AN ADAPTIVE PROJECTED NEWTON NON-CONFORMING DUAL APPROACH FOR TRUST-REGION REDUCED BASIS APPROXIMATION OF PDE-CONSTRAINED PARAMETER OPTIMIZATION

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Abstract. In this contribution we device and analyze improved variants of the non-conforming dual approach for trust-region reduced basis (TR-RB) approximation of PDE-constrained parameter optimization that has recently been introduced in [Keil et al., A non-conforming dual approach for adaptive Trust-Region Reduced Basis approximation of PDE-constrained optimization. arXiv:2006.09297, 2020]. The proposed methods use model order reduction techniques for parametrized PDEs to significantly reduce the computational demand of parameter optimization with PDE constraints in the context of large-scale or multi-scale applications. The adaptive TR approach allows to localize the reduction with respect to the parameter space along the path of optimization without wasting unnecessary resources in an offline phase. The improved variants employ projected Newton methods to solve the local optimization problems within each TR step to benefit from high convergence rates. This implies new strategies in constructing the RB spaces, together with an estimate for the approximation of the hessian. Moreover, we present a new proof of convergence of the TR-RB method based on infinite-dimensional arguments, not restricted to the particular case of an RB approximation and provide an a posteriori error estimate for the approximation of the optimal parameter. Numerical experiments demonstrate the efficiency of the proposed methods.

Introduction

Parametric PDE-constrained optimization problems are of interest in many fields, such as geology, chemistry and engineering. Although the PDE model effectively describes the behavior of the system, these models may lead to difficulties when computing an optimal solution with respect to a given
cost. First, it may not be guaranteed that there exists a unique optimum, due to the fact that the problem may not be (strictly) convex. Second, discretizing the PDE by, e.g., Finite Element (FE) or Finite Volume methods leads to high dimensional full order models (FOM) which might be arbitrarily costly to solve. The latter led to an extensive research activity over the last two decades, particular remedies include mesh adaptivity and/or model order reduction (MOR), see [5, 6, 15, 28, 35, 46] and [7, 26, 44], respectively.

**Model order reduction for PDE-constrained optimization.** MOR techniques are a broad family of methods used to reduce the computational complexity of a given system, by exploiting its underlying structure and by building a reduced order model (ROM). Among these, the Reduced Basis method (RB) is particularly suited for parameter-dependent problems. This projection-based technique consists in reconstructing an approximation to the solution manifold of the PDE in a low-dimensional linear space, spanned by given solutions (snapshots) for carefully selected parameters. One approach to construct a ROM (the so called **offline phase**) is to employ a goal-oriented greedy algorithm based on a posteriori error estimates on the error between FOM and ROM quantities, resulting in quasi-optimally selected snapshots [10, 25]. Alternatively, the ROM can be built by means of a proper orthogonal decomposition (POD) in the method of snapshots; see [24] and the references therein. Once the ROM is built, it can be evaluated quickly (the so-called **online phase**). There exists a large amount of literature using such reduced order surrogate models for optimization methods. A posteriori error estimates for reduced order approximation of linear-quadratic parametric optimization (and optimal control) problems were studied, e.g., in [17, 18, 23, 31, 37, 42]. In particular, in [18, 31] the authors show a posteriori error estimates also for the error between the optimal parameter/control and the approximate one. Although the standard offline/online decomposition is a viable approach for parametric optimization problems, its performance suffers when the dimension of the parameter space increases significantly. For very high dimensional parameter sets, simultaneous parameter and state reduction can be considered [27, 34]. To speed-up the process, it is advantageous to follow the optimization pattern and compute only locally accurate RB models; see, e.g. [9, 22, 52]. In this context, localized RB methods, based on efficient localized a posteriori error control and online enrichment, are particularly well-suited [11, 12, 39, 40, 41]. With respect to the above mentioned works, we are interested in a different, but related approach, which is based on a trust-region (TR) method.

**Trust-Region reduced order models for parametric PDE-constrained optimization.** TR approaches are widely used in optimization, thanks to their robust behavior, which ensures global convergence. The key idea is to define a local approximation of the nonlinear objective, which allows using faster optimization tools; cf. [16, 38]. Obviously, the accuracy of the surrogate model has to be monitored during the TR iterations and possible updates
have to be considered. A well-established method for MOR is the TR-POD algorithm [1, 45]. Furthermore, in [43] a TR-RB algorithm is presented for PDE-constrained optimization problems with unbounded parameter sets. This method is based on [51], where necessary and sufficient conditions are given to guarantee the convergence of the TR method. In this case, the TR is defined accordingly to the a posteriori error estimate for the cost functional. In [32], the TR-RB method of [43] is extended to the case of constrained parameter sets and further improved regarding its convergence.

Main results. In this contribution we present several significant advances for the adaptive TR-RB optimization method presented in [32]:

- We propose higher order TR-RB methods using the projected Newton method to solve the TR sub-problems. The gradient and hessian of the optimization cost functional are approximated using the non-conforming dual (NCD) approach;
- we provide efficiently computable a posteriori error estimates for the ROM error in reconstructing the FOM hessian and the optimal parameter;
- we present a new proof of convergence of the TR-RB method based on infinite-dimensional arguments, not restricted to the particular case of an RB approximation;
- we devise a new adaptive enrichment strategy for the progressive construction of RB spaces, including rigorous conditions for skipping enrichment to ensure the smallest possible ROM dimension;
- we demonstrate in numerical experiments that our new TR-RB methods outperform existing approaches for large scale optimization problems in well defined benchmark problems.

Organization of the article. In Section 1 we introduce the PDE-constrained optimization problem and the necessary and sufficient optimality conditions to characterize local minimizers. In Section 2, we derive the FOM and ROM and furthermore state the a posteriori error estimates to certify the ROM, with particular focus on the approximation of the FOM hessian and the optimal parameter. The improved adaptive TR-RB algorithm is introduced in Section 3, where also the convergence analysis and adaptive Taylor-based enrichment strategy are carried out. Finally, the numerical experiments, in which we compare the algorithm to selected state of the art optimization methods from the literature, are illustrated in Section 4.

1. Problem formulation

Given a real-valued Hilbert space $V$ with inner product $(\cdot, \cdot)$ and its induced norm $\| \cdot \|$, we are interested in efficiently approximating PDE-constrained parameter optimization of a quadratic continuous functional $J : V \times P \to \mathbb{R}$, where the compact and convex admissible parameter set $P \subset \mathbb{R}^P$, with $P \in \mathbb{N}$ is considered to describe bilateral box constraints, i.e.,

$$P := \{ \mu \in \mathbb{R}^P \mid \mu_a \leq \mu \leq \mu_b \} \subset \mathbb{R}^P,$$
for given parameter bounds $\mu_a, \mu_b \in \mathbb{R}^P$, where “$\leq$” has to be understood component-wise. To be more precise, we consider the minimization problem

\[(P.a) \quad \min_{\mu \in \mathcal{P}} J(u_\mu, \mu), \quad \text{with} \quad J(u, \mu) = \Theta(\mu) + j_\mu(u) + k_\mu(u, u),\]

subject to $u_\mu \in V$ being the solution of the state – or primal – equation

\[(P.b) \quad a_\mu(u_\mu, v) = l_\mu(v) \quad \text{for all} \quad v \in V,\]

where $\Theta \in \mathcal{P} \to \mathbb{R}$ denotes a parameter functional. For each admissible parameter $\mu \in \mathcal{P}$, $a_\mu : V \times V \to \mathbb{R}$ denotes a continuous and coercive bilinear form, $l_\mu, j_\mu : V \to \mathbb{R}$ are continuous linear functionals and $k_\mu : V \times V \to \mathbb{R}$ denotes a continuous symmetric bilinear form. The primal residual of $(P.b)$ is key for the optimization as well as for a posteriori error estimation. We define for given $u \in V$, $\mu \in \mathcal{P}$, the primal residual $r^p_\mu(u) \in V'$ associated with $(P.b)$ by

\[(1.1) \quad r^p_\mu(u)[v] := l_\mu(v) - a_\mu(u, v) \quad \text{for all} \quad v \in V.\]

**Remark 1.1.** The Lagrange functional for $(P)$ is given by $\mathcal{L}(u_\mu, \mu, p) = J(u_\mu, \mu) + r^p_\mu(u)[p]$ for $(u_\mu, \mu) \in V \times \mathcal{P}$ and for $p \in V$. In particular we have $J(u_{\mu}, \mu) = \mathcal{L}(u_{\mu}, \mu, p)$ for all $p \in V$.

A standard assumption for the efficient employment of RB methods is the parameter separability from $V$, which we assume in this work. For applications where this assumption does not hold, so-called empirical interpolation (EI) techniques [4, 14, 20] can be utilized.

**Assumption I** (Parameter-separability). For $\Xi^a, \Xi^l, \Xi^j, \Xi^k \in \mathbb{N}$, we assume $a_i, l_i, j_i, k_i$ to be parameter separable with non-parametric components $a_i : V \times V \to \mathbb{R}$ for $1 \leq i \leq \Xi^a$, $l_i \in V'$ for $1 \leq i \leq \Xi^l$, $j_i \in V'$ for $1 \leq i \leq \Xi^j$ and $k_i : V \times V \to \mathbb{R}$ for $1 \leq i \leq \Xi^k$, and respective parameter functionals $\theta^a_i, \theta^l_i, \theta^j_i, \theta^k_i \in \mathcal{P}$, such that

\[
a_\mu(u, v) = \sum_{i=1}^{\Xi^a} \theta^a_i(\mu) a_i(u, v), \quad l_\mu(v) = \sum_{i=1}^{\Xi^l} \theta^l_i(\mu) l_i(v),\]

and analogously for $j_\mu$ and $k_\mu$.

Parameter separability also holds for the primal residual, the cost functional as well as all other linear dependent quantities in this work.

Gradient-based solution methods for problems of type $(P)$ require information about first-order directional derivatives of the cost functional $J$. If second-order derivatives are available, more advanced optimization routines can be applied which generally yields higher local convergence rates.

### 1.1. Notation for differentiability

Assuming the objective functional $J : V \times \mathcal{P} \to \mathbb{R}$ to be Fréchet differentiable w.r.t. $\mu \in \mathcal{P}$, we define the Fréchet derivative of $J$ w.r.t. its second argument in the direction of $\nu \in \mathbb{R}^P$ by $\partial_\nu J(u, \mu) \cdot \nu$ (noting that the dual space of $\mathbb{R}^P$ is itself). Moreover, we refer to $\partial_\mu J(u, \mu)$ as the derivative w.r.t. $\mu$ and for $u \in V$, $\mu \in \mathcal{P}$ we
denote the partial derivative of $J(u, \mu)$ w.r.t. the $i$-th component of $\mu$ by $\partial_{\mu_i}J(u, \mu)$ for $1 \leq i \leq P$. Note that $\partial_{\mu_i}J(u, \mu) = \partial_{\mu_i}J(u, \mu) \cdot e_i$, where $e_i \in \mathbb{R}^P$ denotes the $i$-th canonical unit vector. Furthermore, we denote the gradient of $J$ w.r.t. its second argument – the vector of components $\partial_\mu J(u, \mu)$ – by the operator $\nabla_\mu J : V \times \mathcal{P} \to \mathbb{R}^P$. Similarly, if $J$ is Fréchet differentiable w.r.t. each $u \in V$, for each $u \in V$ and each $\mu \in \mathcal{P}$ there exists a bounded linear functional $\partial_u J(u, \mu) \in V'$, such that the Fréchet derivative of $J$ w.r.t. its first argument in any direction $v \in V$ is given by $\partial_u J(u, \mu)[v]$. We refer to $\partial_u J(u, \mu)$ simply as the derivative w.r.t. $u$. If $J$ is twice Fréchet differentiable w.r.t. each $\mu \in \mathcal{P}$, we denote its hessian w.r.t. its second argument by the operator $\mathcal{H}_\mu J : V \times \mathcal{P} \to \mathbb{R}^{P \times P}$. Finally, we denote the total derivative w.r.t. $\mu_i$ by $d_{\mu_i}$, i.e. $d_{\mu_i} J(u, \mu) = \partial_{\mu_i} J(u, \mu) + \partial_u J(u, \mu)[d_{\mu_i} u]$.

We treat $a, l, k$ and $\mu$ to be twice continuously differentiable as well. We also require all $\mu$-dependent functions to have locally Lipschitz-continuous second derivatives (for locally quadratic convergence of the projected Newton method).

For the continuous and coercive bilinear form $a_\mu(\cdot, \cdot)$, we can define the bounded solution map $S : \mathcal{P} \to V$, $\mu \mapsto u_\mu =: S(\mu)$, where $u_\mu$ is the unique solution to (P.b) for a given $\mu \in \mathcal{P}$. The Fréchet derivatives of $S$ have been used for RB methods for constructing Taylor RB spaces (see [25]) and for deriving optimality conditions for (P) (see [29, 49]).

**Proposition 1.2** (Fréchet derivative of the solution map). *Considering the solution map $S : \mathcal{P} \to V$, $\mu \mapsto u_\mu = S(\mu)$, its Fréchet derivative $d_\nu u_\mu = S'(\mu) \cdot \nu \in V$ w.r.t. a direction $\nu \in \mathbb{R}^P$ is the unique solution of

\begin{equation}
\tag{1.2}
a_\mu(d_\nu u_\mu, v) = \partial_\mu r^{pr}_\mu(u_\mu)[v] \cdot \nu \quad \text{for all } v \in V.
\end{equation}

**Proof.** We refer, e.g., to [29, 49] for the proof of this result. \hfill \Box

1.2. Optimal solution and optimality conditions. Existence of an optimal solution to the non-convex problem (P) follows from [29, Theorem 1.45].

Using first- and second-order optimality conditions we can characterize local optimal solutions. Throughout the paper a bar indicates (local) optimality.

**Proposition 1.3** (First-order necessary optimality conditions). *Let $(\bar{u}, \bar{\mu}) \in V \times \mathcal{P}$ be a local optimal solution to (P). Moreover, let Assumption II hold true. Then there exists an associated unique Lagrange multiplier $\bar{\lambda} \in V$ such that the following first-order necessary optimality conditions hold:

\begin{align}
\tag{1.3a}
r^{pr}_{\mu_i}(\bar{u})[v] &= 0 \quad \text{for all } v \in V, \\
\tag{1.3b}
\partial_u J(\bar{u}, \bar{\mu})[v] - a_\mu(v, \bar{\lambda}) &= 0 \quad \text{for all } v \in V,
\end{align}
Proposition 1.4 \((\text{Fréchet derivative of the dual solution map})\). Considering the dual solution map \(A : P \rightarrow V\), \(\mu \mapsto p_\mu := A(\mu)\), we denote its directional derivative \(d_\nu p_\mu = A'(\mu) \cdot \nu \in V\), which is given as the solution of

\[
(1.6) \quad a_\mu(q, d_\nu p_\mu) = -\partial_\mu a_\mu(q, p_\mu) \cdot \nu + d_\mu \partial_\nu J(u_\mu, \mu)[q] \cdot \nu + 2k_\mu(q, d_\nu u_\mu)
\]

for all \(q \in V\), where the latter equality holds for quadratic \(J\) as in (P.a).

Proof. For a proof we refer to [29, 49], for instance.

We introduce the reduced functional \(\hat{J} : P \rightarrow \mathbb{R}\), \(\mu \mapsto \hat{J}(\mu) := J(u_\mu, \mu) = J(S(\mu), \mu)\). Then problem (P) is equivalent to the so-called reduced problem \((\hat{P})\)

\[
\min_{\mu \in P} \hat{J}(\mu).
\]

In contrast to (P), problem \((\hat{P})\) has only inequality constraints, but no equality ones. Using definitions and notations from above we can compute first-order derivatives of \(\hat{J}\) by means of its gradient \(\nabla_\mu \hat{J} : P \rightarrow \mathbb{R}^P\).

Proposition 1.5 \((\text{Gradient of } \hat{J})\). For given \(\mu \in P\), the gradient of \(\hat{J}\), \(\nabla_\mu \hat{J} : P \rightarrow \mathbb{R}^P\), is given by

\[
\nabla_\mu \hat{J}(\mu) = \nabla_\mu \Theta(\mu) + \nabla_\mu j_\mu(u_\mu) + \nabla_\mu k_\mu(u_\mu, u_\mu) + \nabla_\mu r^{\mu}_{\mu}(u_\mu)[p_\mu].
\]

Proof. This follows from (1.1), (1.2), (1.4) and (P.a), cf. [29].
Remark 1.6. The proof of Proposition 1.5 relies on the fact that both \( u_\mu \) and \( p_\mu \) belong to the same space \( V \); cf. [29]. In particular, for any \( \mu \in \mathcal{P} \), we have \( \nabla_\mu \hat{J}(\mu) = \nabla_\mu \mathcal{L}(u_\mu, \mu, p_\mu) \).

For \( \bar{\mu} \) satisfying the first-order necessary optimality conditions (1.3), we have that \( \bar{\mu} \) is a stationary point of the cost functional \( \hat{J} \). Thus, \( \bar{\mu} \) can be either a local minimum, a saddle point or a local maximum of the cost functional \( \hat{J} \) (and obviously the same relationship occurs between \( (\bar{u}, \bar{\mu}) \) and \( \hat{J} \)). We thus consider second-order sufficient optimality conditions in order to characterize local minima of the functional \( \hat{J} \), requiring its hessian.

**Proposition 1.7** (Hessian of \( \hat{J} \)). The hessian of \( \hat{J} \), \( \hat{H}_\mu := \hat{H}_\mu \hat{J} : \mathcal{P} \to \mathbb{R}^{P \times P} \), is determined by its application to a direction \( \nu \in \mathbb{R}^P \), given by

\[
\hat{H}_\mu(\nu) = \nabla_\mu \left( \partial_\mu \hat{J}(u_\mu, \mu)[d_\nu u_\mu] + r_\mu^p(u_\mu)[d_\nu p_\mu] - a_\mu(d_\nu u_\mu, p_\mu) \right) + \left( \partial_\mu \hat{J}(u_\mu, \mu) + \partial_\mu r_\mu^p(u_\mu)[\nu] \right) \cdot \nu,
\]

where \( u_\nu, p_\mu \in V \) denote the primal and dual solutions, respectively. For a quadratic \( \hat{J} \) as in (P.a) the above formula simplifies to

\[
\hat{H}_\mu(\nu) = \nabla_\mu \left( j_\mu(d_\nu u_\mu) + 2k_\mu(d_\nu u_\mu, u_\mu) + l_\mu(d_\nu p_\mu) - a_\mu(u_\nu, d_\nu p_\mu) \right) - a_\mu(d_\nu u_\mu, p_\mu) + \left( \partial_\mu \hat{J}(u_\mu, \mu) + \partial_\mu l_\mu(p_\mu) - \partial_\mu a_\mu(u_\mu, p_\mu) \right) \cdot \nu.
\]

**Proof.** See, e.g., [29] for the first part. The second one follows from a direct computation. \( \square \)

**Proposition 1.8** (Second-order sufficient optimality conditions). Let Assumption II hold true. Suppose that \( \bar{\mu} \in \mathcal{P} \) satisfies the first-order necessary optimality conditions (1.3). If \( \hat{H}_\mu(\bar{\mu}) \) is positive definite on the critical cone \( \mathcal{C}(\bar{\mu}) \) at \( \bar{\mu} \in \mathcal{P} \), i.e., if \( \nu \cdot (\hat{H}_\mu(\bar{\mu}) \cdot \nu) > 0 \) for all \( \nu \in \mathcal{C}(\bar{\mu}) \setminus \{0\} \), with

\[
\mathcal{C}(\bar{\mu}) := \{ \nu \in \mathbb{R}^P \mid \exists \mu \in \mathcal{P}, c_1 > 0 : \nu = c_1(\mu - \bar{\mu}), \nabla_\mu \hat{J}(\bar{\mu}) \cdot \nu = 0 \},
\]

then \( \bar{\mu} \) is a strict local minimum of \( \hat{P} \).

**Proof.** For this result we refer to [13, 38], for instance. \( \square \)

**Remark 1.9.** For so-called small residual problems (i.e, \( \|\partial_\mu \hat{J}(\bar{u}, \bar{\mu})\|_V \) is small) one can ensure that the second-order sufficient optimality conditions hold. The proof is analogous to [50, Section 3.3].

2. High dimensional discretization and model order reduction

To discretize the optimization problem (P) and the corresponding derivatives of the cost functional we use a classical Ritz-Galerkin projection onto a finite, but possibly high dimensional finite element space \( V_h \subset V \). Based on this FOM we then define a ROM using the reduced basis method with possibly different reduced primal and dual state spaces as well as different
reduced spaces for the primal and dual sensitivity equations. Since the resulting ROM will in general not be equivalent to a Ritz-Galerkin projection of the FOM onto a reduced space $V_r \subset V_h$, we follow the approach from [32], to define a non-conforming dual (NCD) corrected ROM.

2.1. Full order model. Assuming $V_h \subset V$ to be a finite-dimensional subspace, we define a Ritz-Galerkin projection of (P) onto $V_h$ by considering, for each $\mu \in P$, the solution $u_{h,\mu} \in V_h$ of the discrete primal equation

$$a_{\mu}(u_{h,\mu}, v_h) = l_{\mu}(v_h)$$

for all $v_h \in V_h$, which gives $r_{pr}^\mu(u_{h,\mu})[v_h] = 0$ for all $v_h \in V_h, \mu \in P$. We also define, for each $\mu \in P$, the solution $p_{h,\mu} \in V_h$ of the discrete dual equation

$$a_{\mu}(q_h, p_{h,\mu}) = \partial_u J(u_{h,\mu}, \mu)[q_h] = j_{\mu}(q_h) + 2k_{\mu}(q_h, u_{h,\mu}) \quad \forall q_h \in V_h,$$

which results in $r_{du}^\mu(u_{h,\mu}, p_{h,\mu})[q_h] = 0$ for all $q_h \in V_h, \mu \in P$. Similarly, the discrete primal sensitivity equations for solving for $d_{\mu}u_{h,\mu} \in V_h$ as well as discrete dual sensitivity equations for solving for $d_{\mu}p_{h,\mu} \in V_h$ at any direction $\nu \in P$ follow directly analogue to Propositions 1.2 and 1.4. Furthermore, instead of $\tilde{J}$ we define the discrete reduced functional

$$\tilde{J}_h(\mu) := J(u_{h,\mu}, \mu) = L(u_{h,\mu}, \mu, p_h)$$

for all $p_h \in V_h$, where $u_{h,\mu} \in V_h$ is the unique solution of (2.1), and we formulate the discrete optimization problem

$$(\hat{P}_h) \quad \min_{\mu \in P} \tilde{J}_h(\mu).$$

Further, $\hat{\mu}_h$ denotes a locally optimal solution to $$(\hat{P}_h)$$ satisfying first- and second-order optimality conditions.

Remark 2.1. Since $u_{h,\mu}$ and $p_{h,\mu}$ belong to the same space $V_h$, Propositions 1.3-1.5,1.7-1.8 from Section 2.1 hold for the FOM as well, with all quantities replaced by their discrete counterparts.

Analogously to Proposition 1.7 we define a shorthand for the hessian of the discrete reduced functional as $\tilde{H}_{h,\mu} := H_{\mu}\tilde{J}_h : P \to \mathbb{R}^{P \times P}$. As usual in the context of RB methods, we eliminate the issue of “truth” by assuming that the high dimensional space $V_h$ is accurate enough to approximate the true solution.

Assumption III (This is the “truth”). We assume that the primal discretization error $\|u_{\mu} - u_{h,\mu}\|$, the dual error $\|p_{\mu} - p_{h,\mu}\|$, the primal sensitivity errors $\|d_{\mu}u_{\mu} - d_{\mu}u_{h,\mu}\|$ and the dual sensitivity errors $\|d_{\mu}p_{\mu} - d_{\mu}p_{h,\mu}\|$ are negligible for all $\mu \in P, 1 \leq i \leq P$.

To define a suitable ROM for the optimality system, we assume that we have computed problem adapted RB spaces $V_{pr}^r, V_{du}^r \subset V_h$, the construction of which is detailed in Section 3.3. We stress here that $V_{pr}^r$ and $V_{du}^r$ might not coincide, which implies the use of the NCD-corrected approach for reducing the optimality system (1.3).
2.2. NCD-corrected reduced order model. Given problem adapted RB spaces \( V_r^{pr}, V_r^{du} \subset V_h \) of low dimension \( n := \dim V_r^{pr} \) and \( m := \dim V_r^{du} \) we obtain the reduced versions for the optimality system as follows:

- **RB approximation for (1.3a):** For each \( \mu \in \mathcal{P} \) the primal variable \( u_{r,\mu} \in V_r^{pr} \) of the RB approximate primal equation is defined through
  \[
  (2.4a) \quad a_{\mu}(u_{r,\mu}, v_r) = l_{\mu}(v_r) \quad \text{for all } v_r \in V_r^{pr}.
  \]

- **RB approximation for (1.3b):** For each \( \mu \in \mathcal{P} \), \( u_{r,\mu} \in V_r^{pr} \) and \( p_{r,\mu} \in V_r^{du} \) the dual/adjoint variable \( p_{r,\mu} \in V_r^{du} \) satisfies the RB approximate dual equation
  \[
  (2.4b) \quad a_{\mu}(q_r, p_{r,\mu}) = \partial_\mu \mathcal{J}(u_{r,\mu}, \mu)[q_r] = j_{\mu}(q_r) + 2k_{\mu}(q_r, u_{r,\mu}) \quad \forall q_r \in V_r^{du}.
  \]

Analogously to Proposition 1.2, we define the RB solution map \( S_r : \mathcal{P} \to V_r^{pr} \) by \( \mu \mapsto u_{r,\mu} =: S_r(\mu) \) and analogously to Proposition 1.4 the RB dual solution map \( A_r : \mathcal{P} \to V_r^{du} \) by \( \mu \mapsto p_{r,\mu} =: A_r(\mu) \), where \( u_{r,\mu} \) and \( p_{r,\mu} \) denote the primal and dual reduced solutions of (2.4a) and (2.4b), respectively. Note that, in general, (2.4b) is not the dual equation with respect to the optimization problem (2.5), cf. [29, Section 1.6.4], which would only be true if \( V_r^{du} = V_r^{pr} \).

There exist several ways to approximate \( \tilde{P}_h \) in a ROM. The standard way is to simply replace all discretized quantities in the FOM by their respective reduced ones. However, if the reduced primal and dual RB spaces do not coincide, this approach results in inexact gradient and hessian information of the model. In [32], it was shown that this also results in a loss of robustness in the optimization method. Hence, we use a modified approach from [32], i.e. we define the NCD-corrected RB reduced functional by

\[
(2.5) \quad \tilde{\mathcal{J}}_r(\mu) := \mathcal{L}(u_{r,\mu}, \mu, p_{r,\mu}) = \mathcal{J}(u_{r,\mu}, \mu) + r_{\mu}^{pr}(u_{r,\mu})[p_{r,\mu}]
\]

with \( u_{r,\mu} \in V_r^{pr} \) and \( p_{r,\mu} \in V_r^{du} \) being the solutions of (2.4a) and (2.4b) for \( \mu \in \mathcal{P} \), respectively. We then consider the RB reduced optimization problem of finding a locally optimal solution \( \bar{\mu}_r \) of

\[
(\bar{P}_r) \quad \min_{\mu \in \mathcal{P}} \tilde{\mathcal{J}}_r(\mu).
\]

As in Section 1.2 we require the gradient and hessian of \( \tilde{\mathcal{J}}_r \), which can be computed following [29, Section 1.6.2].

**Proposition 2.2** (Gradient of the NCD-corrected RB reduced functional). The \( i \)-th component of the true gradient of \( \tilde{\mathcal{J}}_r \) is given by

\[
(\nabla_\mu \tilde{\mathcal{J}}_r(\mu))_i = \partial_{\mu_i} \mathcal{J}(u_{r,\mu}, \mu) + \partial_{\mu_i} r_{\mu}^{pr}(u_{r,\mu})[p_{r,\mu} + w_{r,\mu}]
\]

\[
- \partial_{\mu_i} v_{\mu}^{du}(u_{r,\mu}, p_{r,\mu})[z_{r,\mu}],
\]

where \( u_{r,\mu} \in V_r^{pr} \) and \( p_{r,\mu} \in V_r^{du} \) denote the RB approximate primal and dual solutions of (2.4a) and (2.4b), \( z_{r,\mu} \in V_r^{du} \) solves

\[
(2.6) \quad a_{\mu}(z_{r,\mu}, q) = -r_{\mu}^{pr}(u_{r,\mu})[q] \quad \forall q \in V_r^{du}
\]
and \( w_{r,\mu} \in V_{pr}^r \) solves
\[
(2.7) \quad a_{\mu}(v, w_{r,\mu}) = r_{\mu}^{pr}(u_{r,\mu}, p_{r,\mu})[v] - 2k_{\mu}(z_{r,\mu}, v), \quad \forall v \in V_{pr}^r. 
\]

We also define the derivatives of the maps \( S_r \) and \( A_r \) in direction \( \nu \in \mathcal{P} \) as the solutions \( d_\nu u_{r,\mu} \in V_{pr}^r \) and \( d_\nu p_{r,\mu} \in V_{du}^r \) of
\[
(2.8) \quad a_{\mu}(d_\nu u_{r,\mu}, v_r) = \partial_\mu \partial_\nu^{pr}(u_{r,\mu})[v_r] \cdot \nu \quad \text{for all } v_r \in V_{pr}^r 
\]
and
\[
(2.9) \quad a_{\mu}(q_r, d_\nu p_{r,\mu}) = d_\mu \partial_\nu J(u_{r,\mu}, \mu)[q_r] \cdot \nu - \partial_\mu a_{\mu}(q_r, p_{r,\mu}) \cdot \nu \quad \text{for all } q_r \in V_{du}^r, 
\]
respectively, analogously to Propositions 1.2 and 1.4, where the last equality holds for quadratic functionals as in (P.a).

**Remark 2.3.** For more accurate reduced derivatives of the solution maps in (2.8) and (2.9) one could again commit a variational crime by introducing problem adapted RB spaces for the primal and dual sensitivities w.r.t. all canonical directions, i.e. \( V_{pr}^{r, d_\mu} \) and \( V_{du}^{r, d_\mu} \). These spaces would then consist of FOM snapshots of the respective derivatives, i.e. solutions of (1.2) and (1.6); cf. [32]. We do not follow this strategy here, since the computational demand for enriching all these spaces scales with the size of the parameter space and quickly becomes unfeasible for large scale applications.

With the help of the reduced derivatives of the primal and dual solution maps, we can also compute the hessian of the NCD-corrected RB reduced functional; cf. [29, Section 1.6.4].

**Proposition 2.4** (Hessian of the NCD-corrected RB reduced functional). Given a direction \( \nu \in \mathcal{P} \), the evaluation of the hessian \( \hat{H}_{r,\mu} \) of \( \hat{J}_r \) is
\[
\hat{H}_{r,\mu}(\mu) \cdot \nu = \nabla_\mu (j_\mu(d_\nu u_{r,\mu} + 2k_{\mu}(z_{r,\mu}, d_\nu u_{r,\mu}) - a_{\mu}(d_\nu u_{r,\mu}, p_{r,\mu} + w_{r,\mu})
+ r_{\mu}^{pr}(u_{r,\mu}, d_\nu p_{r,\mu} + d_\nu w_{r,\mu}) - 2k_{\mu}(z_{r,\mu}, d_\nu u_{r,\mu} + w_{r,\mu})
+ a_{\mu}(z_{r,\mu}, d_\nu p_{r,\mu}) - r_{\mu}^{du}(u_{r,\mu}, p_{r,\mu})[d_\nu w_{r,\mu}]
+ \partial_\mu J(u_{r,\mu}, \mu)[q_r] \cdot \nu - r_{\mu}^{du}(u_{r,\mu}, p_{r,\mu})[\nabla_\mu z_{r,\mu}][d_\nu w_{r,\mu}]) \cdot \nu 
\]
where \( d_\nu u_{r,\mu}, w_{r,\mu} \in V_{pr}^r \) and \( d_\nu p_{r,\mu}, z_{r,\mu} \in V_{du}^r \) solve (2.8), (2.7), (2.9) and (2.6), respectively. Furthermore, \( d_\nu z_{r,\mu} \in V_{du}^r \) solves
\[
(2.10) \quad a_{\mu}(d_\nu z_{r,\mu}, q) = -\partial_\mu (r_{\mu}^{pr}(u_{r,\mu})[q] + a_{\mu}(z_{r,\mu}, q)) \cdot \nu + a_{\mu}(d_\nu u_{r,\mu}, q) 
\]
for all \( q \in V_{du}^r \) and \( w_{r,\mu} \in V_{pr}^r \) solves
\[
(2.11) \quad a_{\mu}(v, d_\nu w_{r,\mu}) = \partial_\mu (r_{\mu}^{du}(u_{r,\mu}, p_{r,\mu})[v] - 2k_{\mu}(z_{r,\mu}, v) - a_{\mu}(v, w_{r,\mu})) \cdot \nu 
+ 2k_{\mu}(v, d_\nu u_{r,\mu} - d_\nu w_{r,\mu}) - a_{\mu}(v, d_\nu p_{r,\mu}), \quad \forall v \in V_{pr}^r. 
\]

There exist multiple possibilities for deducing a reduced hessian. As a straight forward hessian, it is also feasible to consider the FOM hessian from Proposition 1.7 and reducing it by replacing all FOM quantities by
their respective reduced counterpart. While this approach may be a better approximation of the FOM hessian, it is not the true hessian of the NCD-corrected functional which would result in a quasi-Newton type method. In order to prevent an overload of the work at hand, we omit a further discussion of this approach. However, we emphasize that also for this approach an a posteriori error analysis is available. We further remark that the computation of the true hessian $\mathcal{H}_{r,\mu}(\mu)$ can also be realized without the use of auxiliary functions $z_{r,\mu}$ and $w_{r,\mu}$ and their derivatives, respectively. However, this results in having to compute second order derivatives of $u_{r,\mu}$ and $p_{r,\mu}$ which aggravates the computations and makes the hessian inefficiently callable from an optimization point of view because the second direction can not be pulled out. Thus, we also do not follow this approach.

2.3. A posteriori error analysis. For controlling the accuracy of the reduced model, we require a posteriori error estimates of all reduced quantities. Assumption I is the key for the efficient computation of reduced quantities because it enables to assemble FOM matrices offline. In this section, we re-state all estimates that we need for the error aware TR-RB method, and shortly mention an a posteriori result for the hessian of the NCD-corrected RB reduced functional. We also present a bound for the distance to the true functional which would result in a quasi-Newton type method. In order to prevent an overload of the work at hand, we omit a further discussion of this approach. However, we emphasize that also for this approach an a posteriori error analysis is available. We further remark that the computation of the true hessian $\mathcal{H}_{r,\mu}(\mu)$ can also be realized without the use of auxiliary functions $z_{r,\mu}$ and $w_{r,\mu}$ and their derivatives, respectively. However, this results in having to compute second order derivatives of $u_{r,\mu}$ and $p_{r,\mu}$ which aggravates the computations and makes the hessian inefficiently callable from an optimization point of view because the second direction can not be pulled out. Thus, we also do not follow this approach.

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where
\[ \gamma \Delta_{\mu_i} \leq 2 \gamma_{\mu_i} \Delta_{\mu_i} + 2 \gamma \Delta_{\mu_i} \Delta_{\mu_i,pr} \]

We also provide an a posteriori error result for the hessian of the NCD-corrected functional. We emphasize that (just as the sensitivity estimates \( \Delta_{\mu_i,pr} \) and \( \Delta_{\mu_i,du} \)) this error estimator is not a part of our TR-RB method. The proof and a detailed definition is postponed to the appendix.

**Proposition 2.6** (Upper bound on the model reduction error of the hessian of the reduced output). For the hessian \( \hat{H}_{\mu,h}(\mu) \) of \( \hat{J}_h(\mu) \) and the true hessian \( H_{\mu,h}(\mu) \) of the NCD-corrected functional from Proposition 2.4, there exists an a posteriori error bound
\[
|\hat{H}_{\mu,h}(\mu) - H_{\mu,h}(\mu)| \leq \Delta_H(\mu) := \left\| (\Delta_{H,i}(\mu))_{i,l} \right\|_2
\]
which is dependent on the estimators from Proposition 2.5, except \( \Delta_{j_h}(\mu) \).

Following ideas from [19, 31], we derive an error estimation for the optimal parameter consisting of the gradient and hessian of the FOM cost functional. This estimator relies on the following second-order condition for a strict local minima \( \bar{\mu_h} \) of \( \hat{J}_h \), i.e.
\[
(2.14) \quad \nu \cdot (\hat{H}_{\mu,h}(\bar{\mu_h}) \cdot \nu) \geq \lambda_{\min} \left\| \nu \right\|_2^2 \quad \text{for all } \nu \in \mathcal{C}(\bar{\mu_h}) \setminus \{0\},
\]
where \( \lambda_{\min} \) is the smallest eigenvalue of \( \hat{H}_{\mu,h}(\bar{\mu_h}) \), since the parameter space is finite-dimensional. Note that (2.14) is equivalent to the second-order sufficient optimality condition from Proposition 1.8. If (2.14) holds true, we have that for any \( \hat{\lambda} \) such that \( 0 < \hat{\lambda} < \lambda_{\min} \) there exists a radius \( r(\hat{\lambda}) > 0 \) such that for all \( \mu \in B(\bar{\mu}_h, r(\hat{\lambda})) \), the closed ball of radius \( r(\hat{\lambda}) \) centered in \( \bar{\mu}_h \), the following property holds:
\[
\nu \cdot (\hat{H}_{\mu,h}(\mu) \cdot \nu) \geq \hat{\lambda} \left\| \nu \right\|_2^2 \quad \text{for all } \nu \in \mathcal{C}(\bar{\mu_h}) \setminus \{0\}.
\]

**Proposition 2.7** (Upper bound for optimal parameters with the full order model). Let Assumption III be satisfied. Moreover, let \( \bar{\mu}_h \) and \( \bar{\mu}_r \) be strict local minima for the optimization problems \( \hat{P}_h \) and \( \hat{P}_r \), respectively. If \( \bar{\mu}_r \in B(\bar{\mu}_h, r(\lambda_{\min}/2)) \), then it holds
\[
(2.15) \quad \left\| \bar{\mu}_h - \bar{\mu}_r \right\|_2 \leq \Delta_{\mu}(\bar{\mu}_r) := \frac{2}{\lambda_{\min}} \left\| \zeta \right\|_2,
\]
where \( \zeta = (\zeta_i) \in \mathbb{R}^P \) with
\[
\zeta_i := \begin{cases} 
- \min(0, (\nabla \hat{J}_h(\bar{\mu}_r))_i) & \text{if } \bar{\mu}_{r,i} = (\mu_a)_i \\
- \max(0, (\nabla \hat{J}_h(\bar{\mu}_r))_i) & \text{if } \bar{\mu}_{r,i} = (\mu_b)_i \\
-(\nabla \hat{J}_h(\bar{\mu}_r))_i & \text{otherwise}
\end{cases}
\]
for $i = 1, \ldots, P$.

Proof. Note that Assumption III implies that the distance between $\mu_h$ of $(P_h)$ and a strict local minimum $\tilde{\mu}$ of $\tilde{J}$ satisfying (2.14) is negligible, thus we can follow the proof of [31, Theorem 3.4]. □

Remark 2.8. (1) Proposition 2.7 requires the strong assumption that the FOM and RB models are accurate enough to have the parameters $\mu_h$ and $\mu_r$ sufficiently close to a local minimum $\mu$. In [19], a sufficient condition based on the FOM gradient and hessian is given to guarantee this in case $\mu_h, \mu_r \in \text{int } \mathcal{P}$.

(2) Due to Proposition 2.7, we can estimate the distance to the optimal parameter $\mu_h$ without explicitly computing it. Note that the computation of $\zeta$ is not costly for Algorithm 1, since the FOM adjoint solution is available. The computation of $\lambda_{\min}$ would require the evaluation of the FOM hessian, which is a costly procedure instead. This can be sped up with a cheap estimation of the eigenvalue. In [19, Proposition 6], the authors utilize the smallest eigenvalue of the reduced-order hessian under suitable conditions. In our numerical tests, these conditions were never true, implying the inapplicability of the mentioned cheap estimate in our case. For the sake of completeness, let us mention that another technique is to compute $\lambda_{\min}$ in advance on a grid in $\mathcal{P} \subset \mathbb{R}^P$, when $P$ is sufficiently small. This approach can be even performed in parallel, since each eigenvalue computation is independent; cf. [48, Section 6.4.1].

(3) Due to the above-mentioned computational cost, we use estimate (2.15) only as post-processing tool: once the TR-RB algorithm (cf. Section 3) has converged, we check if its solution is close enough to $\mu_h$. If not, we decrease the stopping tolerance $\tau_{\text{FOC}}$ (cf. Algorithm 1) and continue with the algorithm.

3. The improved TR-RB Method

Trust-region methods iteratively compute a first-order critical point of problem (P). For each outer iteration $k \geq 0$ of the TR method, we consider a model function $m^{(k)}$ as a cheap local approximation of the quadratic cost functional $J$ in the so-called trust-region, which has radius $\delta^{(k)}$. We are therefore interested in solving the following constrained optimization subproblem

$$
\min_{s \in \mathbb{R}^P} m^{(k)}(s) \text{ subject to } \|s\|_2 \leq \delta^{(k)}, \quad \bar{\mu} := \mu^{(k)} + s \in \mathcal{P}
$$

and $r_{\bar{\mu}}^P(u_{\bar{\mu}})[v] = 0$ for all $v \in V$.

Under suitable assumptions, problem (3.1) admits a unique solution $\bar{s}^{(k)}$, which is used to compute the next outer TR iterate $\mu^{(k+1)} = \mu^{(k)} + \bar{s}^{(k)}$.

3.1. The projected Newton based TR-RB Method with optional enrichment. Trust-region methods combined with MOR techniques have
been extensively studied in, e.g., [1, 8, 32, 43]. Among these methods, we are interested in TR-RB algorithms. As discussed in [32], it is advantageous to choose the NCD-corrected RB reduced functional as the model function, i.e.,

\[ m(k)(\cdot) = \hat{J}_{\text{r}}(k)(\mu(k) + \cdot) \]

for \( k \geq 0 \), where the super-index \((k)\) indicates that we use different RB spaces \( V^{*}\), \((k)\) in each iteration. We initialize the RB space with the starting parameter \( u_{\mu(0)} \), i.e., \( V_{\text{pr}}^{(0)} = \{u_{h,\mu(0)}\} \) and \( V_{\text{du}}^{(0)} = \{p_{h,\mu(0)}\} \). Like in [32], we consider bilateral parameter constraints but employ a projected Newton method to solve (3.1), which has a faster local convergence compared to the projected BFGS, used in [32, 43]. We first state the TR-RB method suggested in [32, 43], then we remark the further improvements introduced in addition to [32, 43]. The RB version of problem (3.1) is

\[
(3.2) \quad \min_{\tilde{\mu} \in \mathcal{P}} \hat{J}_{\text{r}}(k)(\tilde{\mu}) \quad \text{s.t.} \quad \frac{\Delta \hat{J}(\tilde{\mu})}{\hat{J}_{\text{r}}(k)(\tilde{\mu})} \leq \varrho(k),
\]

where \( \tilde{\mu} := \mu(k) + s \), the equality constraint \( v_{\mu}^{\text{pr}}(u_{\tilde{\mu}})[v] = 0 \) is hidden in the definition of \( \hat{J} \) and the inequality constraints are concealed in the request \( \tilde{\mu} \in \mathcal{P} \). Due to the presence of bilateral constraints on the parameters, we introduce the projection operator \( P_{\mathcal{P}} : \mathbb{R}^{p} \to \mathcal{P} \) defined as

\[
(P_{\mathcal{P}}(\mu))_{i} := \begin{cases} 
(\mu_{a})_{i} & \text{if } \mu_{i} \leq (\mu_{a})_{i}, \\
(\mu_{b})_{i} & \text{if } \mu_{i} \geq (\mu_{b})_{i}, \\
\mu_{i} & \text{otherwise}
\end{cases} \quad \text{for } i = 1, \ldots, P.
\]

The operator \( P_{\mathcal{P}} \) is Lipschitz continuous with Lipschitz constant one; cf. [33]. The additional TR constraint, instead, is treated with a backtracking technique; cf. [43]. For solving (3.2) at iteration \( k \), the projected Newton method uses the approximated generalized Cauchy (AGC) point \( \mu_{\text{AGC}}(k) \) (cf. Definition 3.1) as warm start and generates a sequence \( \{\mu_{\text{AGC}}(k,\ell)\}_{\ell=1}^{L} \), where \( L \) is the last Newton iteration. In what follows, \( \mu^{(k,1)} := \mu_{\text{AGC}}(k) \) and the TR iterate \( \mu^{(k,\ell+1)} := \mu^{(k,\ell)} \). Throughout the paper the index \( k \) refers to the current outer TR iteration, \( \ell \) refers instead to the inner Newton iteration. Note that \( L \) may be different for each iteration \( k \). To simplify the notation, we omit this dependence unless it is strictly necessary to specify it. We define

\[
(3.3) \quad \mu^{(k,\ell)}(j) := P_{\mathcal{P}}(\mu^{(k,\ell)} + \kappa^{\ell}d^{(k,\ell)}) \in \mathcal{P},
\]

where \( \kappa \in (0, 1) \) and \( d^{(k,\ell)} \) is the chosen descent direction at the iteration \((k, \ell)\). In our case, we make the standard choice

\[
d^{(k,\ell)} = -(\mathcal{R}_{\mu}^{(k)}(\mu^{(k,\ell)}))^{-1} \nabla_{\mu} \hat{J}_{\text{r}}^{(k)}(\mu^{(k,\ell)}) \quad \text{for all } k, \ell \in \mathbb{N}, \ell \geq 1,
\]

where

\[
\mathcal{R}^{(k)}_{\mu}(\mu) = \begin{cases} 
\delta_{ij} & \text{if } i \in \mathcal{A}^{c}(\mu) \text{ or } j \in \mathcal{A}^{c}(\mu), \\
(\mathcal{H}_{\mu}(\mu))_{i,j} & \text{otherwise},
\end{cases}
\]

for \( \mu \in \mathcal{P} \).
The function $\delta_{ij}$ indicates the Kronecker delta and the set $A^c$ is the $\varepsilon$-active set for the parameter constraints, i.e.

$$A^c(\mu) = \left\{ i \in \{1, \ldots, P\} \mid (\mu_b)_i - \mu_i \leq \varepsilon \text{ or } \mu_i - (\mu_a)_i \leq \varepsilon \right\}.$$ 

For further details on the projected Newton method, the choice of $\varepsilon$ and its effect on convergence of the method, we refer to [33, Section 5.5]. Note that $\mathcal{H}_{r,\mu}(\mu)$ (and thus $\mathcal{R}_{r}(\mu)$) might not be positive definite for every $\mu \in \mathcal{P}$. Therefore we use a truncated Conjugate Gradient (CG) method to compute $d^{(k,\ell)}$, where the CG terminates when a negative curvature condition criterion is triggered. In such a way, we ensure that $d^{(k,\ell)}$ (resulting from the possible premature termination of the CG) is still a descent direction. The truncated CG is explained in [38, Algorithm 7.1]. Moreover, we enforce an Armijo-type condition

\begin{equation}
\tag{3.4a}
\hat{J}_r^{(k)}(\mu^{(k,\ell)}(j)) - \hat{J}_r^{(k)}(\mu^{(k,\ell)}) \leq -\frac{\kappa_{\text{arm}}}{\kappa^2} \|\mu^{(k,\ell)}(j) - \mu^{(k,\ell)}\|_2^2,
\end{equation}

with $\kappa_{\text{arm}} = 10^{-4}$ and the additional TR constraint on $\hat{J}_r^{(k)}$

\begin{equation}
\tag{3.4b}
q^{(k)}(\mu^{(k,\ell)}(j)) := \frac{\Delta \hat{J}_r^{(k)}(\mu^{(k,\ell)}(j))}{\hat{J}_r^{(k)}(\mu^{(k,\ell)}(j))} \leq \delta^{(k)}
\end{equation}

by selecting $\mu^{(k,\ell+1)} = \mu^{(k,\ell)}(j^{(k,\ell)})$ for $\ell \geq 1$, where $j^{(k,\ell)} < \infty$ is the smallest index for which (3.4) holds. From [32, 43], we recall that the optimization sub-problem will terminate if

\begin{equation}
\tag{3.5a}
\|\mu^{(k,\ell)} - P(\mu^{(k,\ell)} - \nabla^{\mu} \hat{J}_r^{(k)}(\mu^{(k,\ell)}))\|_2 \leq \tau_{\text{sub}}
\end{equation}

or

\begin{equation}
\tag{3.5b}
\beta_2 \delta^{(k)} \leq \frac{\Delta \hat{J}_r^{(k)}(\mu)}{\hat{J}_r^{(k)}(\mu)} \leq \delta^{(k)}
\end{equation}

where $\tau_{\text{sub}} \in (0, 1)$ is a predefined tolerance and $\beta_2 \in (0, 1)$, generally close to one. With condition (3.5b), we prevent the sub-problem to spend too much time close to the boundary of the trust-region, because the model is poor in approximation; cf. [43]. We also report the definition of AGC point for the constrained case.

**Definition 3.1** (AGC point for simple bounds). At the iteration $k$, we define the AGC point as

$$\mu_{\text{AGC}}^{(k)} := \mu^{(k,0)}(j^{(k)}_c) = P(\mu^{(k,0)} + \kappa^{(k)} \delta^{(k)}),$$

where $\mu^{(k,0)} := \mu^{(k)}$, $\delta^{(k)} := -\nabla^{\mu} \hat{J}_r^{(k)}(\mu^{(k,0)})$ and $j^{(k)}_c$ is the smallest non-negative integer $j$ for which $\mu^{(k,0)}(j)$ satisfies (3.4) for $\ell = 0$.

Analogously to [32], as an improvement over [43], we also use a condition to enlarge the TR radius adaptively, which can significantly speed up the TR-RB method. To be more precise, we check whether the sufficient
reduction predicted by the model function $\hat{J}_r^{(k)}$ is realized by the objective function, i.e.

$$\rho^{(k)} := \frac{\hat{J}_h(\mu^{(k)}) - \hat{J}_h(\mu^{(k+1)})}{\hat{J}_r^{(k)}(\mu^{(k)}) - \hat{J}_r^{(k)}(\mu^{(k+1)})} \geq \eta$$

for a tolerance $\eta \in [3/4, 1)$. Note that $\hat{J}_h$ is available, after the enrichment of the RB space [32]. In addition, since the dual solution of (1.4) is included as snapshot, also the FOM gradient $\nabla_\mu \hat{J}_h(\mu^{(k+1)})$ is available at this stage. Thus, we use it for computing the first-order critical condition for the outer TR method and hence to terminate the TR-RB algorithm. Notice that the choice of the (hidden) sub-problem solver differs from the one in [32, 43], which requires the computation of the AGC point in advance, since it is not carried out naturally by the projected Newton method. Although this issue seems disadvantageous with respect to the projected BFGS method, where this computation is normally included in the process (cf. [32, 43]), we remark that the search of the AGC point costs only one projected gradient optimization step and it is used as warm start for the projected Newton method. Therefore, the initial cost is justified by the subsequent advantage of the faster local quadratic convergence of the projected Newton method. It constitutes an improvement with respect to the projected BFGS method, in particular when the optimum is close to the boundary of the parameter set; cf. [33, 38].

Finally, we introduce the possibility of skipping to enrich the model if suitable conditions are satisfied. These conditions can be also used to accept the point $\mu^{(k+1)}$, since they directly imply the error-aware sufficient decrease condition (3.9) for the convergence of the method; cf. [51] and Section 3.2. At first, we define

$$g_h(\mu) := \|\mu - \mathcal{P}(\mu - \nabla_\mu \hat{J}_h(\mu))\|_2$$

and analogously

$$g_r^{(k)}(\mu) := \|\mu - \mathcal{P}(\mu - \nabla_\mu \hat{J}_r^{(k)}(\mu))\|_2$$

for all $\mu \in \mathcal{P}$. Then the sufficient condition for skipping the enrichment at iteration $k$ reads as follows:

$$\text{Skip_enrichment_flag}(k) := \left( q^{(k)}(\mu^{(k+1)}) \leq \beta_3 \delta^{(k+1)} \right) \text{ and } \left( g_h(\mu^{(k+1)}) - g_r^{(k)}(\mu^{(k+1)}) \right) \leq \tau_g \right) \text{ and } \left( \frac{\|\nabla_\mu \hat{J}_h(\mu^{(k+1)}) - \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k+1)})\|_2}{\|\nabla_\mu \hat{J}_h(\mu^{(k+1)})\|_2} \leq \min\{\tau_{\text{grad}}, \beta_3 \delta^{(k+1)}\} \right)$$

for given $\tau_g > 0$ and $\tau_{\text{grad}}, \beta_3 \in (0, 1)$. The first part of (3.8) indicates how much the current RB model is trustworthy in the next iteration $k + 1$, the
second condition is to ensure the convergence of the algorithm (cf. Theorem 3.8) and the third one is to measure the RB accuracy in reconstructing the FOM gradient of $\hat{J}_h$. Note that these conditions require FOM quantities. In [32], they are accessible exactly because of the enrichment, therefore it appears contradictory to request them and then skip a basis update. Here the focus is in fact not to avoid particular FOM solves a-priori, but to exploit them in order to keep the dimension of the RB space small. This is of particular importance when the TR-RB method takes many iterations (as seen in some examples in [32]), where an unconditional enrichment in each iteration would lead to overfitted and too large RB spaces, slowing down the computation in the long run.

3.2. Convergence result for the improved method. In this section, we improve the convergence analysis done in [32], first stating required assumptions from [32]. Condition (3.4b) imposes the following assumption to guarantee the well-posedness of the TR-RB algorithm.

Assumption IV. The cost functional $J(u, \mu)$ is strictly positive for all $u \in V$ and all parameters $\mu \in \mathcal{P}$.

As also remarked in [32], this assumption is not too restrictive. Moreover, as pointed out in [32, 43, 51], it is necessary that an error-aware sufficient decrease condition,

\begin{equation}
\hat{J}_r^{(k+1)}(\mu^{(k+1)}) \leq \hat{J}_r^{(k)}(\mu_{\text{AGC}}^{(k)}) \quad \text{for all } k \in \mathbb{N},
\end{equation}

is fulfilled at each iteration $k$ of the TR-RB algorithm. Cheaply computable sufficient and necessary conditions for (3.9) in Algorithm 1 (Step 5 and Step 17, respectively) are considered to guarantee (3.9). The TR-RB algorithm rejects, then, any computed point which does not satisfy (3.9). Algorithm 1 may be trapped in an infinite loop, where every computed point is rejected and the TR radius is shrunk all time. This situation will not lead to convergence. We point out that this never happened in our numerical tests. On one hand, we consider two safe guards: the first is to force an update of the RB model when the TR radius is below a predefined threshold $0 < \delta_{\text{min}} \ll 1$ and a safety termination criteria, which is triggered when the TR radius is smaller than the double machine precision $\tau_{\text{mac}}$. On the other hand, for showing convergence of Algorithm 1, we assume that this can not happen.

Assumption V. For each $k \geq 0$, there exists a radius $\delta^{(k)} > \tau_{\text{mac}} > 0$ for which there is a solution of (3.2) satisfying (3.9).

Another issue that might appear due to skipping a RB basis update is that at iteration $k - 1$ the optimization subproblem terminates for (3.5b), the point is accepted, the enrichment is skipped and the radius is enlarged to $\delta^{(k)} = \beta_1^{-1} \delta^{(k-1)}$, but then at iteration $k$ the point $\mu^{(k+1)}$ is rejected, implying to shrink the radius to the old value $\delta^{(k-1)}$. If the model is not updated
Algorithm 1: TR-RB algorithm

1. Initialize the ROM at $\mu(0)$, set $k = 0$ and Loop_flag=True

2. while Loop_flag do

3.  Compute the AGC point $\mu^{(k)}_{\text{AGC}}$

4.  Compute $\mu^{(k+1)}$ as solution of (3.2) with stopping criteria (3.5)

5.  if $\tilde{J}_{\text{r}}^{(k)}(\mu^{(k+1)}) + \Delta_{\tilde{J}_{\text{r}}^{(k)}}(\mu^{(k+1)}) < \tilde{J}_{\text{r}}^{(k)}(\mu_{\text{AGC}}^{(k)})$ then

6.  Accept $\mu^{(k+1)}$, set $\delta^{(k+1)} = \delta^{(k)}$, compute $g^{(k)}$ and $g_{h}(\mu^{(k+1)})$

7.  if $g_{h}(\mu^{(k+1)}) \leq \tau_{\text{FOC}}$ then

8.  Set Loop_flag=False

9.  else

10.     if $g^{(k)} \geq \eta_{\theta}$ then

11.         Enlarge the TR radius $\delta^{(k+1)} = \beta_{1}^{-1}\delta^{(k)}$

12.     end

13.     if not Skip_enrichment_flag(k) then

14.         Update the RB model at $\mu^{(k+1)}$

15.     end

16.  else if $\tilde{J}_{\text{r}}^{(k)}(\mu^{(k+1)}) - \Delta_{\tilde{J}_{\text{r}}^{(k)}}(\mu^{(k+1)}) > \tilde{J}_{\text{r}}^{(k)}(\mu_{\text{AGC}}^{(k)})$ then

17.     if $\beta_{1}\delta^{(k)} \leq \delta_{\text{min}}$ or Skip_enrichment_flag(k - 1) then

18.         Update the RB model at $\mu^{(k+1)}$

19.     end

20.     Reject $\mu^{(k+1)}$, shrink the radius $\delta^{(k+1)} = \beta_{1}\delta^{(k)}$ and go to 4;

21. else

22.     Compute $\hat{J}_{h}(\mu^{(k+1)})$, $g_{h}(\mu^{(k+1)})$, $g^{(k)}$ and set $\delta^{(k+1)} = \beta_{1}^{-1}\delta^{(k)}$

23.     if $g_{h}(\mu^{(k+1)}) \leq \tau_{\text{FOC}}$ then

24.         Set Loop_flag=False

25.     else

26.         if Skip_enrichment_flag(k) and $g^{(k)} \geq \eta_{\theta}$ then

27.             Accept $\mu^{(k+1)}$

28.         else if $\hat{J}_{h}(\mu^{(k+1)}) \leq \hat{J}_{r}^{(k)}(\mu_{\text{AGC}}^{(k)})$ then

29.             Accept $\mu^{(k+1)}$ and update the RB model

30.             if $g^{(k)} < \eta_{\theta}$ then

31.                 Set $\delta^{(k+1)} = \delta^{(k)}$

32.             end

33.         else

34.             if $\beta_{1}\delta^{(k)} \leq \delta_{\text{min}}$ or Skip_enrichment_flag(k - 1) then

35.                 Update the RB model at $\mu^{(k+1)}$

36.             end

37.             Reject $\mu^{(k+1)}$, set $\delta^{(k+1)} = \beta_{1}\delta^{(k)}$ and go to 4;

38.         end

39.     end

40.     end

41. end

42. Set $k = k + 1$;
also at this step, we are solving again the same subproblem at the next iteration starting at a point which was already triggering (3.5b), therefore our step would be to compute only the AGC point. Although the method will converge anyway, this situation might repeat several times before we escape this “problematic” region, resulting in a waste of computational time, which contrasts all the time gained by the possibility of not enriching. Therefore, we impose an enrichment of the RB model, when the radius is shrunk at iteration \( k \) and we skipped the basis update at iteration \( k - 1 \); cf. Step 18 and Step 35 of Algorithm 1. Note that to improve the convergence results, we required an additional assumption with respect to [32] (namely locally Lipschitz-continuous second derivatives in Assumption II), which we also require from the ROM.

**Assumption VI.** The ROM gradient \( \nabla_{\mu} \hat{J}_{r}^{(k)} \) is uniformly Lipschitz-continuous, i.e. there exists a constant \( C_{L} > 0 \) independent of \( k \) such that
\[
\| \nabla_{\mu} \hat{J}_{r}^{(k)}(\mu) - \nabla_{\mu} \hat{J}_{r}^{(k)}(\nu) \|_{2} \leq C_{L} \| \mu - \nu \|_{2}
\]
holds for all \( \mu, \nu \in \mathcal{P} \) and all \( k \in \mathbb{N} \). Similarly, the ROM second derivatives of \( \hat{J}_{r}^{(k)} \) are locally Lipschitz-continuous.

This assumption restricts the set of cost functionals, nevertheless it guarantees a locally faster convergence behavior for this class. Algorithm 1 is anyway still applicable to the general class of quadratic functionals – and also converges in this case. We remark that Assumption VI is needed for proving convergence of the method in an infinite-dimensional perspective. In the particular case of the RB model function, it is possible to show that this is satisfied. The proof follows from the fact that the RB model will exactly approximate the cost functional \( \hat{J}_{h} \) after a finite number of updates. As a direct consequence of Assumption VI, we have the following result:

**Corollary 3.2.** Let Assumption VI be satisfied. Then there exists a constant \( C > 0 \) such that for any \( k \in \mathbb{N} \) it holds
\[
\| \nabla_{\mu} \hat{J}_{r}^{(k)}(\mu^{(k)}) \|_{2} \leq C.
\]
Furthermore, the following property of the projection operator \( P_{\mathcal{P}} \) holds:

**Lemma 3.3.** Let \( \mu \in \mathcal{P} \) and \( d \in \mathbb{R}^{P} \) be arbitrary. Then it holds
\[
(3.10) \quad \| \mu - P_{\mathcal{P}}(\mu - td) \|_{2} \geq t \| \mu - P_{\mathcal{P}}(\mu - d) \|_{2}
\]
for all \( t \in [0, 1] \).

**Proof.** Let \( \mu \in \mathcal{P}, d \in \mathbb{R}^{P} \) and \( t \in [0, 1] \) be arbitrary. We prove the statement by showing that
\[
(3.11) \quad |\mu_{i} - (P_{\mathcal{P}}(\mu - td))_{i}| \geq t |\mu_{i} - (P_{\mathcal{P}}(\mu - d))_{i}|
\]
holds for all components \( i = 1, \ldots, P \). Let \( i \in \{1, \ldots, P\} \) be arbitrary.

**Case (1):** \( (P_{\mathcal{P}}(\mu - td))_{i} \in \{(\mu_{a})_{i}, (\mu_{b})_{i}\} \).
It clearly holds \((P \rho (\mu - td))_i = (P \rho (\mu - d))_i\), so that
\[
|\mu_i - (P \rho (\mu - td))_i| = |\mu - (P \rho (\mu - d))_i| \geq t |\mu - (P \rho (\mu - d))_i|.
\]

**Case (2a):** \((P \rho (\mu - td))_i \in ((\mu_a)_i, (\mu_b)_i)\) and \((P \rho (\mu - d))_i \in ((\mu_a)_i, (\mu_b)_i)\).

We can conclude
\[
|\mu_i - (P \rho (\mu - td))_i| = t |d_i| = t |\mu_i - (P \rho (\mu - d))_i|,
\]
which is what we have to show.

**Case (2b):** \((P \rho (\mu - td))_i \in ((\mu_a)_i, (\mu_b)_i)\) and \((P \rho (\mu - d))_i \in \{(\mu_a)_i, (\mu_b)_i\}\).

We define \(\bar{t} := \frac{\mu_i - (\rho \mu_b)_i}{d_i}\). Note that \(t < \bar{t} \leq 1\). Then it holds
\[
|\mu_i - (P \rho (\mu - td))_i| = t |d_i| = \frac{t}{\bar{t}} |\mu_i - (P \rho (\mu - td))_i| \\
= \frac{t}{\bar{t}} |\mu_i - (P \rho (\mu - d))_i| \geq t |\mu_i - (P \rho (\mu - d))_i|.
\]

Thus, in all cases, for any component \(i \in \{1, \ldots, P\}\) the inequality (3.11) holds. Now it can be immediately concluded that (3.10) holds as well. 

The next lemma is needed to show convergence of the algorithm.

**Lemma 3.4.** For every iterate \(\mu^{(k)} (k \in \mathbb{N})\) of Algorithm 1, it holds

\begin{equation}
q^{(k)}(\mu^{(k)}) \leq \beta_3 \delta^{(k)} \quad \text{and} \quad \frac{|g_r^{(k)}(\mu^{(k)}) - g_h(\mu^{(k)})|}{g_r^{(k)}(\mu^{(k)})} \leq \tau_g
\end{equation}

**Proof.** We show this statement by induction over \(k \in \mathbb{N}\). For \(k = 0\) we trivially have
\[
q^{(0)}(\mu^{(0)}) = 0 \quad \text{and} \quad \frac{|g_r^{(0)}(\mu^{(0)}) - g_h(\mu^{(0)})|}{g_r^{(0)}(\mu^{(0)})} = 0,
\]

since the RB model was constructed at \(\mu^{(0)}\).

Now assume that (3.12) is satisfied for all \(1 \leq l \leq k\) for some \(k \in \mathbb{N}\) and let \(\mu^{(k+1)}\) be the new accepted iterate.

(1) \(\mu^{(k+1)}\) is accepted in line 6:

Then the RB model is updated in line 14, if
\[
q^{(k)}(\mu^{(k+1)}) > \beta_3 \delta^{(k+1)} \quad \text{or} \quad \frac{|g_r^{(k)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})|}{g_r^{(k)}(\mu^{(k+1)})} > \tau_g
\]

or
\[
\left( \frac{\|\nabla_\mu J_h(\mu^{(k+1)}) - \nabla_\mu J_r^{(k)}(\mu^{(k+1)})\|_2}{\|\nabla_\mu J_h(\mu^{(k+1)})\|_2} \right) > \min\{\tau_{grad}, \beta_3 \delta^{(k+1)}\}.
\]

So, on one hand, if the RB model is not updated in line 14, this implies that
\[
q^{(k+1)}(\mu^{(k+1)}) = q^{(k)}(\mu^{(k+1)}) \leq \beta_3 \delta^{(k+1)}
\]
and
\[
\frac{g_r^{(k+1)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})}{g_r^{(k+1)}(\mu^{(k+1)})} = \frac{g_r^{(k)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})}{g_r^{(k)}(\mu^{(k+1)})} \leq \tau g
\]
hold. On the other hand, if the RB model is updated, we have
\[
q^{(k+1)}(\mu^{(k+1)}) = 0 \quad \text{and} \quad \frac{g_r^{(k+1)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})}{g_r^{(k+1)}(\mu^{(k+1)})} = 0,
\]
so that the claim follows in both cases.

(2) \(\mu^{(k+1)}\) is accepted in line 28:
In this case the RB model is not updated. Thus, we can directly conclude from the previous if-condition in line 27 and the enlarged TR radius
\[
q^{(k+1)}(\mu^{(k+1)}) = q^{(k)}(\mu^{(k+1)}) \leq \beta_3 \beta_1^{-1} g(k) = \beta_3 g(k+1)
\]
and
\[
\frac{g_r^{(k+1)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})}{g_r^{(k+1)}(\mu^{(k+1)})} = \frac{g_r^{(k)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})}{g_r^{(k)}(\mu^{(k+1)})} \leq \tau g.
\]
Hence, the claim holds also in this case.

(3) \(\mu^{(k+1)}\) is accepted in line 30:
Then the RB model is updated at \(\mu^{(k+1)}\), so that we have
\[
q^{(k+1)}(\mu^{(k+1)}) = 0 \quad \text{and} \quad \frac{g_r^{(k+1)}(\mu^{(k+1)}) - g_h(\mu^{(k+1)})}{g_r^{(k+1)}(\mu^{(k+1)})} = 0.
\]
Thus, the claim holds trivially. In total, we have shown the claim for every possible case, which concludes the proof.

We continue the convergence analysis by showing a result about the AGC point \(\mu^{(k)}_{AGC}\). We recall the following results from [33, Corollary 5.4.4]:

**Lemma 3.5.** For all \(j, k \in \mathbb{N}\) and \(\kappa \in (0, 1)\), we have
\[
\|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa j \nabla_{\mu} \tilde{J}_r^{(k)}(\mu^{(k)}))\|_2^2 \leq \kappa^j \nabla_{\mu} \tilde{J}_r^{(k)}(\mu^{(k)}) \cdot (\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa^j \nabla_{\mu} \tilde{J}_r^{(k)}(\mu^{(k)})))
\]
To proceed, we assume that the error indicator \(q^{(k)}\) in the TR condition (3.4b) is uniformly continuous.

**Assumption VII.** The function \(q^{(k)} : \mathcal{P} \to \mathbb{R}\) defined in (3.4b) is uniformly continuous in \(\mathcal{P}\) uniformly in \(k\), i.e.
\[
\forall \varepsilon > 0 : \exists \eta = \eta(\varepsilon) > 0 : \forall \mu, \nu \in \mathcal{P} \quad \|\mu - \nu\|_2 < \eta \Rightarrow \left| q^{(k)}(\mu) - q^{(k)}(\nu) \right| < \varepsilon.
\]
Also this last assumption is needed for proving convergence of the method in an infinite-dimensional perspective. In the particular case of the RB model, since $\mathcal{P}$ is compact, one can apply the Heine-Cantor theorem [47] to show that $q^{(k)}$ is uniformly continuous for each $k \in \mathbb{N}$. Then the independence from $k$ follows from the fact that the RB model approximation is exact (after a sufficient number of enrichments) and $q^{(k)} = q^{(k+1)}$ when the enrichment is not performed. Finally, the next result gives a lower and upper bound for the line-search of the AGC point. This is important, because it shows that at each iteration $k$ the ACG point can be computed in a finite number of line-search steps.

**Theorem 3.6.** Let Assumptions I-V be satisfied and let $\mu^{(k)}(j) := P_{\mathcal{P}}(\mu^{(k)} - \kappa \nabla_{\mu} \hat{J}^{(k)}(\mu^{(k)}))$ for $j \in \mathbb{N}$. Then we have that $\mu^{(k)}(j)$ satisfies (3.4) for all

$$j \geq \log_\kappa \left( \min \left\{ \frac{2(1 - \kappa_{\text{arm}})}{C_L}, \frac{\eta((1 - \beta_3)\tau_{\text{mac}})\kappa}{C} \right\} \right)$$

where $\kappa \in (0,1)$ is the backtracking constant introduced in (3.3) and $C_L, C$ and $\eta$ are introduced in Assumption VI, Corollary 3.2 and Assumption VII, respectively. Furthermore, for the step-length of the AGC points, it holds

$$j_c^{(k)} \leq \log_\kappa \left( \min \left\{ \frac{2(1 - \kappa_{\text{arm}})\kappa}{C_L}, \frac{\eta((1 - \beta_3)\tau_{\text{mac}})\kappa}{C} \right\} \right).$$

**Proof.** We need to prove only (3.13), since (3.14) is a direct consequence of it. Let $j$ satisfying (3.13) be arbitrary and consider $y := \mu^{(k)} - \mu^{(k)}(j)$, then it holds

$$\hat{J}^{(k)}(\mu^{(k)}) - \hat{J}^{(k)}(\mu^{(k)}(j)) = - \int_0^1 \frac{d}{ds} \hat{J}^{(k)}(\mu^{(k)} - sy) \, ds$$

$$= \int_0^1 \nabla_{\mu} \hat{J}^{(k)}(\mu^{(k)} - sy) \cdot y \, ds$$

$$= \nabla_{\mu} \hat{J}(\mu^{(k)}) \cdot y + \int_0^1 \left( \nabla_{\mu} \hat{J}^{(k)}(\mu^{(k)} - sy) - \nabla_{\mu} \hat{J}^{(k)}(\mu^{(k)}) \right) \cdot y \, ds$$

Now, the integral term can be estimated exploiting the Lipschitz continuity of $\nabla_{\mu} \hat{J}^{(k)}$ (cf. Assumption VI) as follows:

$$\left| \int_0^1 \left( \nabla_{\mu} \hat{J}^{(k)}(\mu^{(k)} - sy) - \nabla_{\mu} \hat{J}(\mu^{(k)}) \right) \cdot y \, ds \right|$$

$$\leq C_L \int_0^1 \|sy\|_2 \|y\|_2 \, ds = \frac{C_L}{2} \|\mu^{(k)}(j) - \mu^{(k)}\|_2^2$$
Multiplying (3.15) by \( \kappa^j \) and using (3.16) together with Lemma 3.5, we obtain
\[
\kappa^j \left( \hat{J}_r^{(k)}(\mu^{(k)}) - \hat{J}_r^{(k)}(\mu^{(k)}(j)) \right)
\geq \kappa^j \nabla \mu \hat{J}_r^{(k)}(\mu^{(k)}) \cdot (\mu^{(k)} - \mu^{(k)}(j)) - \frac{C_L \kappa^j}{2} \| \mu^{(k)}(j) - \mu^{(k)} \|^2_2
\geq \left( 1 - \frac{C_L \kappa^j}{2} \right) \| \mu^{(k)}(j) - \mu^{(k)} \|^2_2.
\]
Thus, we have
\[
\hat{J}_r^{(k)}(\mu^{(k)}(j)) - \hat{J}_r^{(k)}(\mu^{(k)}) \leq -\frac{1}{\kappa^j} \left( 1 - \frac{C_L \kappa^j}{2} \right) \| \mu^{(k)}(j) - \mu^{(k)} \|^2_2.
\]
Since \( j \) satisfies (3.13), we have that \( \kappa^j \leq \frac{2(1-\tau_{\text{mac}})}{C_L} \). Therefore, the Armijo-type condition (3.4a) is satisfied. It remains to show that (3.4b) holds as well. Note that
\[
\| \mu^{(k)}(j) - \mu^{(k)} \|^2_2 \leq \| \kappa^j \nabla \mu \hat{J}_r^{(k)}(\mu^{(k)}) \|^2_2 \leq \eta((1-\beta_3)\tau_{\text{mac}})
\]
by the choice of \( j \) and Corollary 3.2. Now, Assumption V, Lemma 3.4 and Assumption VII imply that
\[
q^{(k)}(\mu^{(k)}(j)) \leq |q^{(k)}(\mu^{(k)}(j)) - q^{(k)}(\mu^{(k)})| + q^{(k)}(\mu^{(k)}) < (1-\beta_3)\tau_{\text{mac}} + \beta_3 \delta^{(k)} \leq \delta^{(k)},
\]
which completes the proof. \( \square \)

In the next step we show that Algorithm 1 ensures that the error-aware sufficient decrease condition (3.9) is satisfied for every successful iteration.

**Lemma 3.7.** Let the iterate \( \mu^{(k+1)} \) be accepted by Algorithm 1. Then the error-aware sufficient decrease condition (3.9) is satisfied.

**Proof.** When the RB model is updated, we can proceed as in [43, Section 4.1]. If the model is not enriched we have to distinguish two cases:

1. \( \mu^{(k+1)} \) is accepted in line 6 and **Skip_enrichment_flag** is true, we have
   \[
   \hat{J}_r^{(k+1)}(\mu^{(k+1)}) = \hat{J}_r^{(k)}(\mu^{(k+1)}) \leq \hat{J}_r^{(k)}(\mu^{(k+1)}) + \Delta \hat{J}_r^{(k)}(\mu^{(k+1)}) < \hat{J}_r^{(k)}(\mu^{(k)}_{\text{AGC}}).
   \]
2. \( \mu^{(k+1)} \) is accepted in line 28:
   Note that it always holds \( \hat{J}_r^{(k)}(\mu^{(k+1)}) \leq \hat{J}_r^{(k)}(\mu^{(k)}_{\text{AGC}}) \), since the truncated CG projected Newton method for solving the TR subproblem (3.2) is a descent method and the AGC point \( \mu^{(k)}_{\text{AGC}} \) is used as a warm start. Since the RB model is not updated, this implies
   \[
   \hat{J}_r^{(k+1)}(\mu^{(k+1)}) = \hat{J}_r^{(k)}(\mu^{(k+1)}) \leq \hat{J}_r^{(k)}(\mu^{(k)}_{\text{AGC}}),
   \]
   so that (3.9) is satisfied.

Thus, whenever \( \mu^{(k+1)} \) is accepted, regardless updating the RB model or not, the error-aware sufficient decrease condition (3.9) is satisfied. \( \square \)
We are now able prove our improved (w.r.t. [32]) convergence results also taking into consideration the possibility of skipping RB model updates.

**Theorem 3.8.** Let the hypotheses of Theorem 3.6 be satisfied. Then every accumulation point $\bar{\mu}$ of the sequence $\{\mu^{(k)}\}_{k\in\mathbb{N}} \subset \mathcal{P}$ generated by Algorithm 1 is an approximate first-order critical point for $\hat{J}_h$, i.e., it holds

\[
\|\bar{\mu} - P_{\mathcal{P}}(\bar{\mu} - \nabla_\mu \hat{J}_h(\bar{\mu}))\|_2 = 0.
\]

**Proof.** Let $k \in \mathbb{N}$ be arbitrary. From Definition 3.1, (3.4a) and (3.9) due to Lemma 3.7, we have

\[
\hat{J}_r^{(k)}(\mu^{(k)}) - \hat{J}_r^{(k+1)}(\mu^{(k+1)}) \geq \hat{J}_r^{(k)}(\mu^{(k)}) - \hat{J}_r^{(k)}(\mu^{(k)}_{\text{AGC}}) \geq \frac{k_{\text{arm}}}{k_{\text{j}}^{(k)}} \|\mu^{(k)} - \mu^{(k)}_{\text{AGC}}\|_2^2 \geq \frac{k_{\text{arm}}}{k_{\text{j}}^{(k)}} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2^2.
\]

By summing both sides of the previous inequality from $k = 0$ to $K$, we obtain

\[
\hat{J}_r^{(0)}(\mu^{(0)}) - \hat{J}_r^{(K+1)}(\mu^{(K+1)}) \geq \sum_{k=0}^{K} \frac{k_{\text{arm}}}{k_{\text{j}}^{(k)}} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2^2 \geq 0.
\]

For $K \to +\infty$ the term on the left-hand side is bounded from above, due to Assumption IV. Thus

\[
\lim_{k \to +\infty} \frac{k_{\text{arm}}}{k_{\text{j}}^{(k)}} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2^2 = 0.
\]

From Theorem 3.6, we have that $\kappa_{\text{j}}^{(k)} \geq \min \left\{ \frac{2(1-\kappa_{\text{arm}})}{C_L}, \frac{\eta((1-\beta_3)_\text{mac}}{C} \right\} : = \tilde{\kappa}$ for all $k \in \mathbb{N}$. Furthermore, we also have that $\kappa_{\text{j}}^{(k)} \leq 1$ for all $k \in \mathbb{N}$, because $\kappa \in (0, 1)$. Hence,

\[
\lim_{k \to +\infty} \kappa_{\text{arm}} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2^2 \leq \lim_{k \to +\infty} \frac{k_{\text{arm}}}{k_{\text{j}}^{(k)}} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2^2 = 0
\]

which clearly implies

\[
\lim_{k \to +\infty} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2 = 0.
\]

Lemma 3.3 shows that

\[
\|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \kappa_{\text{j}}^{(k)} \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2 \geq \tilde{\kappa} \|\mu^{(k)} - P_{\mathcal{P}}(\mu^{(k)} - \nabla_\mu \hat{J}_r^{(k)}(\mu^{(k)}))\|_2.
\]
holds for all $k \in \mathbb{N}$. Thus, we can conclude

$$\lim_{k \to \infty} \left\| \mu^{(k)} - P_{\mathcal{P}} \left( \mu^{(k)} - \nabla \hat{J}_r (\mu^{(k)}) \right) \right\|_2 = 0. \tag{3.18}$$

By Lemma 3.4 we have

$$\left\| \mu^{(k)} - P_{\mathcal{P}} \left( \mu^{(k)} - \nabla \hat{J}_r (\mu^{(k)}) \right) \right\|_2 - \left\| \mu^{(k)} - P_{\mathcal{P}} \left( \mu^{(k)} - \nabla \hat{J}_h (\mu^{(k)}) \right) \right\|_2 \leq \left\| \mu^{(k)} - P_{\mathcal{P}} \left( \mu^{(k)} - \nabla \hat{J}_r (\mu^{(k)}) \right) \right\|_2 \tau_g \to 0 \text{ as } k \to \infty,$$

which, together with (3.18), implies

$$\lim_{k \to \infty} \left\| \mu^{(k)} - P_{\mathcal{P}} \left( \mu^{(k)} - \nabla \hat{J}_h (\mu^{(k)}) \right) \right\|_2 = 0. \tag{3.19}$$

Now let $\bar{\mu}$ be an accumulation point of the sequence $\{\mu^{(k)}\}_{k \in \mathbb{N}} \subset \mathcal{P}$, i.e., it holds

$$\mu^{(k_i)} \to \bar{\mu} \quad \text{as } i \to \infty$$

for some subsequence $\{\mu^{(k_i)}\}_{i \in \mathbb{N}}$. Using (3.19), we have by the continuity of the gradient $\nabla \hat{J}_h$ and of the projection operator $P_{\mathcal{P}}$

$$\left\| \bar{\mu} - P_{\mathcal{P}} \left( \bar{\mu} - \nabla \hat{J}_h (\bar{\mu}) \right) \right\|_2 = \lim_{i \to \infty} \left\| \mu^{(k_i)} - P_{\mathcal{P}} \left( \mu^{(k_i)} - \nabla \hat{J}_h (\mu^{(k_i)}) \right) \right\|_2 = 0,$$

which concludes the proof. $\square$

Remark 3.9. (1) The biggest improvement in comparison to the convergence proof from [32] consists in the fact that we proved that any accumulation point of the sequence $\{\mu^{(k)}\}_{k \in \mathbb{N}}$ is an actual critical point for $\hat{J}_h$ and not an approximated one up to the tolerance $\tau_{sub}$.

(2) Note that there is no direct use of the RB model properties in Theorem 3.8, as it is in [32]. This opens the possibility of considering different model functions, similarly to [51] for unconstrained parameter sets, provided that the requested (and shown) properties hold.

(3) In contrast to [32], we make use of the error-aware sufficient decrease condition (3.9) in the proof of convergence and not only to guarantee that the accumulation point is not a local maximum of $\hat{J}_h$. As also remarked in [32], $\bar{\mu}$ can still be a saddle point as well as a local minimum. In the numerical experiments, to verify that the computed point $\bar{\mu}$ is actually a local minimum, we check the second-order sufficient optimality conditions (cf. Proposition 1.8) as soon as the algorithm terminates.

(4) Algorithm 1 is also an improvement with respect to [32, Algorithm 1] by allowing to skip updates of the RB model. This prevents the dimension of the RB space to grow excessively and, thus, helps to overcome the dimension of the FOM model. This feature is particularly relevant in applications which require many iterations, such as PDE-constrained multiobjective optimization by scalarization methods [2, 21, 30]. In there many optimization problems have to be solved iteratively, so that it is crucial for an efficient algorithm to keep the dimension of the RB space reasonably small.
3.3. Construction of RB spaces. For the construction of the required RB spaces $V_{pr}^r, V_{du}^r$ the numerical experiments in [32] have shown that Lagrangian RB spaces are more favorable compared to aggregated RB spaces (i.e. non separated primal and dual spaces), since the use of the used NCD-corrected cost functional fully overcomes the approximation error that comes with separating the RB spaces. Thus, using aggregated RB spaces unnecessarily increases the size of the RB spaces which is particularly problematic when the number of iterations of Algorithm 1 is large. For this reason, we only focus on enrichment approaches where the NCD-corrected functional is required. We state the Lagrangian RB spaces and introduce an additional enrichment strategy which is of particular interest for a projected Newton method. After solving a sub-problem of the TR-algorithm 1, we (optionally) enrich with the primal and dual solutions $u_{h,\mu(k)}, p_{h,\mu(k)} \in V_h$, where $\mu(k) \in P$ is the current iterate. In addition, we potentially also have access to their respective sensitivities w.r.t a direction $\eta$, i.e. $d_\eta u_{h,\mu}, d_\eta p_{h,\mu} \in V_h$. For the projected Newton method, we also require directional derivatives of the primal and dual solutions. However, it can not be guaranteed that a reduced solution $d_\eta u_{r,\mu}$ is a good approximation of $d_\eta u_{h,\mu}$; cf. [32]. On the other hand, computing snapshots $d_\eta u_{h,\mu}$ component-wise (e.g. for full Taylor RB spaces) results in a prohibitively large computational effort for a high dimension of the parameter space. Instead, we suggest to only add snapshots of a wisely-chosen direction $\eta$. As discussed earlier, it is cheap to compute the gradient $\nabla_\mu \hat{J}_h(\mu)$ if $u_{h,\mu}, p_{h,\mu} \in V_h$ are already available. On top of that, we know that we need the directional sensitivities of $u_{h,\mu}$ and $p_{h,\mu}$ in the direction $\eta = \nabla_\mu \hat{J}_r(\mu)$ in order to proceed with the next sub-problem of the TR-RB algorithm. Thus, we propose the following two enrichment strategies.

(a) Lagrangian RB spaces: Following [32], we simply add each FOM solution to the corresponding RB space, i.e. for a given $\mu \in P$, we enrich by $V_{pr}^{r,k} = V_{pr}^{r,k-1} \cup \{u_{h,\mu}\}, V_{du}^{r,k} = V_{du}^{r,k-1} \cup \{p_{h,\mu}\}$.

(b) Directional Taylor RB space We compute a direction $\eta := \nabla_\mu \hat{J}_r(\mu)$ from $u_{h,\mu}$ and $p_{h,\mu}$ and include the directional derivatives to the respective RB space, i.e. $V_{pr}^{r,k} = V_{pr}^{r,k-1} \cup \{u_{h,\mu}\} \cup \{d_\eta u_{h,\mu}\}, V_{du}^{r,k} = V_{du}^{r,k-1} \cup \{p_{h,\mu}\} \cup \{d_\eta p_{h,\mu}\}$.

For the sake of brevity, in Section 4, we present only the results for strategy (b). At [3] one can find the results also for the strategy (a).

4. NUMERICAL EXPERIMENTS

In this section, we show the numerical performance of the improved Algorithm 1 in comparison to the one described in [32]. We further study how the a posteriori error estimate for the optimal parameter approximation can be used as a post-processing tool. The simulations have been performed with a python implementation, using pyMOR [36] for the numpy/scipy-based discretization and the RB part. The code for this section can be
found on [3], where we also provide jupyter-notebooks\(^1\) with the results (and explanations) of the numerical tests presented below.

### 4.1. Computational details

We define the discrete space \(V_h\) as a piece-wise linear FE space on a triangular mesh \(\tau_h\), with a fine enough grid to fulfill Assumption III. From a MOR point of view, the choice of the inner product \((\cdot, \cdot)_h\) has a large impact on the coercivity and continuity constants used in the error estimates in Section 2.3. For this reason we define the inner product to be spanned by the energy product with respect to a fixed reference parameter \(\hat{\mu}\), i.e. \((\cdot, \cdot)_h := a_{\hat{\mu}}(\cdot, \cdot)\). For this product, it is easy to compute a lower bound for the coercivity constant of the bilinear form \(a_{\mu}\) for all parameters in \(P\). In particular, we can make use of the min-theta approach (see [25, Proposition 2.35]). The continuity constants \(\gamma_{a_{\mu}}, \gamma_{\partial_{\mu}a_{\mu}}, \gamma_{k_{\mu}}, \gamma_{\partial_{\mu}k_{\mu}}, \gamma_{\partial_{\mu}j_{\mu}}\) and \(\gamma_{\partial_{\mu}l_{\mu}}\) can be computed using a max-theta approach (see [25]).

Another important technical detail is the preassembly of all high dimensional parts of the model in Section 2.2 and the corresponding error estimators in Section 2.3, which can be carried out as usual with RB methods (see, e.g., [25, 26, 44]). For all experiments, we use an initial TR radius of \(\delta_0 = 0.1\), a TR shrinking factor \(\beta_1 = 0.5\), an Armijo step-length \(\kappa = 0.5\), a safeguard for the TR boundary of \(\beta_2 = 0.95\), a tolerance for enlarging the TR radius of \(\eta_\varrho = 0.75\), a stopping tolerance for the TR sub-problems of \(\tau_{\text{sub}} = 10^{-8}\), a maximum number of TR iteration \(K = 60\), a maximum number of sub-problem iteration \(K_{\text{sub}} = 400\), a maximum number of Armijo iteration of 50, \(\varepsilon = 10^{-8}\) for the \(\varepsilon\)-active set and optional enrichment parameters \(\tau_g = \tau_{\text{FOC}}/\tau_{\text{sub}}\), \(\beta_3 = 0.5\) and \(\tau_{\text{grad}} = 0.01\). We also point out that the stopping tolerance for the FOC condition \(\tau_{\text{FOC}}\) is specified in each experiment. We compare four Algorithms:

- **FOM TR-Newton-CG** [38]: following [38, Algorithm 7.2], this method considers a standard FOM quadratic approximation for \(\tilde{J}_h\) as model function and includes the computation of the Cauchy point as well as a way to handle the box constraints of \(P\), following [38, Section 16.7].

- **BFGS NCD TR-RB (UE)** [32]: this is the NCD-corrected method with BFGS sub-problem solver and Lagrange RBs following [32, Algorithm 1] with unconditional enrichment (UE) of the RB spaces, where no reduced hessian or sensitivities of the primal and dual solutions are required.

- **Newton NCD TR-RB (UE)**: this is the NCD-corrected method from [32] with directional Taylor RB spaces, a projected Newton method for the TR sub-problems and unconditional enrichment (UE) of the RB spaces.

- **Newton NCD TR-RB (OE)** [Alg. 1]: this is the NCD-corrected method with directional Taylor RB spaces, a projected Newton method for the TR sub-problems and optional enrichment (OE) of the RB spaces from Algorithm 1.

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\(^1\)See https://github.com/TiKeil/Proj-Newton-NCD-corrected-TR-RB-for-pde-opt.
4.2. Model problem: Quadratic objective functional with elliptic PDE constraints. For our experiments we set the objective functional to be a weighted $L^2$-misfit on a domain of interest $D \subseteq \Omega$ and a weighted Tikhonov term, i.e.

$$J(v, \mu) = \frac{\sigma_d}{2} \int_D (v - u^d)^2 + \frac{1}{2} \sum_{i=1}^M \sigma_i (\mu_i - \mu_i^d)^2 + 1,$$

with a desired state $u^d$ and desired parameter $\mu^d$. With respect to the formulation in (P.a), we have

$$\Theta(\mu) = \frac{\sigma_d}{2} \sum_{i=1}^M \sigma_i (\mu_i - \mu_i^d)^2 + \frac{\sigma_d}{2} \int_D u^d u^d,$$

$$j_\mu(u) = -\sigma_d \int_D u^d u, \quad \text{and} \quad k_\mu(u, u) = \frac{\sigma_d}{2} \int_D u^2.$$

Note that the formulation of $J(v, \mu)$ is a very general choice. It is applicable to design optimization, optimal control as well as to inverse problems. We remark that the constant term 1 is added to fulfill Assumption IV and does not influence the position of the local minima. As PDE-constraint, we consider the weak formulation of the parameterized equation

$$-\nabla \cdot (\kappa_\mu \nabla u_\mu) = f_\mu \quad \text{in } \Omega,$$
$$c_\mu(\kappa_\mu \nabla u_\mu \cdot n) = (u_{out} - u_\mu) \quad \text{on } \partial \Omega.$$  \hfill (4.1)

with parametric diffusion coefficient $\kappa_\mu$ and source $f_\mu$, outside temperature $u_{out}$ and robin function $c_\mu$. Accordingly, we have

$$a_\mu(v, w) = \int_\Omega \kappa_\mu \nabla v \cdot \nabla w \, dx + \int_{\partial \Omega} \frac{1}{c_\mu} vw \, dS,$$
$$l_\mu(v) = \int_\Omega f_\mu v \, dx + \int_{\partial \Omega} \frac{1}{c_\mu} u_{out} v \, dS.$$

and, in addition, we set the parameter box constraints $\mu_i \in [\mu_i^{min}, \mu_i^{max}]$.

A possible application is the stationary distribution of heat in a building. Inspired by the blueprint of a building with windows, heaters, doors and walls, we consider a parameterized diffusion problem which is displayed in Figure 1. We picked a certain domain of interest $D$ and we enumerated all windows, walls, doors and heaters separately. For simplicity we omit a realistic modeling of temperature and restrict ourselves to academic numbers of the diffusion and heat source quantities. We set the computational domain to $\Omega := [0, 2] \times [0, 1] \subset \mathbb{R}^2$ and we model boundary conditions by incorporating all walls and windows that touch the boundary of the blueprint to the robin function $c_\mu$. All other diffusion components enter the diffusion coefficient $\kappa_\mu$, whereas the heaters work as a source term on the right hand side $f_\mu$. Moreover, we assume an outside temperature of $u_{out} = 5$. For our discretization we choose a mesh size $h = \sqrt{2}/200$ which resolves all features.
from the given picture and results in \( \dim V_h = 80601 \) degrees of freedom.

We consider two scenarios.

- **Experiment 1:** optimize 12 Parameters (3 walls, 2 doors, 7 heaters) to reach the target \( u^d(x) = 18 \chi_D(x) \) and \( \mu^d \equiv 0 \) using also the a posteriori error estimate for the optimal parameter (Proposition 2.15) as post-processing (cf. Section 4.3),

- **Experiment 2:** optimize 28 Parameters (8 walls, 8 doors, 12 heaters) with target \( u^d = S_h(\mu^d) \) where \( \mu^d \in \mathcal{P} \) is given (cf. Section 4.4).

Both experiments are computed with 10 different random samples for the starting parameter \( \mu^{(0)} \). For the sake of brevity, we omit the details on the data for the experiment and refer to [3] on how to reproduce them.

### 4.3. Experiment 1: A posteriori error estimate for optimal parameter.

This experiment shows the usability of the a posteriori error estimate (2.15) and shows the limitations of the projected BFGS method. We focus, at first, on the behavior of the methods for a given starting parameter \( \mu^{(0)} \).

In Fig. 2 the error at each iteration \( k \) is reported for Algorithm 1 and for the TR-RB method from [32]. We omit the FOM TR-Newton-CG, due to its larger computational time. We compute the solution with a tolerance \( \tau_{\text{FOC}} = 5 \times 10^{-4} \) (Fig. 2.A). When the methods reach this tolerance, we evaluate the a posteriori error estimate and if this is greater than the value \( \tau_\mu = 10^{-4} \), we decrease the tolerance \( \tau_{\text{FOC}} \) by two orders of magnitude and repeat the procedure until the a posteriori estimate is below the desired tolerance \( \tau_\mu \) (Fig. 2.A). In Fig. 2.B, we do not use the a posteriori estimate and directly compute the solution with a tolerance \( \tau_{\text{FOC}} = 10^{-7} \). This test shows that the possibility of skipping enrichments improve the TR-RB algorithm. We point out that in this particular figure, the cost of computing the a posteriori error estimate (2.15) is included in the computational time (as dashed horizontal line), which also includes the costly computation of the smallest eigenvalue of the FOM hessian affecting the real performances of the method. In fact, when directly considering a smaller \( \tau_{\text{FOC}} \), Algorithm 1
Figure 2. Error decay and performance of selected algorithms defined in Section 4.1 for experiment 1 from Section 4.2 with unconditional enrichment (UE) vs. optional enrichment (OE) for a single optimization run with random initial guess \( \mu(0) \) for two choices of \( \tau_{FOC} \) (solid lines) with optional intermediate parameter control according to (2.15) (dotted lines): for each algorithm each marker corresponds to one (outer) iteration of the optimization method and indicates the absolute error in the current parameter, measured against the computed FOM optimum. The dashed black horizontal lines indicate the time taken for the post-processing of the parameter control.

Table 1. Performance and accuracy of the algorithms defined in Section 4.1 (abbreviated in order of definition) for experiment 1 from Section 4.2 with unconditional enrichment (UE) vs. optional enrichment (OE) for ten optimization runs with random initial guess \( \mu(0) \) together with the relative error in reconstructing the local minimizer and the FOC condition at which the method is the fastest as visible from Fig. 2.B. This demonstrates how the a posteriori estimate is important as post-processing tool to verify the correct choice of the tolerances. Another important issue that emerges from this numerical test is how a BFGS-based method (as the one in [32]) struggles to reach smaller values of the FOC condition, resulting in a high increase of the computational time and stagnating error, as can be seen in Figures 2.A and 2.B. In Tab. 1 we report the average computational time and iterations for ten random starting parameters \( \mu(0) \) together with the relative error in reconstructing the local minimizer and the FOC condition at which the method
4.4. **Experiment 2: Large parameter set.** In this experiment we apply the TR-RB algorithm to a 28 dimensional parameter set. This large number of parameters is prohibitive for the standard RB implementation based on a greedy algorithm for the offline phase. This problem can be easily overcome by our adaptive algorithm, as also remarked in [32, 43]. What might still be problematic is the increase of the number of iterations, which would lead to large RB spaces with the unconditional enrichment from [32]. The purpose of this experiment is to demonstrate that skipping enrichment yields similar convergence behavior (in terms of iterations), but at a lower cost.

Tab. 2 reports the average runtime and iterations for the tested TR methods together with the relative error in reconstructing $\mu^d$ and at which FOC condition the method stops. One can note that all the adaptive TR-RB stops. Also here, one can see how the possibility of skipping enrichments and the choice of a projected Newton method improve the results obtained with the algorithm from [32]. In particular, the projected BFGS method struggles to reach the given $\tau_{\text{FOC}}$ in all experiments, showing its limitation. We remark that for larger tolerances the method from [32] is still valid and might converge faster, depending on the given example.

### Table 2

| Method            | runtime [s] avg. (min/max) | speed-up | iterations $k$ avg. (min/max) | rel. error | FOC cond. |
|-------------------|---------------------------|----------|------------------------------|------------|-----------|
| FOM               | 2423 (1962/3006)          |          | 18.5 (16/23)                 | 5.1e-9     | 4.57e-6   |
| BFGS (UE)         | 197 (156/272)             | 12.3     | 12.1 (10/14)                 | 3.65e-9    | 2.38e-6   |
| Newton (UE)       | 258 (202/387)             | 9.4      | 8.1 (7/9)                    | 5.83e-9    | 1.93e-6   |
| Newton (OE)       | 168 (145/191)             | 14.4     | 8.4 (7/12)                   | 1.22e-8    | 3.36e-6   |

Figure 3. Error decay w.r.t. the desired parameter $\bar{\mu} = \mu^d$ and performance (left) and number of sub-problem iterations in each TR iteration (right) of selected algorithms defined in Section 4.1 for experiment 2 from Section 4.2 with unconditional enrichment (UE) vs. optional enrichment (OE) for a single optimization run with random initial guess $\mu^{(0)}$ for $\tau_{\text{FOC}} = 1 \cdot 10^{-5}$. 

We remark that for larger tolerances the method from [32] is still valid and might converge faster, depending on the given example.
algorithm are a valid tool for speeding up the computational time w.r.t. the FOM TR-New.-CG. Among all, the best performances are achieved by Algorithm 1. The effect of skipping an enrichment can be seen comparing Algorithm 1 with the method from [32] with the projected Newton method as sub-problem solver. The numbers of outer iterations are the same, while the computational time is decreased. This is due to two reasons: skipping an enrichment implies no preparation of the new RB space (like preassembling the new a posteriori estimate $\Delta_j^\mathcal{J}$) and faster computations having a smaller RB space. In Fig. 3 (left), one can see the error between the desired parameter $\mu^d$ and each iteration of the different adaptive TR-RB methods for the same random starting parameter $\mu^{(0)}$, which confirms what is mentioned above. Fig. 3 (right) shows instead the number of iterations needed to solve each TR sub-problem at the outer iteration $k$ of the method. One can deduce that the advantages of Algorithm 1 with respect to [32] based on projected Newton are not due to different inner iterations number, but have to be associated to the reduction of the dimension of the RB space. From Fig. 3 (right) we also see that the BFGS method might lose its super-linear convergence according to the approximation of the hessian carried out by the method, which might deteriorate for an increasing number of active components of the parameter $\mu^{(k)}$; see [33].

5. Conclusion

In this work we proposed a new variant of adaptive TR-RB method for PDE-constrained parameter optimization. As major improvement we included the possibility of skipping basis updates according to rigorous criteria, which ensures the convergence of the method while preventing the RB space from growing indefinitely. We further made use of a projected Newton method for solving the TR sub-problem and of a post-processing operation based on an a posteriori error estimate for the optimal parameter. These features made the algorithm robust (in terms of convergence) and comparable with other methods presented in the literature, which performed slower than Algorithm 1 in our numerical experiments. In future works, we are interested in adopting (spatially) localized RB methods to only locally enriching the RB model, allowing for faster computations and even smaller local dimensions of the ROM.

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A Appendix

Proof of Proposition 2.6 (Upper bound on the model reduction error of the hessian of the reduced output). For the hessian $\hat{H}_{h,\mu}(\mu)$ of $\hat{J}_h(\mu)$ and the true hessian $\hat{H}_{r,\mu}(\mu)$ of the NCD-corrected functional from Proposition 2.4, we have the following a posteriori error bound

$$\left| \hat{H}_{h,\mu}(\mu) - \hat{H}_{r,\mu}(\mu) \right| \leq \Delta_H(\mu) := \left\| (\Delta H_{i,j}(\mu))_{i,j} \right\|_2$$

with

$$\Delta H_{i,j}(\mu)$$

$$:= \Delta_{pr}(\mu) \left( \gamma \partial_{\mu_i} \partial_{\mu_j} u_r,\mu u_{r,\mu} + 2 \gamma \partial_{\mu_i} \partial_{\mu_j} a_{r,\mu} \right)$$

$$+ 2 \gamma \partial_{\mu_i} \partial_{\mu_j} \| d_{r,\mu} u_r,\mu \| + \gamma \partial_{\mu_i} \partial_{\mu_j} \| d_{r,\mu} a_{r,\mu} \|$$

$$+ \Delta_{du,r}(\mu) \left( \gamma \partial_{\mu_i} \partial_{\mu_j} a_r,\mu + 2 \gamma \partial_{\mu_i} \partial_{\mu_j} u_r,\mu \right)$$

$$+ \gamma \partial_{\mu_i} \partial_{\mu_j} a_{r,\mu} \| d_{r,\mu} u_r,\mu \|$$

$$+ \Delta_{d_a}(\mu) \left( \gamma \partial_{\mu_i} \partial_{\mu_j} u_r,\mu + \gamma \partial_{\mu_i} \partial_{\mu_j} a_r,\mu \right)$$

$$+ \gamma \partial_{\mu_i} \partial_{\mu_j} a_{r,\mu} \| d_{r,\mu} a_{r,\mu} \|$$
\[
+ \Delta_{d_{ij}} d_{ij}(\mu) \left( \gamma_{\partial_{ij} \gamma_{ij}} + \gamma_{\partial_{ij} \gamma_{ij}} \| u_{r,\mu} \| \right) + (\Delta_{pr})^2(\mu) \left( \gamma_{\partial_{ij} \gamma_{ij}} \right)
+ \Delta_{pr}(\mu) \Delta_{d_{ij}}(\mu) \left( \gamma_{\partial_{ij} \gamma_{ij}} + \Delta_{pr}(\mu) \Delta_{d_{ij}}(\mu) \right) \left( 2 \gamma_{\partial_{ij} \gamma_{ij}} \right)
+ \Delta_{pr}(\mu) \Delta_{d_{ij}}(\mu) \left( \gamma_{\partial_{ij} \gamma_{ij}} \right) + \Delta_{d_{ij}}(\mu) \Delta_{d_{ij}}(\mu) \left( \gamma_{\partial_{ij} \gamma_{ij}} \right)
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij}(\mu) \| d_{ij} w_{r,\mu} \| \| w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} w_{r,\mu} \| u_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| u_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| d_{ij} w_{r,\mu} \|
+ 2 \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} w_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
+ \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} d_{ij} u_{r,\mu} \| \| d_{ij} w_{r,\mu} \|
\]

where \( \| \cdot \|_2 \) denotes the spectral norm for matrices. The norms of the auxiliary functions \( \| w_{r,\mu} \|, \| z_{r,\mu} \| \) and the norms of their sensitivities \( d_{ij} w_{r,\mu} \) and \( d_{ij} z_{r,\mu} \) can be estimated by

\[
\begin{align*}
\text{(i) } & \| z_{r,\mu} \| \leq a_{\mu}^{-1} \| r_{pr}(u_{r,\mu}) \|, \\
\text{(ii) } & \| w_{r,\mu} \| \leq a_{\mu}^{-1} \left( \| r_{st}_{dij}(u_{r,\mu}, p_{\mu} r, \mu) \| + 2 \gamma_{\partial_{ij} \gamma_{ij}} \| z_{r,\mu} \| \right), \\
\text{(iii) } & \| d_{ij} z_{r,\mu} \| \leq a_{\mu}^{-1} \left( \| r_{pr}_{dij}(u_{r,\mu}, d_{ij} u_{r,\mu}) \| + \gamma_{\partial_{ij} \gamma_{ij}} \| z_{r,\mu} \| \right), \\
\text{(iv) } & \| d_{ij} w_{r,\mu} \| \leq a_{\mu}^{-1} \left( \| r_{st}_{dij}(u_{r,\mu}, p_{\mu} r, \mu, d_{ij} u_{r,\mu}, d_{ij} p_{\mu} r, \mu) \| + 2 \gamma_{\partial_{ij} \gamma_{ij}} \| d_{ij} z_{r,\mu} \| \right) + \gamma_{\partial_{ij} \gamma_{ij}} \| z_{r,\mu} \| + \gamma_{\partial_{ij} \gamma_{ij}} \| w_{r,\mu} \|. 
\end{align*}
\]

\textbf{Proof.} To prove the hessian estimate, we recall that for all \( i, l \) we have

\[
(\hat{H}_{r,\mu}(\mu))_{i,l} = \partial_{l} (j_{i}(d_{ij} u_{r,\mu} + 2k_{ij}(u_{r,\mu}, d_{ij} u_{r,\mu}) - a_{ij}(d_{ij} u_{r,\mu}, p_{\mu} r, \mu + w_{r,\mu}) + r_{st}_{pr}(u_{r,\mu}, d_{ij} u_{r,\mu}) - 2k_{ij}(z_{r,\mu}, d_{ij} u_{r,\mu})) + \partial_{ij}(\mathcal{J}(u_{r,\mu}, \mu) + r_{st}_{pr}(u_{r,\mu}, u_{r,\mu}) - r_{st}_{dij}(u_{r,\mu}, p_{\mu} r, \mu)) \cdot e_{i}) \cdot e_{i},
\]

and

\[
(\hat{H}_{h,\mu}(\mu))_{i,l} = \partial_{l} (\partial_{uj}(u_{h,\mu})[d_{ij} u_{h,\mu}] + r_{st}_{pr}(u_{h,\mu}, p_{\mu} h, \mu) - a_{ij}(d_{ij} u_{h,\mu}, p_{\mu} h, \mu) + \partial_{ij}(\mathcal{J}(u_{h,\mu}, \mu) + r_{st}_{pr}(u_{h,\mu}, p_{\mu} h, \mu)) \cdot e_{i}) \cdot e_{i}.
\]

We get

\[
\| (\hat{H}_{h,\mu}(\mu) - \hat{H}_{r,\mu}(\mu))_{i,l} \|
\leq \| \partial_{l} (\partial_{uj}(u_{h,\mu})[d_{ij} u_{h,\mu}] - \partial_{uj}(u_{r,\mu})[d_{ij} u_{r,\mu}] + l_{i}(d_{ij} p_{h,\mu})
- l_{i}(d_{ij} p_{h,\mu}) - a_{ij}(d_{ij} u_{h,\mu}, p_{h,\mu}) + a_{ij}(d_{ij} u_{r,\mu}, p_{r,\mu}) - a_{ij}(u_{h,\mu}, d_{ij} p_{h,\mu})
+ a_{ij}(d_{ij} u_{r,\mu}, d_{ij} p_{r,\mu}) + a_{ij}(d_{ij} w_{r,\mu}, u_{r,\mu} - r_{st}_{pr}(u_{r,\mu})) + 2k_{ij}(z_{r,\mu}, d_{ij} u_{r,\mu}) - a_{ij}(z_{r,\mu}, d_{ij} p_{r,\mu}) + a_{ij}(d_{ij} u_{r,\mu}, p_{\mu} r, \mu) + \partial_{ij}(\mathcal{J}(u_{h,\mu}, \mu) - \mathcal{J}(u_{r,\mu}, \mu)) + l_{i}(p_{h,\mu}) - l_{i}(p_{r,\mu}) - a_{ij}(u_{h,\mu}, p_{h,\mu})
\|.
\]
+ a_\mu(u_{r,\mu}, p_{r,\mu}) + r^\text{pr}_\mu(u_{r,\mu})[w_{r,\mu}] - r^\text{dual}_\mu(u_{r,\mu}, p_{r,\mu})[z_{r,\mu}] \cdot e_1 \right) \cdot e_i.

For the first terms we see that

\[ \partial_\mu(\partial_u \mathcal{J}(u_{h,\mu}, \mu)[d_{\mu}u_{h,\mu}] - \partial_u \mathcal{J}(u_{r,\mu}, \mu)[d_{\mu}u_{r,\mu}]) \cdot e_i = \partial_\mu(j_\mu(d_{\mu}e_{\text{pr}}_{h,\mu} + 2k_\mu(d_{\mu}e_{\text{pr}}_{h,\mu}, u_{h,\mu}) + 2k_\mu(d_{\mu}u_{r,\mu}, e_{\text{pr}}_{h,\mu}))) \cdot e_i. \]

Obviously, this equation still incorporates the norm of the FOM solution \( u_{h,\mu} \). However, we can simply estimate these FOM quantities by \( \|u_{h,\mu}\| \leq \Delta_{pr}(\mu) + \|u_{r,\mu}\| \). For the second terms we have

\[ \partial_\mu(l_{\mu}(d_{\mu}p_{h,\mu}) - l_{\mu}(d_{\mu}p_{r,\mu})) \cdot e_i = \partial_\mu(l_{\mu}(d_{\mu}e_{\text{dual}}_{h,\mu})) \cdot e_i. \]

The third terms can be determined by

\[ -\partial_\mu(a_\mu(d_{\mu}u_{h,\mu}, p_{h,\mu}) - a_\mu(d_{\mu}u_{r,\mu}, p_{r,\mu})) \cdot e_i = -\partial_\mu(a_\mu(d_{\mu}e_{\text{pr}}_{h,\mu}, p_{h,\mu}) - a_\mu(d_{\mu}u_{r,\mu}, e_{\text{dual}}_{h,\mu})) \cdot e_i \]

and similarly we get for the fourth term

\[ -\partial_\mu(a_\mu(u_{h,\mu}, d_{\mu}p_{h,\mu}) - a_\mu(u_{r,\mu}, d_{\mu}p_{r,\mu})) \cdot e_i = -\partial_\mu(a_\mu(e_{\text{pr}}_{h,\mu}, d_{\mu}p_{h,\mu}) - a_\mu(u_{r,\mu}, d_{\mu}e_{\text{dual}}_{h,\mu})) \cdot e_i. \]

With the same strategy as above, we have for the first part of the second derivatives that

\[
\partial_\mu\left(\partial_\mu(\mathcal{J}(u_{h,\mu}, \mu) - \mathcal{J}(u_{r,\mu}, \mu) + l_{\mu}(p_{h,\mu}) - l_{\mu}(p_{r,\mu})
-a_\mu(u_{h,\mu}, p_{h,\mu}) + a_\mu(u_{r,\mu}, p_{r,\mu})) \cdot e_i \right) \cdot e_i
= \partial_\mu\left(\partial_\mu(j_\mu(e_{\text{pr}}_{h,\mu} + 2k_\mu(e_{\text{pr}}_{h,\mu}, u_{h,\mu}) + 2k_\mu(u_{r,\mu}, e_{\text{pr}}_{h,\mu}) + l_{\mu}(e_{\text{dual}}_{h,\mu})
-a_\mu(e_{\text{dual}}_{h,\mu}, p_{h,\mu}) - a_\mu(u_{r,\mu}, e_{\text{dual}}_{h,\mu})) \cdot e_i \right) \cdot e_i.
\]

For the rest of the proof we simply use the Cauchy-Schwarz inequality for all terms and sum all pieces together to get \( \Delta_{H,1}(\mu) \).

For a proof of (i) and (ii) we refer to [32, Proposition 2.7]. For the first sensitivity estimation (iii) we use the equations (2.10) and (2.12) to get

\[ a_\mu \|d_{\mu}z_{r,\mu}\|^2 \leq a_\mu(d_{\mu}z_{r,\mu}, d_{\mu}z_{r,\mu}) \]
\[ = -\partial_\mu(r^\text{pr}_\mu(u_{r,\mu})[d_{\mu}z_{r,\mu}] + a_\mu(z_{r,\mu}, d_{\mu}z_{r,\mu})) \cdot \nu + a_\mu(d_{\mu}u_{r,\mu}, d_{\mu}z_{r,\mu}) \]
\[ = -r^\text{pr}_\mu(d_{\mu}u_{r,\mu}, d_{\mu}u_{r,\mu})[d_{\mu}z_{r,\mu}] - \partial_\mu a_\mu(z_{r,\mu}, d_{\mu}z_{r,\mu}) \cdot \nu \]
\[ \leq \left( \|r^\text{pr}_\mu(d_{\mu}u_{r,\mu}, d_{\mu}u_{r,\mu})\| + \gamma \partial_\mu a_\mu \|z_{r,\mu}\| \right) \|d_{\mu}z_{r,\mu}\|. \]

For (iv), we instead use (2.11) and (2.13) and yield

\[ a_\mu \|d_{\mu}w_{r,\mu}\|^2 \leq a_\mu(d_{\mu}w_{r,\mu}, d_{\mu}w_{r,\mu}) \]
\[ = \partial_\mu(r^\text{dual}_\mu(u_{r,\mu}, p_{r,\mu})[d_{\mu}w_{r,\mu}] - 2k_\mu(z_{r,\mu}, d_{\mu}w_{r,\mu}) - a_\mu(d_{\mu}w_{r,\mu}, w_{r,\mu})) \cdot \nu \]
\[ + 2k_\mu(d_{\mu}w_{r,\mu}, u_{r,\mu} - d_{\nu}z_{r,\mu}) - a_\mu(d_{\mu}w_{r,\mu}, d_{\nu}p_{r,\mu}) \]
\[ r_{\mu}^{d_{\mu}, d_{\mu}, (u_{r, \mu}, p_{r, \mu}, d_{\mu}, u_{r, \mu}, d_{\mu}, p_{r, \mu})[d_{\mu}, w_{r, \mu}] - 2k_{\mu}(d_{\mu}, w_{r, \mu}, d_{\nu}, z_{r, \mu}) \]
\[ - \partial_{\mu}(2k_{\mu}(z_{r, \mu}, d_{\mu}, w_{r, \mu}) - a_{\mu}(d_{\mu}, w_{r, \mu}, w_{r, \mu}) \cdot \nu \]
\[ \leq \left( \| r_{\mu}^{d_{\mu}, d_{\mu}, (u_{r, \mu}, p_{r, \mu}, d_{\mu}, u_{r, \mu}, d_{\mu}, p_{r, \mu})\| + 2\gamma k_{\mu} \| d_{\mu}, z_{r, \mu} \| \right) \]
\[ + 2\gamma a_{\mu} \| z_{r, \mu} \| + \gamma a_{\mu} \| w_{r, \mu} \| \right) \| d_{\mu}, w_{r, \mu} \|. \]

□

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