be used for (3.4) to provide the following result: Let $\partial_{\mu_i} \boldsymbol{\alpha}^k(\mu)$ be the coefficient vector of $\partial_{\mu_i} \chi^k_N(\mu)$, then

$$\left[\sum_{q=1}^{Q_{\mathcal{A}_Y}} \sigma^q_{\mathcal{A}_Y}(\mu) \boldsymbol{\mathcal{A}}^q_Y\right] \partial_{\mu_i} \boldsymbol{\alpha}^k(\mu) = \sum_{q=1}^{Q_{\mathcal{F}^k_Y}} \partial_{\mu_i} \sigma^q_{\mathcal{F}^k_Y}(\mu) \boldsymbol{\mathcal{F}}^k_Y - \left[\sum_{q=1}^{Q_{\mathcal{A}_Y}} \partial_{\mu_i} \sigma^q_{\mathcal{A}_Y}(\mu) \boldsymbol{\mathcal{A}}^q_Y\right] \boldsymbol{\alpha}^k(\mu),$$

where we make use of the fact that due to the affine decompositions, the partial derivatives directly apply to the σ-functions. The most important remark here is that the above expression does not contain any addition offline data in comparison to the reduced model for the cell problems. Thus, the overall computational efford to calculate the parameter derivatives is neglectable.

A similar result can be given for $u^0_N(\mu)$: For the coefficient vector $\partial_{\mu_i} \boldsymbol{\beta}(\mu)$ of $\partial_{\mu_i} u^0_N(\mu)$ we have

$$\left[\sum_{q=1}^{Q_{\mathcal{A}_N}} \sigma^q_{\mathcal{A}_N}(\mu) \boldsymbol{\mathcal{A}}^q_N\right] \partial_{\mu_i} \boldsymbol{\beta}(\mu) = \sum_{q=1}^{Q_{\mathcal{F}}} \partial_{\mu_i} \sigma^q_{\mathcal{F}}(\mu) \boldsymbol{\mathcal{F}}^q - \left[\sum_{q=1}^{Q_{\mathcal{A}_N}} \partial_{\mu_i} \sigma^q_{\mathcal{A}_N}(\mu) \boldsymbol{\mathcal{A}}^q_N\right] \boldsymbol{\beta}(\mu).$$

Again, no addition offline efford is needed. Higher order derivatives allow similar splittings as above, also with no extra data that has to be generated in the offline phase.

3.3. Optimization with reduced models. Our aim was to give a reduced basis approximation of the optimization problem (1.1). At this point we have all the neccessary ingredients to do this. First of all, we introduce the RB approximations of the functionals J and C_j as

$$\left.\begin{aligned} J_N(\mu) &:= J(u_N^0(\mu), \mu) \\ C_{N,j}(\mu) &:= C_j(u_N^0(\mu), \mu) \end{aligned}\right\} \tag{3.9}$$

Then, the *reduced optimization problem* reads

$$\left.\begin{aligned} \text{Find} \quad & \mu_N^* = \arg\min J_N(\mu) \\ \text{subject to} \quad & C_{N,j}(\mu) \leq 0 \quad \forall j = 1, \dots, N, \\ & \mu \in \mathcal{P} \end{aligned}\right\} \tag{3.10}$$

In order to solve this problem efficiently, we need offline-online splittings for the involved functionals. To that end we assume that J_N and $C_{N,j}$ allow an expansion similar to the affine decomposition above; in detail, we require

$$\left.\begin{aligned} J_N(\mu) &= \sum_{q=1}^{Q_{J_N}} \sigma_{J_N}^q(\mu) J_N^q(\varphi_1, \dots, \varphi_N), \\ C_{N,j}(\mu) &= \sum_{q=1}^{Q_{C_{N,j}}} \sigma_{C_{N,j}}^q(\mu) C_{N,j}^q(\varphi_1, \dots, \varphi_N), \end{aligned}\right\} \tag{3.11}$$

i.e. the reduced functionals can be decomposed into parameter-dependent parts only, and into reduced-basis-dependent parts.[2] Notice that J_N^q and $C_{N,j}^q$ can be arbitrary mappings. These decompositions ensure that the functionals as well as their parameter derivatives allow an offline-online splitting and are therefore efficiently computable for many different parameters.

REMARK 3.4. *There is a huge variaty of functionals that allow such a decomposition. Here are some examples:*

- *Solution $u_N^0(\mu)$ not involved: $J_N(\mu) = c(\mu)$ with an arbitrary $c : \mathcal{P} \to \boldsymbol{R}$*
- *Polynomial integral expressions: $J_N(\mu) = \int_\Omega (u_N^0(\mu) - u_{ref})^p \, dx$ for some $p \in \boldsymbol{N}$ and a given reference configuration $u_{ref} : \Omega \to \boldsymbol{R}$*
- *Point evaluations: $J_N(\mu) = u_N^0(x_{ref}; \mu)$ for some $x_{ref} \in \Omega$*

REMARK 3.5. *In addition to* (3.11) *– which is needed for computational efficiency – further restrictions might be needed to ensure existence (and uniqueness) of μ_N^* in* (3.10)*, see for example [8].*

4. Numerical experiments. We consider $\Omega = (0, 0.6) \times (0, 0.2) \subset \boldsymbol{R}^2$, with $\Gamma_{R_1} = [0, 0.2] \times \{0.2\}, \Gamma_{R_2} = [0.4, 0.6] \times \{0.2\}$ and $\Gamma_N = \partial\Omega \setminus (\Gamma_{R_1} \cup \Gamma_{R_2})$. For the source term we define two circular bubbles $W_i = \{x \in \Omega \mid ||x - c_i|| < r_i\}$ with $c_1 = (0.15, 0.1), c_2 = (0.45, 0.1)$ and $r_1 = r_2 = 0.025$. We introduce four scalar parameters $\mu = (\mu_1, \dots, \mu_4)$ and the parameter space is $\mathcal{P} = [0.001, 1]^4 \subset \boldsymbol{R}^4$. As data functions we specify

$$\begin{aligned} f(x) &= 500 \cdot \mathbf{1}_{W_1}(x) + 800 \cdot \mathbf{1}_{W_2}(x) && (x \in \Omega) \\ g(x; \mu) &= 300 \left(\mu_3 \cdot \mathbf{1}_{\Gamma_{R_1}}(x) + \mu_4 \cdot \mathbf{1}_{\Gamma_{R_2}}(x)\right) && (x \in \Gamma_{R_1} \cup \Gamma_{R_2}) \end{aligned}$$

[2] This is actually a restriction to J and C_J, cf. (3.9)

and the microscopic diffusion

$$A(y;\mu) = 16(\mu_2 - \mu_1)y_1^2(1-y_1)^2 + \mu_1 \qquad (y \in Y),$$

extended to $\boldsymbol{R}^d$ by periodicity w.r.t. Y. Our test problem then is (1.2) with A and f as above where the Dirichlet condition is replaced by a no-flow condition on Γ_N and Robin condition on the rest of $\partial\Omega$ (with right hand side g).[3] It should be mentioned that in this special case all cell solutions $\chi^2(\mu)$ vanish, since the diffusion tensor depends only on y_1, cf. (2.2).

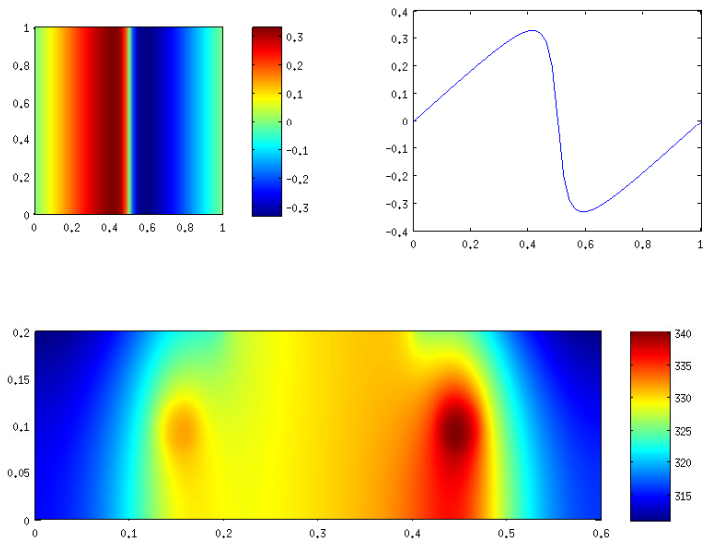

FIG. 4.1. *Example of a reduced solution of the test problem for* $\mu = (0.2, 0.01, 0.3, 0.4)$. *Top left:* $\chi_h^1(\mu)$, *top right: cross-section plot of* $\chi_h^1(\mu)$ *in* y_1*-direction; bottom:* $u_h^0(\mu)$. *The effective diffusion tensor is* $A_h^0(\mu) = \mathrm{diag}(0.013, 0.094)$.

As discretization for the high-dimensional computations we chose piecewise linear finite elements on uniform grids with $N_Y = 5,000$ and $N_\Omega = 60,000$ triangles. An example of a possible solution is given in Figure 4.1. The reduced spaces were assembled by a walk-through of a uniform grid in parameter space. Table 4.1 shows computational times for both detailed and reduced simulations, as well as reduction errors for the macroscopic solution and one of the cell problems, calculated as the average over 100 randomly chosen parameters μ.

4.1. Reduced multiscale optimization experiment. We test our method with two different optimization problems. The first one has linear constraints and an objective functional depending only on the parameter μ, while the second one is unconstrained with a quadratic objective functional. More precisely, we define

$$J_1(u^0(\mu),\mu) := \sum_{i=1}^{4} \omega_i (1+\mu_i)^{\beta_i}, \quad C_1(u^0(\mu),\mu) := \frac{1}{|\Omega|}\int_\Omega u^0(\mu)\,\mathrm{d}x - T_{\max}$$

[3] It can be shown that the homogenization theory is valid for this setting, too.

TABLE 4.1
Comparison between detailed and reduced simulations for different sizes of the reduced bases (averaged over 100 parameters).

(N_Y, N_Ω)	time det.	time red.	$\|\|u_h^0 - u_N^0\|\|$	$\|\|\chi_h^1 - \chi_N^1\|\|$
$(5, 10)$	1.30s	23.20ms	$7.36 \cdot 10^{-2}$	$7.22 \cdot 10^{-3}$
$(10, 20)$	1.38s	23.65ms	$3.64 \cdot 10^{-4}$	$8.09 \cdot 10^{-5}$
$(15, 30)$	1.47s	29.27ms	$4.69 \cdot 10^{-5}$	$1.93 \cdot 10^{-7}$

for the first and

$$J_2(u^0(\mu), \mu) := \int_\Omega \left(u^0(\mu) - u_{\text{ref}}\right)^2 \, \mathrm{d}x + \frac{\alpha}{2}||\mu||^2, \quad C_2(u^0(\mu), \mu) :\equiv 0$$

for the second problem. Here, $\omega_i, \beta_i, T_{\max}, \alpha \in \boldsymbol{R}$ are given constants and $u_{\text{ref}} : \Omega \to \boldsymbol{R}$ is a reference configuration. For the upcoming results we used $\omega_i = 1, \beta_i = 2, T_{\max} = 650$, $u_{\text{ref}} \equiv T_{\max}$ and $\alpha = 2$. The results are given in tables 4.2 and 4.3. We see that the relative error between the reduced optimum μ_N^* and the detailed one μ_h^* is not too big even for very small reduced bases and drops significantly for larger ones. We also see that our method (including all offline calculations) is very efficient compared to the detailed method, which finds expression in the speed-up factors. Note that the online phase for the second setting increases stronger with the RB size than for the first one. This is due to the fact that for the functional J_2 the number of terms in the affine decomposition scales quadratically with the basis size, while for C_1 this dependence is linear. Nevertheless, computational time is in both cases independent of the dimension of the underlying high dimensional FEM solutions.

The resulting nonlinear programs are solved using the Matlab routine `fmincon` with a built-in interior-point algorithm that can handle both linear and nonlinear equality and inequality constraints as well as box constraints.

TABLE 4.2
Results of both optimization settings for different sizes of the reduced bases. In column 4, μ_h^* stands for the optimal parameter calculated with a detailed optimization. The runtime includes only the online phase.

	(N_Y, N_Ω)	μ_N^*	$\frac{\|\|\mu_N^* - \mu_h^*\|\|}{\|\|\mu_h^*\|\|}$	runtime [s]
S.1	$(5, 10)$	(0.0040, 0.0081, 0.0212, 0.0245)	1.77e-2	2.9
	$(10, 20)$	(0.0037, 0.0085, 0.0213, 0.0246)	8.63e-4	2.8
	$(15, 30)$	(0.0037, 0.0086, 0.0213, 0.0246)	3.76e-4	3.7
S.2	$(5, 10)$	(0.2109, 0.2313, 0.0149, 0.0216)	4.42e-3	10.4
	$(10, 20)$	(0.2098, 0.2303, 0.0147, 0.0218)	4.40e-4	17.6
	$(15, 30)$	(0.2099, 0.2304, 0.0147, 0.0218)	6.14e-5	30.5

5. Conclusion. In this contribution we investigated in model reduction for paramter optimization of elliptic multiscale problems. We introduced the reduced basis method in this context and demonstrated in numerical experiments the accuracy and efficiency of this model reduction approach in multi-query optimization scenarios for multiscale problems.

TABLE 4.3

Computational time for detailed and reduced optimization, with the size of the reduced bases being $(N_Y, N_\Omega) = (15, 30)$. *In columns 3 and 4, the given values are without resp. with offline phase.*

	detailed [s]	reduced [s]	speed-up factor
S.1	670.7	3.7 / 32.0	181.3 / 21.0
S.2	1528.0	27.5 / 98.7	55.6 / 15.5

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