Adaptive Reduced Basis Methods for PDE-Constrained Optimization and Optimal Input Design

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Abstract: In this paper we propose an algorithm for the bi-level optimal input design involving a parameter-dependent evolution problem. In the inner cycle a control is fixed and the parameter is optimized in order to minimize a cost function that measure the discrepancy from some data. In the outer cycle the found parameter is fixed and the control is now optimized in order to minimize a suitable measure of uncertainty of the parameters. The inner cycle uses a trust-region reduced basis approximation of the model with creation and enrichment of the reduced basis on-the-fly. Numerical examples illustrate the efficiency of the proposed approach.

Keywords: Reduced basis methods, a-posteriori error, trust-region optimization, evolution problems, optimal input design.

1. INTRODUCTION

PDE modelling is relevant in many fields, such as medicine and engineering, and optimization methods are useful when dealing with real-life problems. It is not uncommon for some models to depend on underlying unknown parameters, while we might have some controls (either finite or infinite-dimensional) that we are able to change in real time. Parameter estimation (PE) comprehends methods and algorithms able to find or approximate the underlying parameters using empirical data or observations. It is often the case that the choice of a particular control speeds up or slows down the parameter estimation, hence being an important choice when the temporal or computational costs are limited.

In this work two problems are discussed. First, the step of parameter estimation is not trivial: usually such problems are ill-posed or non-convex, hence resulting in non-unique or non-global solutions. Even when well-posed, some applications deal with such high-dimensional discretizations that the solution is prohibitively costly. For this reason model order reduction (MOR) methods were developed, where the "expensive" models are replaced by cheaper and less accurate surrogates; cf., e.g., Benner et al. (2020a,b,c) and Benner et al. (2014). In our case the reduced basis (RB) is used, creating a reduced-order model on the optimization path in such a way that the local minimum found by our taylored optimization method in the reduced space is very close to a local minimum in the full space.

The second problem belongs to the optimal input/experimental design (OED); see e.g. Goodwin and Payne (1977); Atkinson et al. (2007); Bock et al. (2013); Körkel et al. (2004); Pozzi et al. (2019); Reddy et al. (2019); Alexanderian et al. (2016). We want to find the "best" control, namely the one that gives us a better parameter estimation in a bi-level algorithm. In particular, assuming there are measurement error in the observations, the "best" control is the one that minimizes the uncertainty given by the parameter optimization.

The article is organized as follows: In Section 2 the parameter estimation problem is introduced. Its discretization and the a-posteriori error analysis is discussed in Section 3. The trust-region method for the parameter optimization is explained in Section 4. The OED is described in Section 5, whereas Section 6 is devoted for numerical experiments.

2. PARAMETER ESTIMATION PROBLEM

We assume that all parameters are stacked in a vector $\mu \in \mathbb{R}^d$, and belong to the compact (admissible) set

$$\mathcal{P}_{\mathsf{ad}} = \left\{ \mu \in \mathbb{R}^d \,\middle|\, \mu_i^{\mathsf{a}} \le \mu_i \le \mu_i^{\mathsf{b}} \text{ for } i = 1, \dots, d \right\}$$

The *state* variable y satisfies the evolution problem

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t} \langle y(t), \varphi \rangle_H + a_\mu(y(t), \varphi) &= \langle f_\mu(t; u), \varphi \rangle_{V',V} \\ y(0) &= y_\circ \quad \text{in } H \end{aligned} \tag{1}$$

for all $\varphi \in V$ and $t \in (0, T]$ a.a., where $y_\circ \in H$, V, H are Hilbert spaces with $V \hookrightarrow H \hookrightarrow V'$ (Gelfand triple) and u denotes the *control* belonging to a convex, bounded, closed subset $\mathcal{U}_{\mathsf{ad}}$ of a Hilbert space $\mathcal{U}$. For any $\mu \in \mathcal{P}_{\mathsf{ad}}$ the bilinear form $a_\mu : V \times V \to \mathbb{R}$ is

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- symmetric:
$$a_\mu(\varphi,\phi) = a_\mu(\phi,\varphi) \quad \text{for all } \varphi,\phi \in V;$$
- continuous: there exists a constant $\overline{\gamma}_\mu > 0$ satisfying
$$|a_\mu(\varphi,\phi)| \le \overline{\gamma}_\mu \|\varphi\|_V \|\phi\|_V \quad \text{for all } \varphi,\phi \in V;$$
- coercive: there is $\underline{\alpha}_\mu > 0$ such that
$$a_\mu(\varphi,\varphi) \ge \underline{\alpha}_\mu \|\varphi\|_V^2 \quad \text{for all } \varphi \in V.$$

Moreover, $f_\mu(\cdot\,;u) \in L^2(0;T;V')$ holds for any $(\mu,u) \in \mathcal{X}_{\mathsf{ad}} = \mathcal{P}_{\mathsf{ad}} \times \mathcal{U}_{\mathsf{ad}}$.

For any $\mu \in \mathcal{P}_{\mathsf{ad}}$ it follows that (1) admits a unique solution $y = y_\mu \in \mathcal{Y}$ with
$$\mathcal{Y} = W(0,T) = L^2(0,T;V) \cap H^1(0,T;V');$$
cf., e.g., Hinze et al. (2009); Tröltzsch (2010). Recall that
$$\tfrac{\mathrm{d}}{\mathrm{d}t} \langle \varphi(t), \phi \rangle_H = \langle \varphi_t(t), \phi \rangle_{V',V} \quad \text{for all } (\varphi,\phi) \in \mathcal{Y} \times V$$
and $\mathcal{Y} \hookrightarrow C([0,T];H)$. We assume that a_μ and f_μ depend affinely on the parameters:
$$a_\mu = \sum_{l=1}^{m_a} \vartheta_l^a(\mu)\hat{a}_l, \quad f_\mu(t;u) = \sum_{l=1}^{m_f} \vartheta_l^f(\mu)\hat{f}_l(t;u) \tag{2}$$
for any $(\mu,u) \in \mathcal{X}_{\mathsf{ad}}$ and $t \in [0,T]$. Otherwise, we apply the *(discrete) empirical interpolation method* to get approximations satisfying (2); cf., e.g., Barrault et al. (2004); Chaturantabut and Sorensen (2010, 2012); Hesthaven et al. (2016).

The goal is to estimate unknown model parameters $\mu \in \mathcal{P}_{\mathsf{ad}}$, where the control input should be chosen in an optimal way explained later. Here, we suppose that $u \in \mathcal{U}_{\mathsf{ad}}$ is fixed and consider
$$\min J(y,\mu) \text{ subject to } (y,\mu) \in \mathcal{Y} \times \mathcal{P}_{\mathsf{ad}} \text{ satisfies (1)} \quad (\mathbf{P})$$
As (1) is uniquely solvable, we can define the *reduced cost* $\hat{J}(\mu) = J(y_\mu,\mu)$, where y_μ solve (1). Then, $(\mathbf{P})$ is equivalent to
$$\min \hat{J}(\mu) \quad \text{subject to (s.t.)} \quad \mu \in \mathcal{P}_{\mathsf{ad}} \qquad (\hat{\mathbf{P}})$$

In our application the cost quantifies the discrepancy to a given desired (or observed) state $\hat{y} \in L^2(0,T;H)$:
$$\hat{J}(\mu) = 1 + \tfrac{1}{2}\int_0^T \|y_\mu(t) - \hat{y}(t)\|_H^2 \,\mathrm{d}t + \tfrac{\sigma}{2}\|\mu - \hat{\mu}\|_2^2 \tag{3}$$
where $\|\cdot\|_2$ stands for the Euclidean norm, σ is a non-negative weight and $\hat{\mu} \in \mathbb{R}^d$ is a reference parameter. Existence of an optimal solution $\bar{\mu}$ can be ensured under continuity for $\mu \to a_\mu$ and $\mu \to f_\mu$, but – due to non-convexity – there are possibly many local solutions; cf., e.g., Hinze et al. (2009). A local optimal solution $\bar{\mu}$ to $(\hat{\mathbf{P}})$ is characterized by first-order necessary optimality conditions. Let $\bar{y} = y_{\bar{\mu}}$ be the optimal state associated with $\bar{\mu}$ and the *adjoint variable* $\bar{p} = p_{\bar{\mu}} \in \mathcal{Y}$ the solution of the *adjoint equation*
$$\begin{aligned} -\tfrac{\mathrm{d}}{\mathrm{d}t}\langle \bar{p}(t), \varphi \rangle_H + a_{\bar{\mu}}(\bar{p}(t),\varphi) &= \langle \hat{y}(t) - \bar{y}(t), \varphi \rangle_H \\ \bar{p}(T) &= 0 \quad \text{in } H \end{aligned}$$
for all $\varphi \in V$ and $t \in [0,T)$. Using the *adjoint approach* the gradient of the cost functional at $\bar{\mu}$ is given as
$$\begin{aligned} \nabla\hat{J}(\bar{\mu}) = \sigma(\bar{\mu} - \hat{\mu}) &+ \int_0^T \sum_{i=1}^{m_a} \nabla\vartheta_i^a(\mu)\hat{a}_q(\bar{y}(t),\bar{p}(t))\,\mathrm{d}t \\ &- \int_0^T \sum_{i=1}^{m_f} \nabla\vartheta_i^f(\mu)\langle \hat{f}_i(t;u), p(t)\rangle_{V',V}\,\mathrm{d}t \in \mathbb{R}^d. \end{aligned}$$

The derivation is based on the Lagrangian
$$\begin{aligned} \mathcal{L}(y,\mu,p;u) = J(y,\mu) &+ \int_0^T \langle y_t(t), p(t)\rangle_{V',V}\,\mathrm{d}t \\ &+ \int_0^T a_\mu(y(t),p(t)) - \langle f_\mu(t;u), p(t)\rangle_{V',V}\,\mathrm{d}t \end{aligned}$$
for $(\mathbf{P})$.

3. DISCRETIZATION

Next we introduce a high-dimensional discretization, called *full-order model* (FOM), which we assume to be accurate enough, but however expensive to solve. To reduce significantly the computational costs a further approximation is applied, the *reduced-order model* (ROM), faster to solve but less accurate.

3.1 FOM

Let $\varphi_1,\dots,\varphi_N \in V$ be given linearly independent functions and $V^N = \operatorname{span}\{\varphi_1,\dots,\varphi_N\} \subset V$. The FOM for (1) reads: for given $\mu \in \mathcal{P}_{\mathsf{ad}}$ the function $y_\mu^N(t) \in V^N$ solves
$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t}\langle y_\mu^N(t), \varphi \rangle_H + a_\mu(y_\mu^N(t),\varphi) &= \langle f_\mu(t;u), \varphi \rangle_{V',V} \\ y_\mu^N(0) &= \mathcal{P}^N y_\circ \end{aligned} \tag{4}$$
for all $\varphi \in V^N$ and $t \in (0,T]$, where $\mathcal{P}^N : H \to V^N$ is a projection. Due to $y_\mu^N(t) \in V^N$ we have
$$y_\mu^N(t) = \sum_{i=1}^N \mathrm{y}_{\mu,i}(t)\varphi_i \quad \text{for } t \in [0,T]$$
so that (4) reduces into finding the coefficient vector $\mathrm{y}_\mu(t) = (\mathrm{y}_{\mu,i}(t))_{1\le i\le N}$ solving
$$\begin{aligned} \mathrm{M}\dot{\mathrm{y}}_\mu(t) + \mathrm{A}_\mu \mathrm{y}_\mu(t) &= \mathrm{f}_\mu(t;u), \quad t \in (0,T] \\ \mathrm{M}\mathrm{y}_\mu(0) &= \mathrm{y}_\circ \end{aligned} \tag{5}$$
for $\mathrm{f}_\mu(t;u) = (\langle f_\mu(t;u), \varphi_i\rangle_{V';V}) \in \mathbb{R}^N$, $\mathrm{y}_\circ = (\langle y_\circ, \varphi_i\rangle_H) \in \mathbb{R}^N$, $\mathrm{A}_\mu = ((a_\mu(\varphi_j,\varphi_i))) \in \mathbb{R}^{N\times N}$, $\mathrm{M} = ((\langle \varphi_j,\varphi_i\rangle_H)) \in \mathbb{R}^{N\times N}$.

Remark 1. Due to (2) both A_μ and f_μ satisfy
$$\mathrm{A}_\mu = \sum_{l=1}^{m_a} \vartheta_l^a(\mu)\hat{\mathrm{A}}_l, \quad \mathrm{f}_\mu(t;u) = \sum_{l=1}^{m_f} \vartheta_l^f(\mu)\hat{\mathrm{f}}_l(t;u)$$
for $\hat{\mathrm{A}}_l = ((\hat{a}_l(\varphi_j,\varphi_i)))$ and $\hat{\mathrm{f}}_l(t;u) = (\langle \hat{f}_l(t;u), \varphi_i\rangle_{V';V})$. $\diamond$

For solving (5) we apply the implicit Euler method for the time integration; cf., e.g., Quarteroni (2017). To simplify the presentation we utilize an equidistant time grid $t_k = (k-1)\Delta t$, $k = 1,\dots,K$ and $\Delta t = T/(K-1)$. Then, the problem is to find $\{\mathrm{y}_\mu^k\}_{k=1}^K \subset \mathbb{R}^N$ solving
$$\begin{aligned} (\mathrm{M} + \Delta t\mathrm{A}_\mu)\mathrm{y}_\mu^k &= \mathrm{M}\mathrm{y}_\mu^{k-1} + \Delta t\mathrm{f}_\mu^k(u) \\ \mathrm{M}\mathrm{y}_\mu^1 &= \mathrm{y}_\circ \end{aligned} \tag{6}$$
for $k = 2,\dots,K$ and $\mu \in \mathcal{P}_{\mathsf{ad}}$ with $\mathrm{f}_\mu^k(u) = \mathrm{f}_\mu(t^k;u) \in \mathbb{R}^N$. Note that y_μ^k is the coefficient vector of the approximation $y_\mu^k \in V^N$ of $y_\mu^N(t_k) \in V^N$; cf. (13).

Remark 2. Similarly, we get the Galerkin approximations for the adjoint state, the reduced cost, and the reduced cost gradient. More precisely, the discrete adjoint sequence $\{\mathrm{p}_\mu^k\}_{k=1}^K \subset \mathbb{R}^N$ satisfies:
$$\begin{aligned} (\mathrm{M} + \Delta t\mathrm{A}_\mu)\mathrm{p}_\mu^k &= \mathrm{M}\big(\mathrm{p}_\mu^{k+1} + \Delta t(\hat{\mathrm{y}}^k - \mathrm{y}_\mu^k)\big) \\ \mathrm{p}_\mu^K &= 0 \end{aligned}$$

where $k = 1, \dots, K-1$, $\{\mathrm{y}_\mu^k\}_{k=1}^K$ solves (6) and $\hat{y}^k = \sum_{i=1}^N \hat{y}_i^k \varphi_i \approx \hat{y}(t_k)$ holds. Further, the reduced cost $\hat{J}$ is approximated by

$$\hat{J}^N(\mu) = 1 + \tfrac{1}{2} \sum_{k=1}^K \alpha_k \left(\mathrm{y}_\mu^k - \hat{\mathrm{y}}^k\right)^\top \mathrm{M}\left(\mathrm{y}_\mu^k - \hat{\mathrm{y}}^k\right) + \tfrac{\sigma}{2} \|\mu - \hat{\mu}\|_2^2 \tag{7}$$

where the α_k's are trapezoidal weights. The gradient of the reduced cost is then given by

$$\nabla \hat{J}^N(\mu) = \sum_{k=1}^K \alpha_k \Big[\sum_{l=1}^{m_a} \nabla \vartheta_l^a(\mu) \hat{\mathrm{A}}_l \mathrm{y}_\mu^k - \sum_{l=1}^{m_f} \nabla \vartheta_l^f(\mu) \hat{\mathrm{f}}_l^k(u)\Big]^\top \mathrm{p}_\mu^k + \sigma(\mu - \hat{\mu})$$

◇

3.2 ROM

The reduced order modelling is based on the projection of the model onto a smaller dimension space: in particular, we call the reduced-order space $V^\ell = \operatorname{span}\{\psi_i\}_{i=1}^\ell \subset V^N$ for $\ell \ll N$. We use the method of *proper orthogonal decomposition* (POD), that consists in finding such basis using the snapshots $\{\mathrm{y}_\mu^k\}_{k=1}^K \subset \mathbb{R}^N$, or equivalently $\{y_\mu^k\}_{k=1}^K \subset V^N$, satisfying the problem

$$\begin{aligned} &\min_{\{\psi_j\}_{j=1}^\ell} \sum_{k=1}^K \alpha_k \Big\| y_\mu^k - \sum_{i=1}^\ell \langle y_\mu^k, \psi_i\rangle_V \ \psi_i \Big\|_V^2 \\ &\text{subject to } \langle \psi_i, \psi_j\rangle_V = \delta_{ij} \qquad \forall\ 1 \le i, j \le \ell. \end{aligned} \tag{8}$$

A solution to (8) is given by the eigenvectors corresponding to the ℓ biggest eigenvalues of the matrix $R = \mathrm{YDY}^\top \mathrm{W}$, where $\mathrm{Y} = [\mathrm{y}_\mu^1, \dots, \mathrm{y}_\mu^K] \in \mathbb{R}^{N\times K}$ is the matrix of snapshots, D is the diagonal matrix of the trapezoidal weights

$$\mathrm{D} = \begin{pmatrix} \alpha_1 & & \\ & \ddots & \\ & & \alpha_K \end{pmatrix}$$

and $\mathrm{W} = ((\langle \varphi_j, \varphi_i\rangle_V)) \in \mathbb{R}^{N\times N}$.

Remark 3. These ℓ eigenvectors can be evaluated by defining $\bar{\mathrm{Y}} = \mathrm{W}^{1/2}\mathrm{YD}^{1/2}$ and solving the eigenvalue problem

$$\begin{aligned} &\bar{\mathrm{Y}}^\top \bar{\mathrm{Y}} \mathrm{v}_i = \lambda_i \mathrm{v}_i, && 1 \le i \le \ell, \\ &\text{s.t. } \langle \mathrm{v}_i, \mathrm{v}_j\rangle_{\mathbb{R}^N} = \delta_{ij}, && 1 \le i, j \le \ell, \end{aligned}$$

where the matrix $\bar{\mathrm{Y}}^\top \bar{\mathrm{Y}} = \mathrm{D}^{1/2}\mathrm{YWYD}^{1/2}$ is relatively easy to evaluate (i.e. there is actually no need to evaluate the square root of W and the square root of a diagonal matrix is straightforward), and then defining the vectors

$$\Psi_i = \frac{1}{\sqrt{\lambda_i}} \mathrm{YD}^{1/2} \mathrm{v}_i \in \mathbb{R}^N$$

as the coefficient vectors of the reduced basis element ψ_i in the FOM basis $\{\varphi_i\}_{i=1}^N$, for $i = 1, \dots, \ell$. ◇

Furthermore, we have the following error formula:

$$\sum_{k=1}^K \alpha_k \Big\| y_\mu^k - \sum_{i=1}^\ell \langle y_\mu^k, \psi_i\rangle_V \ \psi_i \Big\|_V^2 = \sum_{j=\ell+1}^d \lambda_i. \tag{9}$$

We define the coefficient matrix $\Psi \in \mathbb{R}^{N\times\ell}$ satisfying $\psi_j = \sum_{i=1}^N \Psi_{ij}\varphi_i$ for $j = 1, \dots, \ell$. We notice how each column Ψ_i is the coefficient vector of ψ_i, coherently as defined before.

Before defining the RB approximations of the variables, let us use a variation of the standard POD: instead of finding one RB (for both state and adjoint variables) by solving the problem (8) (eventually also using the adjoint variable's snapshots), we find two different set of basis, one for the state variable and one for the adjoint variable. The former is found by solving

$$\begin{aligned} \min_{\{\psi_j\}_{j=1}^\ell} \Bigg\{ &\sum_{k=1}^K \alpha_k \Big\| y_\mu^k - \sum_{i=1}^\ell \langle y_\mu^k, \psi_i\rangle_V \ \psi_i \Big\|_V^2 \\ &+ \sum_{k=2}^K \Delta t \Big\| \bar{\partial} y^k - \sum_{i=1}^\ell \langle \bar{\partial} y^k, \psi_i\rangle_V \ \psi_i \Big\|_V^2 \Bigg\} \\ \text{s.t.} &\langle \psi_\mathrm{i}, \psi_\mathrm{j}\rangle_\mathrm{V} = \delta_\mathrm{ij} \qquad \forall\ 1 \le \mathrm{i}, \mathrm{j} \le \ell. \end{aligned}$$

Here, we have used the notation

$$\bar{\partial} y^k = \tfrac{y_\mu^k - y_\mu^{k-1}}{\Delta t} \approx (y_\mu)_t(t_k)$$

and in the same way we define

$$\bar{\partial} p^k = \tfrac{p_\mu^k - p_\mu^{k-1}}{\Delta t} \approx (p_\mu)_t(t_k)$$

for $k = 2, \dots, K$, to impose a certain level accuracy of the reduced basis also with respect to the approximations of the derivative of the states; cf. Gubisch and Volkwein (2017); Kunisch and Volkwein (2001). Indeed, defining

$$\mathrm{Z} = [\mathrm{y}_\mu^1, \dots, \mathrm{y}_\mu^K, \bar{\partial}\mathrm{y}_\mu^2, \dots, \bar{\partial}\mathrm{y}_\mu^K] \in \mathbb{R}^{N\times(2K-1)} \tag{10}$$

and

$$\bar{\mathrm{D}} = \operatorname{diag}(\mathrm{D}, \Delta t I_{K-1})$$

where I is the identity matrix, we solve the eigenvalue problem

$$\begin{aligned} &\bar{\mathrm{Z}}^\top \bar{\mathrm{Z}} \tilde{\mathrm{v}}_i = \tilde{\lambda}_i \tilde{\mathrm{v}}_i, && 1 \le i \le \ell, \\ &\text{s.t. } \langle \tilde{\mathrm{v}}_i, \tilde{\mathrm{v}}_j\rangle_{\mathbb{R}^N} = \delta_{ij}, && 1 \le i, j \le \ell, \end{aligned} \tag{11}$$

where $\bar{\mathrm{Z}} = \mathrm{W}^{1/2}\mathrm{Z}\bar{\mathrm{D}}^{1/2}$. Hence, the error formula (9) becomes

$$\begin{aligned} &\sum_{k=1}^K \alpha_k \Big\| y_\mu^k - \sum_{i=1}^\ell \langle y_\mu^k, \psi_i\rangle_V \ \psi_i \Big\|_V^2 \\ &+ \sum_{k=2}^K \Delta t \Big\| \bar{\partial} y^k - \sum_{i=1}^\ell \langle \bar{\partial} y^k, \psi_i\rangle_V \ \psi_i \Big\|_V^2 \\ &= \sum_{i=\ell+1}^d \tilde{\lambda}_i. \end{aligned}$$

Similarly, for the adjoint variable's reduced basis, we define

$$\mathrm{Z} = [\mathrm{p}_\mu^1, \dots, \mathrm{p}_\mu^K, \bar{\partial}\mathrm{p}_\mu^2, \dots, \bar{\partial}\mathrm{p}_\mu^K] \in \mathbb{R}^{N\times(2K-1)}$$

and proceed as before. For more details, see Kunisch and Volkwein (2001, 2002).

Hence, we are given $\Psi_y \in \mathbb{R}^{N,\ell_y}$ RB matrix for the state variable and $\Psi_p \in \mathbb{R}^{N,\ell_p}$ RB matrix for the adjoint variable, where $\ell_y, \ell_p \in \mathbb{R}$ are the dimensions of the reduced bases. Then, the ROM for (4) reads as follows: find $\{\mathrm{y}_\mu^{k,\ell}\}_{k=1}^K \subset \mathbb{R}^\ell$ such that

$$\begin{aligned} \big(\mathrm{M}^{\ell_y} + \Delta t \mathrm{A}_\mu^{\ell_y}\big)\mathrm{y}_\mu^{k,\ell} &= \mathrm{M}^{\ell_y}\mathrm{y}_\mu^{k-1,\ell} + \Delta t \mathrm{f}_\mu^{k,\ell_y}(u) \\ \mathrm{M}^{\ell_y}\mathrm{y}_\mu^{1,\ell} &= \mathrm{y}_\circ^{\ell_y} \end{aligned} \tag{12}$$

with the RB matrices are given as

$$\begin{aligned} \mathrm{y}_\circ^{\ell_y} &= \Psi_y^\top \mathrm{y}_\circ, \\ \mathrm{M}^{\ell_y} &= \Psi_y^\top \mathrm{M} \Psi_y, \\ \mathrm{A}_\mu^{\ell_y} &= \sum_{l=1}^{m_a} \vartheta_l^a(\mu) \Psi_y^\top \hat{\mathrm{A}}_l \Psi_y, \\ \mathrm{f}_\mu^{k,\ell_y}(u) &= \sum_{l=1}^{m_f} \vartheta_l^f(\mu) \Psi_y^\top \hat{\mathrm{f}}_l^k(u). \end{aligned}$$

The solution $\{\mathrm{y}_\mu^{k,\ell}\}_{k=1}^K$ uniquely exists (see Kunisch and Volkwein (2001)) and it is interpreted as a reduced-order approximation for $\{\mathrm{y}_\mu^k\}_{k=1}^K$:

$$\mathrm{y}_\mu^k \approx \tilde{\mathrm{y}}_\mu^{k,\ell} := \Psi_y \mathrm{y}_\mu^{k,\ell} \in \mathbb{R}^N$$

For $1 \le k \le K$ we also use the additional notations

$$y_\mu^k = \sum_{i=1}^N \mathrm{y}_{\mu,i}^k \varphi_i \in V^N \text{ and } y_\mu^{k,\ell} = \sum_{i=1}^\ell \mathrm{y}_{\mu,i}^{k,\ell} \psi_i \in V^\ell \quad (13)$$

Similarly, we construct a reduced-order adjoint approximation $\{\mathrm{p}_\mu^{k,\ell}\}_{k=1}^K \subset \mathbb{R}^\ell$ by solving

$$\big(\mathrm{M}^{\ell_p} + \Delta t \mathrm{A}_\mu^{\ell_p}\big)\mathrm{p}_\mu^{k,\ell} = \mathrm{M}^{\ell_p}\mathrm{p}_\mu^{k+1,\ell} + \Delta t\big(\hat{\mathrm{y}}^{k,\ell_p} - \mathrm{M}^{\ell_{py}}\mathrm{y}_\mu^{k,\ell}\big)$$
$$\mathrm{p}^{K,\ell} = 0$$

where

$$\mathrm{M}^{\ell_p} = \Psi_p^\top \mathrm{M}\Psi_p, \qquad \mathrm{M}^{\ell_{py}} = \Psi_p^\top \mathrm{M}\Psi_y,$$
$$\mathrm{A}_\mu^{\ell_p} = \sum_{l=1}^{m_a} \vartheta_l^a(\mu)\hat{\mathrm{A}}_l^{\ell_p}, \qquad \hat{\mathrm{A}}_l^{\ell_p} = \Psi_p^\top \hat{\mathrm{A}}_l \Psi_p,$$
$$\hat{\mathrm{y}}^{k,\ell} = \Psi_p^\top \mathrm{M}\hat{\mathrm{y}}^k.$$

Then, since

$$\|y_\mu^{k,\ell} - \hat{y}^k\|_H^2 = \big(\mathrm{y}_\mu^{k,\ell}\big)^\top \mathrm{M}^{\ell_y}\mathrm{y}_\mu^{k,\ell} - 2\big(\mathrm{y}_\mu^{k,\ell}\big)^\top \hat{\mathrm{y}}^{k,\ell} + \big(\hat{\mathrm{y}}^k\big)^\top \mathrm{M}\hat{\mathrm{y}}^k,$$

the reduced cost function is approximated by

$$\begin{aligned}\hat{J}^\ell(\mu) = {} & \tfrac{1}{2}\sum_{k=1}^K \alpha_k \Big[\big(\mathrm{y}_\mu^{k,\ell}\big)^\top \mathrm{M}^\ell \mathrm{y}_\mu^{k,\ell} - 2\big(\mathrm{y}_\mu^{k,\ell}\big)^\top \hat{\mathrm{y}}^{k,\ell}\Big] \\ & + \tfrac{1}{2}\sum_{k=1}^K \alpha_k \big(\hat{\mathrm{y}}^k\big)^\top \mathrm{M}\hat{\mathrm{y}}^k + \tfrac{\sigma}{2}\|\mu - \hat{\mu}\|_2^2 + 1,\end{aligned} \quad (14)$$

where the element

$$\frac{1}{2}\sum_{k=1}^K \alpha_k \big(\hat{\mathrm{y}}^k\big)^\top \mathrm{M}\hat{\mathrm{y}}^k \approx \frac{1}{2}\|\hat{y}\|^2_{L^2(0,T;H)}$$

can be evaluated and stored as soon as the data $\hat{y}$ is evaluated. Finally, the gradient of the reduced cost function is given by

$$\nabla \hat{J}^\ell(\mu) = \sum_{k=1}^K \alpha_k \Big[\sum_{l=1}^{m_a} \nabla\vartheta_l^a(\mu)\hat{\mathrm{A}}_l^{\ell_{py}}\mathrm{y}_\mu^{k,\ell} - \sum_{l=1}^{m_f} \nabla\vartheta_l^f(\mu)\hat{\mathrm{f}}_l^{k,\ell_p}(u)\Big]^\top \mathrm{p}_\mu^{k,\ell} + \sigma(\mu - \hat{\mu}),$$

where

$$\hat{\mathrm{A}}_l^{\ell_{py}} = \Psi_p^\top \hat{\mathrm{A}}_l \Psi_y, \qquad \text{for } l = 1, \dots, m_a$$
$$\hat{\mathrm{f}}_l^{k,\ell_p}(u) = \Psi_p^\top \hat{\mathrm{f}}_l^k, \qquad \text{for } l = 1, \dots, m_f.$$

3.3 A-posteriori RB error estimates

Now we present a-posteriori error estimates for the error of the ROM without evaluating the full-order solution. For our TR algorithm we will need estimates for the state and for the cost function.

Let us define the μ-dependent space-time energy norm for the sequence $\{y^k\}_{k=1}^K \subset V^N$ as

$$\|y^j\|_\mu = \Big(\|y^j\|_H^2 + \Delta t \sum_{k=2}^j a_\mu(y^k, y^k)\Big)^{1/2}$$

for $j = 2, \dots, K$, and $\|y^1\|_\mu = \|y^1\|_H$. Then we can define the error estimates in this norm in the following propositions.

Proposition 4. Let $\{y_\mu^k\}_{k=1}^K$ and $\{y_\mu^{k,\ell}\}_{k=1}^K$ be given by (13) and $\mathsf{err}_\mu^k = y_\mu^k - y_\mu^{k,\ell} \in V^N$ for $k = 1, \dots, K$. For $\varphi \in V^N$ we define the residual

$$\langle \mathsf{res}_\mu^k, \varphi\rangle_{(V^N)',V^N} = \Big\langle \tfrac{y_\mu^{k-1,\ell} - y_\mu^{k,\ell}}{\Delta t}, \varphi\Big\rangle_H - a_\mu(y_\mu^{k,\ell}, \varphi) + \langle f_\mu(t_k; u), \varphi\rangle_{V',V}$$

and

$$\varepsilon_\mu^k = \|\mathsf{res}_\mu^k\|_{(V^N)'} = \sup_{\varphi \in V^N \setminus \{0\}} \frac{\langle \mathsf{res}_\mu^k, \varphi\rangle_{(V^N)',V^N}}{\|\varphi\|_V}$$

Then $\|\mathsf{err}_\mu^j\|_\mu \le \Delta_\mu^j$ for $j \in \{1, \dots, K\}$, where

$$\Delta_\mu^j = \left(\|\mathsf{err}_\mu^1\|_H^2 + \tfrac{\Delta t}{\underline{\alpha}_\mu}\sum_{k=2}^j \big|\varepsilon_\mu^j\big|^2\right)^{1/2} \quad (15)$$

Proof. We refer to Grepl and Patera (2005). □

Proposition 5. Let $\{y_\mu^k\}_{k=1}^K$ and $\{y_\mu^{k,\ell}\}_{k=1}^K$ be given by (13), the reduced cost functions $\hat{J}^N(\mu)$ and $\hat{J}^\ell(\mu)$ be given by (7) and (14) respectively, the estimator Δ_μ^j be defined by (15), and the cost error defined by

$$\mathsf{err}_\mu^{\hat{J}} = \hat{J}^N(\mu) - \hat{J}^\ell(\mu).$$

Then we have

$$|\mathsf{err}_\mu^{\hat{J}}| \le \Delta_\mu^{\hat{J}} \quad (16)$$

where

$$\Delta_\mu^{\hat{J}} = \tfrac{1}{2}\sum_{k=1}^K \alpha_k\big((\Delta_\mu^k)^2 + 2\Delta_\mu^k \|y_\mu^{k,\ell} - \hat{y}^k\|_H\big), \quad (17)$$

which, again, does not require the evaluation of the full-order solution $\{y_\mu^k\}_{k=1}^K$.

Proof. First, we can write

$$\begin{aligned}&\|\hat{y}^k - y_\mu^k\|_H^2 - \|\hat{y}^k - y_\mu^{k,\ell}\|_H^2 \\ &= \langle \hat{y}^k - y_\mu^k, \hat{y}^k - y_\mu^k\rangle_H - \langle \hat{y}^k - y_\mu^{k,\ell}, \hat{y}^k - y_\mu^{k,\ell}\rangle_H \\ &= \langle \hat{y}^k - y_\mu^k, y_\mu^{k,\ell} - y_\mu^k\rangle_H - \langle y_\mu^k - y_\mu^{k,\ell}, \hat{y}^k - y_\mu^{k,\ell}\rangle_H \\ &= \langle \mathsf{err}_\mu^k, y_\mu^k + y_\mu^{k,\ell} - 2\hat{y}^k\rangle_H \\ &= \langle \mathsf{err}_\mu^k, \mathsf{err}_\mu^k + 2y_\mu^{k,\ell} - 2\hat{y}^k\rangle_H \\ &= \|\mathsf{err}_\mu^k\|_H^2 + 2\langle \mathsf{err}_\mu^k, y_\mu^{k,\ell} - \hat{y}^k\rangle_H.\end{aligned}$$

Moreover, using the Cauchy-Schwarz inequality

$$\big|\langle \mathsf{err}_\mu^k, y_\mu^{k,\ell} - \hat{y}^k\rangle_H\big| \le \|\mathsf{err}_\mu^k\|_H \|y_\mu^{k,\ell} - \hat{y}^k\|_H$$

Then,

$$\begin{aligned}|\mathsf{err}_\mu^{\hat{J}}| &\le \tfrac{1}{2}\sum_{k=1}^K \alpha_k \Big|\|\hat{y}^k - y_\mu^k\|_H^2 - \|\hat{y}^k - y_\mu^{k,\ell}\|_H^2\Big| \\ &\le \tfrac{1}{2}\sum_{k=1}^K \alpha_k \Big|\|\mathsf{err}_\mu^k\|_H^2 + 2\langle \mathsf{err}_\mu^k, y_\mu^{k,\ell} - \hat{y}^k\rangle_H\Big| \\ &\le \tfrac{1}{2}\sum_{k=1}^K \alpha_k \big(\|\mathsf{err}_\mu^k\|_H^2 + 2\|\mathsf{err}_\mu^k\|_H \|y_\mu^{k,\ell} - \hat{y}^k\|_H\big) \\ &\le \tfrac{1}{2}\sum_{k=1}^K \alpha_k \big((\Delta_\mu^k)^2 + 2\Delta_\mu^k \|y_\mu^{k,\ell} - \hat{y}^k\|_H\big)\end{aligned}$$

Together with (17) we get (16).

4. TRUST-REGION RB APPROXIMATION

It is fairly easy to find a reduced basis for one fixed parameter, as we see in the next subsection. But when the parameter changes, the basis found before is not

necessarily a good reduced basis for the new state. For this reason, a Greedy algorithm is often used (in the offline phase) to find a "common" reduced basis for all the parameters in the admissible set $\mathcal{P}_{\mathsf{ad}}$ so that in the online phase a fast computation of a state for a new admissible parameter is possible. This leads to the well-known offline/online decomposition (see, e.g., Grepl and Patera (2005), Binev et al. (2011), Haasdonk (2013)). In the context of optimization the offline computation might not be very suitable, because during the optimization method only parameters from a small (but a-priorily unknown) subset of $\mathcal{P}_{\mathsf{ad}}$ are required. In Qian et al. (2017), Keil et al. (2021), Banholzer et al. (2020)) the RB space is built during a trust-region (TR) optimization process, where – following the optimization path – the RB space is enriched if it is necessary. We will utilize these ideas to develop our algorithm for the optimal experimental design. The full algorithm is presented in Algorithm 1, called for short *trust region reduced basis optimization* (TRRB-O), but for further details we refer to Banholzer et al. (2020) for further information. See also the recent paper Banholzer et al. (2022), where the TR approach is used in a multi-objective parameter optimization problem. Finally, we would like to refer to earlier work on methods based on TR proper orthogonal decomposition (TR-POD); see Arian et al. (2000); Sachs et al. (2014); Rogg et al. (2017).

4.1 Finding a reduced basis

For a fixed $\mu \in \mathcal{P}_{\mathsf{ad}}$ we compute a reduced-order approximation of y^k by the proper orthogonal decomposition (POD) method through the use of multiple snapshots, as explained previously. Taking for the moment in consideration the state variable only we find, then, a reduced basis $V^{\ell_y} = \operatorname{span}\{\psi_1^y, \dots, \psi_\ell^y\}$ that can be characterized by the matrix Ψ_y,

$$\psi_i^y = \sum_{i=1}^{N} (\Psi_y)_{ij} \varphi_i \in V^N,\ \langle \psi_j^y, \psi_i^y \rangle_V = \delta_{ij},\ 1 \le i, j \le \ell \tag{18}$$

The choice for the dimension of the reduced space ℓ may vary; for example, it can be fixed a-priorily or it can be chosen based on the eigenvalue decay in the POD method; see, e.g., Gubisch and Volkwein (2017). In our case, we decided to determine ℓ depending on the eigenvalues: given $\tilde{\lambda}_1 \ge \tilde{\lambda}_2 \ge \dots$ solutions of (11), we take the ℓ biggest eigenvalues such that $\lambda_{\ell+1}/\lambda_1 < \varepsilon_{rel}$. This means that in the worst case possible $\sum_{i=\ell+1}^{K} \tilde{\lambda}_i < K\lambda_1 \cdot \varepsilon_{rel}$; looking at our numerical examples, where $K = 201$ and $\varepsilon_{rel} = 10^{-7}$, it is guaranteed that at least $\sum_{i=\ell+1}^{K} \tilde{\lambda}_i < 2\lambda_1 \cdot 10^{-5}$. In our numerical experiment we have also fixed the maximum initial basis dimension to 10; we have observed that this does not impact on the overall accuracy.

4.2 Enriching a reduced basis

Assume that we already have computed RB spaces for the state and adjoint variables, characterized by the matrices Ψ_y and Ψ_p (see (18)). Let us suppose that we want to enrich the basis in the parameter $\mu_+ \in \mathcal{P}_{\mathsf{ad}}$. Then, the enrichment consists of finding another matrices $\Psi_y^+ \in \mathbb{R}^{N \times \ell_{y+}}$ and $\Psi_p^+ \in \mathbb{R}^{N \times \ell_{p+}}$ using POD on the subspace that is

Initialize the ROM at $\mu^{(0)}$, set $k = 0$, $\delta^{(0)} = \delta_0$, $Loop\_flag = True$.
while *Loop_flag* **do**
  BFGS sub-problem: find $\tilde{\mu}$ solution of (20) with stopping criteria (21). Store $\mu_{AGC}^{(k)}$ in the meantime.
  if (24) *is True* **then**
    Parameter is accepted: $\mu^{(k+1)} = \tilde{\mu}$.
    Set $\delta^{(k+1)} = \delta^{(k)}$.
    $\hat{J}^N$, $\nabla \hat{J}^N$, $\rho^{(k)}$, g^N, and $g^{\ell,(k)}$ are evaluated in $\mu^{(k+1)}$.
    if $g^N(\mu^{(k+1)}) \le \varepsilon_{tr}$ **then**
      Set $Loop\_flag = False$.
    else
      if $\rho_k \ge \beta_2$ **then**
        Set $\delta^{(k+1)} = 2\delta^{(k)}$.
      end
      if (27) is *False* **then**
        The model is enriched at $\mu^{(k+1)}$.
      end
    end
  else if (26) is *False* **then**
    The parameter $\tilde{\mu}$ is rejected.
    if (27) was *True* in the previous iteration **then**
      The model is enriched in $\tilde{\mu}$.
    end
    Set $\delta^{(k+1)} = \delta^{(k)}/2$.
  else
    $\hat{J}^N$, $\nabla \hat{J}$, $\rho^{(k)}$, g^N, and $g^{\ell,(k)}$ are evaluated in $\tilde{\mu}$.
    if $g^N(\tilde{\mu}) \le \varepsilon_{tr}$ **then**
      Set $\mu^{(k+1)} = \tilde{\mu}$.
      Set $Loop\_flag = False$.
    else
      if (27) is *True* and $\rho_k \ge \beta_2$ **then**
        The parameter is accepted: $\mu^{(k+1)} = \tilde{\mu}$.
        Set $\delta^{(k+1)} = 2\delta^{(k)}$.
      else if $\hat{J}^N(\mu^{(k+1)}) \le \hat{J}^{\ell,(k)}(\mu_{ACG}^{(k)})$ **then**
        The parameter is accepted: $\mu^{(k+1)} = \tilde{\mu}$.
        The model is enriched in $\mu^{(k+1)}$.
        if $\rho_k \ge \beta_2$ **then**
          Set $\delta^{(k+1)} = 2\delta^{(k)}$
        else
          Set $\delta^{(k+1)} = \delta^{(k)}$.
        end
      else
        The parameter $\tilde{\mu}$ is rejected.
        if (27) was *True* in the previous iteration **then**
          The model is enriched in $\tilde{\mu}$.
        end
        Set $\delta^{(k+1)} = \delta^{(k)}/2$.
      end
    end
  end
  Set $k = k + 1$.
end

Algorithm 1: Adaptive TR-RB optimization

orthogonal to the reduced space, namely substituting Z in (10) with $\tilde{\mathrm{Z}}$, whose columns are defined by

$$\tilde{\mathrm{Z}}_k = \mathrm{Z}_k - \sum_{i=1}^{\ell} \langle \mathrm{Z}_k, \Psi_i \rangle_{\mathrm{W}} \ \Psi_i,$$

where $\Psi = \Psi_y$ or Ψ_p. Once we found the matrices Ψ_y^+, Ψ_p^+, we merge them respectively with Ψ_y and Ψ_p, using Gram-Schmidt numerical W-orthonormalization, if necessary.

4.3 TR framework

The TR optimization method computes iteratively a first-order critical point of $(\hat{\mathbf{P}})$. At each iteration $k \geq 0$ of the optimization algorithm, we call such approximated optimal parameter $\mu^{(k)}$. We consider a cheaply computable model $m^{(k)}$ (approximation of the reduced cost) that can be trusted to accurately represent the function $\hat{J}$ in a reasonable neighborhood of $\mu^{(k)}$, called *trust region* $\mathcal{T}(\delta^{(k)}) = \{\mu : \|\mu - \mu^{(k)}\|_2 \leq \delta^{(k)}\}$, where $\delta^{(k)}$ is called *TR radius*. The TR method finds $\mu^{(k+1)}$ by solving the problem

$$\min_{s \in \mathbb{R}^d} m^{(k)}(s) \quad \text{s.t.} \quad \|s\|_2 \leq \delta^{(k)},\ \mu^{(k)} + s \in \mathcal{P}_{\mathsf{ad}} \tag{19}$$

Setting $\tilde{\mu} = \mu^{(k)} + s$ the RB version of (19) is

$$\min_{\tilde{\mu} \in \mathcal{P}_{\mathsf{ad}}} \hat{J}^{\ell,(k)}(\tilde{\mu}) \quad \text{s.t.} \quad q^{(k)}(\tilde{\mu}) = \frac{\Delta_{\tilde{\mu}}^{\hat{J},(k)}}{\hat{J}^{\ell,(k)}(\tilde{\mu})} \leq \delta^{(k)} \tag{20}$$

Here and whenever some quantity depends on the iteration k, we show it in the superscript, like the RB cost $\hat{J}^{\ell,(k)}$.The so-called efficiency $q^{(k)}$ helps us to quantify the accuracy of the RB and to define the TR.

How the model behaves in the TR tells us if we need to enrich the basis, or reduce the TR radius (in case the model is not accurate enough), or if we can enlarge the RB basis and even skip the enrichment process, in case the model is already accurate enough in the trust region.

4.4 TR subproblem

Let us suppose that we have fixed a TR radius $\delta^{(k)}$. Then a proposed parameter, solution of (20), is evaluated using a projected Armijo-BFGS algorithm (we refer to Kelley (1999) for the details). The iterations of the BFGS algorithm are indicated in the second subscript of the parameter: $\{\mu^{(k,j)}\}_{j=1}^{m_k}$ is the sequence of BFGS iterates and $\tilde{\mu} = \mu^{(k,m_k)}$ is the result of the BFGS algorithm. The maximum number of BFGS iterates is fixed at 400, and the algorithm finishes automatically when one of the termination criterion is satisfied:

$$q^{(k)}(\mu^{(k,j)}) \geq \beta_1 \cdot \delta^{(k)} \tag{21a}$$

$$\|\mu^{(k,j)} - \mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}(\mu^{(k,j)} + \nabla \hat{J}^{\ell,(k)}(\mu^{(k,j)}))\|_2 \leq \varepsilon_{sub}, \tag{21b}$$

where $\beta_1 \in (0, 1]$ is generally close to 1 and ε_{sub} is the tolerance of the sub-problem. Equation (21a) tells us if we are too close to the border of the trust region (where the RB model is less accurate), so we choose a β_1 pretty close to 1, such that the the numerical inequality approximates the real TR boundary. The projection $\mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}$ onto $\mathcal{P}_{\mathsf{ad}}$ is defined as

$$\mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}(\mu)_i = \begin{cases} \mu_i^a \ \text{if } \mu_i < \mu_i^a \\ \mu_i^b \ \text{if } \mu_i > \mu_i^a \\ \mu_i \ \text{otherwise} \end{cases} \qquad i = 1, \ldots, d.$$

Once that the projected BFGS method evaluates the descent direction $d^{(k,j)}$ for the parameter $\mu^{(k,j)}$, the Armijo backtracking finds $\mu^{(k,j+1)}$ as:

$$\mu^{(k,j+1)} = \mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}(\mu^{(k,j)} + \alpha_{(k,j)} d^{(k,j)}) \in \mathcal{P}_{\mathsf{ad}}$$

where $\alpha_{(k,j)} = 0.5^{\beta}$ and the power $\beta = \beta(k,j)$ is the smallest integer such that the sufficient decrease and the TR constraint are satisfied:

$$\begin{aligned} &\hat{J}^{\ell,(k)}(\mu^{(k,j+1)}) - \hat{J}^{\ell,(k)}(\mu^{(k,j)}) \\ &\qquad \leq -\tfrac{\alpha_\circ}{\alpha_{(k,j)}} \|\mu^{(k,j+1)} - \mu^{(k,j)}\|_2^2 \end{aligned} \tag{22a}$$

with $\alpha_\circ = 10^{-4}$ and

$$q^{(k)}(\mu^{(k,j+1)}) \leq \delta^{(k)} \tag{22b}$$

4.5 Modification of the trust region

Once that the sub-problem has found a suitable candidate $\tilde{\mu} := \mu^{(k,m_k)}$, there are different possibilities: for example, we might realize that the candidate is on the border of the trust region, and since the model is not accurate there, we could shrink the TR radius and find a new candidate or just enrich the basis; on the other hand, if we notice that some "predicted sufficient reduction" is satisfied, we can enlarge the TR radius.

The approximated generalized Cauchy point (AGC) is defined as $\mu_{AGC}^{(k)} = \mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}(\mu^{(k)} - \alpha^{(k,0)} \nabla \hat{J}^{\ell,(k)}(\mu^{(k)}))$, with $\alpha^{(k,0)}$ chosen such that (22a) and (22b) are satisfied. The cost of the evaluation of this parameter is "free", since it is evaluated in the first iteration of the BFGS algorithm. Then, an error-aware sufficient decrease condition (EASDC) is introduced (Qian et al. (2017)):

$$\hat{J}^{\ell,(k+1)}(\mu^{(k+1)}) \leq \hat{J}^{\ell,(k)}\big(\mu_{AGC}^{(k)}\big) \tag{23}$$

where we highlight that $\hat{J}^{\ell,(k)}$ refers to the reduced model at iteration k, while $\hat{J}^{\ell,(k+1)}$ refers instead to the model after the $(k+1)$-th (eventual) enrichment. This condition is central in the proof of convergence and the "sufficient" and "necessary" conditions we will see in the algorithm refer to the verification of it. Let us say explicitly that this condition is not straightforward to verify. Indeed, the left-hand side requires the evaluation of the cost function post-enhancement on the new parameter. We want to avoid this evaluation if some other conditions are not satisfied. For this reason, we postpone the evaluation of the FOM solution until we have to check the termination criterion or we want to enrich the RB.

To ensure that the candidate is a good parameter, a sufficient condition is analyzed:

$$\hat{J}^{\ell,(k)}(\tilde{\mu}) + \Delta_{\tilde{\mu}}^{\hat{J},(k)} < \hat{J}^{\ell,(k)}(\mu_{AGC}^{(k)}). \tag{24}$$

If (24) is satisfied, the candidate is accepted, $\mu^{(k+1)} = \tilde{\mu}$ and the model is "updated" (that means, the basis is enriched) there. Then, the TR radius is doubled if the predicted sufficient reduction (of model $m^{(k)}$) is realized, namely if

$$\rho^{(k)} = \tfrac{\hat{J}^N(\mu^{(k)}) - \hat{J}^N(\mu^{(k+1)})}{\hat{J}^{\ell,(k)}(\mu^{(k)}) - \hat{J}^{\ell,(k)}(\mu^{(k+1)})} \geq \beta_2, \tag{25}$$

where $\beta_2 \in [3/4, 1)$. This condition is called sufficient predicted reduction, because it confronts the real reduction of cost $\hat{J}^N$ with the reduction $\hat{J}^{\ell,(k)}$ of the approximated model.

If the sufficient condition (24) does not hold, we check a necessary condition:

$$\hat{J}^{\ell,(k)}(\tilde{\mu}) - \Delta_{\tilde{\mu}}^{\hat{J},(k)} < \hat{J}^{\ell,(k)}\big(\mu_{AGC}^{(k)}\big) \tag{26}$$

If this also fails, it means that the point $\tilde{\mu}$ probably needs an enhancement too big to satisfy the error-aware sufficient decrease condition (23). Then it must be rejected, the model must be enriched and the TR radius shrunken. If, on the other hand, the sufficient condition fails and the necessary condition holds, we enrich the model and check (23) on the candidate parameter:

$$\hat{J}^{\ell,(k+1)}(\tilde{\mu}) \leq \hat{J}^{\ell,(k)}\big(\mu_{AGC}^{(k)}\big)$$

If this holds, the candidate and the enrichment are accepted (and again, if (25) holds the radius is doubled), while if it fails both the parameter and the enrichment are rejected and the radius is shrunken.

Defining

$$g^N(\mu^{(k+1)}) = \|\mu^{(k+1)} - \mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}(\mu^{(k+1)} - \nabla \hat{J}^N(\mu^{(k+1)}))\|_2$$

the stopping criterion for the parameter estimation is $g^N(\mu^{(k+1)}) \leq \varepsilon_{tr}$, where ε_{tr} is the overall tolerance.

4.6 Skipping the enrichment

Enriching the basis often leads to reduced bases with too many elements, hence wasting the reduced-order model purpose. For this reason, in Banholzer et al. (2020) the possibility of skipping the enrichment was included. In particular, this happens when all these three conditions are true:

$$q^{(k)}(\mu^{(k+1)}) \leq \beta_3 \delta^{(k+1)} \tag{27a}$$

$$\frac{|g^N(\mu^{(k+1)}) - g^{\ell,(k)}(\mu^{(k+1)})|}{g^{\ell,(k)}(\mu^{(k+1)})} \leq \tau_g \tag{27b}$$

$$\frac{\|\nabla \hat{J}^N(\mu^{(k+1)}) - \nabla \hat{J}^{\ell,(k)}(\mu^{(k+1)})\|_2}{\|\nabla \hat{J}^N(\mu^{(k+1)})\|_2} \leq \min\left\{\tau_{grad}, \beta_3 \delta^{(k+1)}\right\} \tag{27c}$$

with $\beta_3 \in (0,1)$ and $g^{\ell,(k)}(\mu) = \|\mu - \mathcal{P}_{\mathcal{P}_{\mathsf{ad}}}(\mu - \nabla \hat{J}^{\ell,(k)}(\mu))\|_2$. Inequality (27a) indicates how much the model $m^{(k+1)}$ is trustworthy, inequality (27b) checks the convergence criterion of the reduced model, and inequality (27c) checks the RB accuracy of the cost gradient.

4.7 Some comments on the convergence of the algorithm

The convergence of the algorithm to a first-order critical point of $\hat{J}^N$ is showed in Keil et al. (2021) and Banholzer et al. (2020), Theorem 3.8, for the elliptic case. In our case the algorithm is the same, so we just have to make sure that the assumptions required for the convergence are satisfied. First of all, Assumption I of parameter separability of a_μ and f_μ is satisfied in (2). Then, we can assume a_μ, f_μ and J to be twice continuously Fréchet differentiable w.r.t. μ, as in Assumption II, which requires all the continuous functions ϑ_l^a and ϑ_l^f to be regular enough for $l = 1, \dots, m_a$ and $l = 1, \dots, m_f$, respectively. Assumption III simply requires the FOM to be accurate enough so that we can neglect its error. Assumption IV requires the cost functional $J(y, \mu)$ to be strictly positive for all $y \in \mathcal{Y}$ and $\mu \in \mathcal{P}_{\mathsf{ad}}$, which has been guaranteed by adding 1 in the cost formula. Assumption V is a technical safeguard that we do not need to discuss more than it is in the original paper. Assumption VI requires the ROM gradient to be uniformly Lipschitz-continuous and its second derivatives to be locally Lipschitz-continuous, guaranteed in our case by the quadratic form (14). We also assume the function $q^{(k)}$ to be uniformly continuous in $\mathcal{P}_{\mathsf{ad}}$ uniformly in k as in Assumption VII, which is in our case satisfied by the continuity of $q^{(k)}$ and the compactness of $\mathcal{P}_{\mathsf{ad}}$. Finally, let us make a comment on Lemma 3.4 of Banholzer et al. (2020). In the elliptic case, every time the model is enriched the following conditions are satisfied:

$$q^{(k+1)}(\mu^{(k+1)}) = 0, \quad \frac{\left|g^{\ell,(k+1)}(\mu^{(k+1)}) - g^N(\mu^{(k+1)})\right|}{g^{\ell,(k)}(\mu^{(k+1)})} = 0,$$

but in our case this is not the case. For us it is sufficient, though, to require

$$q^{(k+1)}(\mu^{(k+1)}) \leq \beta_3 \delta^{(k+1)}$$

and

$$\frac{\left|g^{\ell,(k+1)}(\mu^{(k+1)}) - g^N(\mu^{(k+1)})\right|}{g^{\ell,(k)}(\mu^{(k+1)})} \leq \tau_g$$

every time the model is enriched (i.e. two of the necessary conditions to skip the enrichment process) to satisfy Lemma 3.4.

5. OPTIMAL INPUT DESIGN

The result of the parameter estimation can depend strongly on the chosen control, even leading to convergence errors. In order to gain confidence in the accuracy of the parameter estimation, we want to find a "optimal" control, with the purpose of minimizing the uncertainty of the estimated parameter.

Following standard ideas of the optimal experimental/input design (Goodwin and Payne (1977), Atkinson et al. (2007)), we use an adaptive algorithm that starts from some initial guesses $u^{[1]}$ and $\mu^{[1]}$ and finds a new parameter and a new control at each iteration $n > 1$, trying to get closer to the true parameter μ^* and to the optimal control.

The superscript $[n]$ on objects like data vectors, state variables and cost functions specifies the experiment index, namely what control function it is being considered. The adaptive algorithm starts from initial guesses. Then, for $n > 1$, the algorithm iterates on three phases:

- The first phase is the simulation of some data $\hat{\mathrm{y}}^{[n-1]}$ using the control $u^{[n-1]}$ and the true parameter μ^*.
- The second phase is the TR-RB approximation, from which we obtain the parameter $\mu^{[n]}$.
- The third phase is the optimal input design, whose purpose is to find a new control $u^{[n]}$. The algorithm stops when the control just found is very close to the previous one.

Next, we will see how we incorporate the memory idea (i.e. storing all controls and data from past iterations) in our framework. Then we will see how can measure the uncertainty of the parameter estimation solution and

finally we will see how to evaluate this measure in our discretized setting.

5.1 Memory framework

As discussed, many objects depend on the control function, and we will indicate with the subscript $[n]$ when they depend on the control $u^{[n]}$. For example, $\{\mathrm{y}_\mu^{k,[n]}\}_{k=1}^K \subset \mathbb{R}^N$ and $\{\mathrm{y}_\mu^{k,\ell,[n]}\}_{k=1}^N \subset \mathbb{R}^{\ell_y}$ will be, respectively, the solution of (6) and (12) with parameter μ and control $u^{[n]}$.

Simulating measurement errors, for $n \geq 1$ (experiment index) we assume that the data is a random variable presenting some additive noise on its coefficients, i.e.

$$\hat{\mathrm{y}}_i^{k,[n]} = \mathrm{y}_{\mu^* i}^{k,[n]} + \eta_{n,k,i}, \tag{28}$$

where $\eta_{n,k,i} \sim \mathcal{N}(0, \sigma_{\mathrm{d}}^2)$ for all $k = 1, \dots, K$ (temporal index) and $i = 1, \dots, N$ (coefficient index in the FOM basis). So, in a way, we assume we are able to measure the FOM coefficient of the state variable corresponding to the true parameter at each time step, plus some error. The data collected at each iteration, $\hat{\mathrm{y}}^{[n]} \in \mathbb{R}^{NK}$, is a vector stacked with all entries $\hat{\mathrm{y}}_i^{k,[n]}$ for $k = 1, \dots, K$ and $i = 1, \dots, N$.

The approximated FOM discrepancy from the data for a single experiment is then

$$\hat{J}^{N,[n]}(\mu) = \tfrac{1}{2} \sum_{k=1}^{K} \alpha_k \big(\mathrm{y}_\mu^{k,[n]} - \hat{\mathrm{y}}^{k,[n]}\big)^\top \mathrm{M} \big(\mathrm{y}_\mu^{k,[n]} - \hat{\mathrm{y}}^{k,[n]}\big),$$

and the FOM cost function (7) becomes

$$\hat{J}^N(\mu) = 1 + \tfrac{1}{N_{ex}} \sum_{n=1}^{N_{ex}} \hat{J}^{N,[n]}(\mu) + \tfrac{\sigma}{2} \|\mu - \hat{\mu}\|_2.$$

Its gradient is then

$$\begin{aligned} \nabla \hat{J}^N(\mu) = \tfrac{1}{N_{ex}} \sum_{n=1}^{N_{ex}} \sum_{k=1}^{K} \alpha_k \Big[\sum_{l=1}^{m_a} \nabla \vartheta_l^a(\mu) \hat{\mathrm{A}}_l \mathrm{y}_\mu^{k,[n]} \\ - \sum_{l=1}^{m_f} \nabla \vartheta_l^f(\mu) \hat{\mathrm{f}}_l^k(u^{[n]}) \Big]^\top \mathrm{p}_\mu^{k,[n]} + \sigma(\mu - \hat{\mu}), \end{aligned}$$

and the RB approximations $\hat{J}^{\ell,[n]}, \hat{J}^\ell, \nabla \hat{J}^\ell$ are defined in a similar way.

5.2 Uncertainty measure

At iteration $n \geq 1$, the stacked data vector $\hat{\mathrm{y}}^{[n]} \in \mathbb{R}^{NK}$ is a realization of the nonlinear model

$$\hat{\mathrm{y}}^{[n]} = \mathcal{F}^{[n]}(\mu^*) + \nu,$$

where $\nu \sim \mathcal{N}(0, \sigma_{\mathrm{d}}^2 \mathrm{I}_{NK})$ is a NK-dimensional Gaussian random variable and $\mathcal{F}^{[n]} : \mathbb{R}^d \to \mathbb{R}^{NK}$ is the non-linear map defined by

$$\mathcal{F}^{[n]}_{(k-1)N+i}(\mu) = \mathrm{y}_{\mu,i}^{k,[n]},$$

for $k = 1, \dots, K$ and $i = 1, \dots, N$. The solution of the second phase $\mu^{[n]}$ will be then an estimator of the true parameter μ^*. To evaluate the quality of such estimator we use the Fisher's information matrix (cf., e.g., Goodwin and Payne (1977)), which quantifies how informative an experiment is.

The Fisher's information matrix $\mathrm{M}_\mu \in \mathbb{R}^{d \times d}$ of the estimator μ is defined as

$$\mathrm{M}_\mu = \mathbb{E}_{\hat{\mathrm{y}}^{[n]}|\mu} \left[\left(\frac{\partial \log p(\hat{\mathrm{y}}^{[n]}|\mu)}{\partial \mu} \right)^\top \left(\frac{\partial \log p(\hat{\mathrm{y}}^{[n]}|\mu)}{\partial \mu} \right) \right].$$

Since $\hat{\mathrm{y}}^{[n]}|\mu \sim \mathcal{N}(\mathcal{F}^{[n]}(\mu), \sigma_{\mathrm{d}}^2 \mathrm{I}_{NK})$,

$$p(\hat{\mathrm{y}}^{[n]}|\mu) = ((2\pi)^{NK} \sigma_{\mathrm{d}}^2)^{-1/2} \exp\big(-\tfrac{1}{2\sigma_{\mathrm{d}}^2} \|\hat{\mathrm{y}}^{[n]} - \mathcal{F}^{[n]}(\mu)\|_2^2 \big),$$

$$\log p(\hat{\mathrm{y}}^{[n]}|\mu) = -\tfrac{1}{2} \log((2\pi)^{NK} \sigma_{\mathrm{d}}^2) - \tfrac{1}{2\sigma_{\mathrm{d}}^2} \|\hat{\mathrm{y}}^{[n]} - \mathcal{F}^{[n]}(\mu)\|_2^2,$$

$$\tfrac{\partial \log p(\hat{\mathrm{y}}^{[n]}|\mu)}{\partial \mu} = \tfrac{1}{\sigma_{\mathrm{d}}^2} (\hat{\mathrm{y}}^{[n]} - \mathcal{F}^{[n]}(\mu))^\top \tfrac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu},$$

where the Jacobian matrix $\frac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu} \in \mathbb{R}^{NK \times 2}$ is given as

$$\big(\tfrac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu}\big)_{(k-1)N+i,j} = \tfrac{\partial \mathrm{y}_{\mu,i}^{k,[n]}}{\partial \mu_j},$$

for $k = 1, \dots, K$, $j = 1, \dots, N$, and $j = 1, \dots, d$. The derivative of the state variable with respect to the j-th parameter is called the j-th sensitivity of the state variable. In particular, in the infinite-dimensional setting, the j-th sensitivity variable $s_j = s_{\mu,j} \in \mathcal{Y}$ is the unique solution of the j-th sensitivity equation, defined as

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t} \langle s_j(t), \varphi \rangle_H + a_\mu(s_j(t), \varphi) \\ + a_\mu^{s,j}(y_\mu(t), \varphi) = \langle f_\mu^{s,j}(t; u), \varphi \rangle_{V',V} \\ s_j(0) = 0 \quad \text{in } H, \end{aligned} \tag{29}$$

for all $\varphi \in V$ and $t \in (0, T]$, where

$$a_\mu^{s,j} = \tfrac{\partial}{\partial \mu_j} a_\mu = \sum_{l=1}^{m_a} \tfrac{\partial \vartheta_l^a(\mu)}{\partial \mu_j} \hat{a}_l,$$

$$f_\mu^{s,j}(t; u) = \tfrac{\partial}{\partial \mu_j} f_\mu(t; u) = \sum_{l=1}^{m_f} \tfrac{\partial \vartheta_l^f(\mu)}{\mu_j} \hat{f}_l(t; u).$$

Then, in the FOM approximation coefficients, the derivative w.r.t. μ_j of $\mathrm{y}_{\mu,i}^{k,[n]}$ is $\mathrm{s}_{\mu,j,i}^{k,[n]}$, where the superscript $[n]$ means that $u^{[n]}$ is used in the sensitivity equation, and as before k is the time index and i is the coefficient index.

The Fisher's information matrix is then

$$\begin{aligned} \mathrm{M}_\mu &= \mathbb{E}_{\hat{\mathrm{y}}^{[n]}|\mu} \left[\left(\tfrac{\partial \log p(\hat{\mathrm{y}}^{[n]}|\mu)}{\partial \mu} \right)^\top \left(\tfrac{\partial \log p(\hat{\mathrm{y}}^{[n]}|\mu)}{\partial \mu} \right) \right] \\ &= \tfrac{1}{\sigma_{\mathrm{d}}^4} \tfrac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu}^\top \mathbb{E}_{\hat{\mathrm{y}}^{[n]}|\mu} \left[\|\hat{\mathrm{y}}^{[n]} - \mathcal{F}^{[n]}(\mu)\|_2^2 \right] \tfrac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu} \\ &= \frac{1}{\sigma_{\mathrm{d}}^2} \frac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu}^\top \frac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu}. \end{aligned}$$

For $j_1, j_2 \in \{1, \dots, d\}$,

$$\begin{aligned} (\mathrm{M}_\mu)_{j_1,j_2} &= \frac{1}{\sigma_{\mathrm{d}}^2} \frac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu_{j_1}}^\top \frac{\partial \mathcal{F}^{[n]}(\mu)}{\partial \mu_{j_2}} \\ &= \frac{1}{\sigma_{\mathrm{d}}^2} \sum_{k=1}^{K} \sum_{i=1}^{N} \mathrm{s}_{\mu,j_1,i}^{k,[n]} \, \mathrm{s}_{\mu,j_2,i}^{k,[n]}. \end{aligned}$$

To preserve the physical structure of the time-dependent model, we decide to apply a weighing in time:

$$\begin{aligned} (\mathrm{M}_\mu)_{j_1,j_2} &= \frac{1}{\sigma_{\mathrm{d}}^2} \sum_{k=1}^{K} \sum_{i=1}^{N} \alpha_k \, \mathrm{s}_{\mu,j_1,i}^{k,[n]} \, \mathrm{s}_{\mu,j_2,i}^{k,[n]} \\ &\approx \frac{1}{\sigma_{\mathrm{d}}^2} \int_0^T \sum_{i=1}^{N} \mathrm{s}_{\mu,j_1,i}^{[n]}(t) \, \mathrm{s}_{\mu,j_2,i}^{[n]}(t) \mathrm{d}t. \end{aligned}$$

As a further weighting, we could multiply for the matrix W, so that the product approximates a physically relevant inner product:

$$(\mathrm{M}_\mu)_{j_1,j_2} = \frac{1}{\sigma_\mathrm{d}^2}\sum_{k=1}^{K} \alpha_k\ \mathrm{s}_{\mu,j_1}^{k,[n]}\ \mathrm{W}\ \mathrm{s}_{\mu,j_2}^{k,[n]} \approx \frac{1}{\sigma_\mathrm{d}^2}\int_0^T \langle s_{\mu,j_1}^{[n]}(t), s_{\mu,j_2}^{[n]}(t)\rangle_V \mathrm{d}t.$$

For μ unbiased estimator of μ^* (i.e. $\mathbb{E}(\mu) = \mu^*$) the Cramer-Rao inequality (cf. Goodwin and Payne (1977)) gives a lower bound for the covariance matrix:

$$\mathrm{Cov}(\mu) \succeq \mathrm{M}_\mu^{-1},$$

where the inequality means that $\mathrm{Cov}(\mu) - \mathrm{M}_\mu^{-1}$ is semi-definite positive, and the estimator is called efficient if it achieves the equality. Hence, at each iteration $n > 1$, as a measure of uncertainty we choose then the trace of the inverse of the Fisher's information matrix evaluated in the estimator $\mu^{[n]}$, namely

$$\phi = \mathrm{trace}(\mathrm{M}_{\mu^{[n]}}^{-1}). \tag{30}$$

Minimising the trace of the covariance matrix is equivalent to minimising the average mean square error of the maximum a-posteriori probability estimator, or alternatively it can be seen as the minimisation of the average half-axis length of the confidence ellipsoid with respect to the average variance of the parameters (Atkinson et al. (2007)).

Next, we will see how to use the RB approximation to speed up the evaluation of $\mathrm{M}_{\mu^{[n]}}$.

5.3 Approximating the uncertainty

As discussed before, the uncertainty measure is evaluated through the FOM approximation of the sensitivity variables $\mathrm{s}_{\mu,j}^{k,[n]} \in \mathbb{R}^N$, $k = 1,\dots,K$ and $j = 1,\dots,d$. If we want to incorporate the reduced-basis approximation in this calculation, we need to build a RB. We can do this between the phase two and three of the algorithm, namely when we have a fixed a parameter $\mu^{[n+1]}$. Indeed, using parameter $\mu^{[n+1]}$ and control $u^{[n]}$, we evaluate snapshots of the sensitivities $\mathrm{s}_{\mu,j}^{k,[n]} \in \mathbb{R}^N$ for $j = 1,\dots,d$ and we stack them together with the approximations of the derivatives (as in (10)). Then, using POD we can evaluate a common reduced basis for all the sensitivities.

Since the Fisher's information matrix will be evaluated for many different controls, we could also add snapshots for a set of control function, but in our numerical examples this did not affect greatly the overall algorithm.

Thus, being $\Psi_s \in \mathbb{R}^{N\times \ell_s}$ the POD matrix for the sensitivity variables and $\{\mathrm{s}_{\mu,j}^{k,\ell,[n]}\}_{k=1}^K \in \mathbb{R}^{\ell_s}$ the solution of the ROM approximation of (29), the Fisher's information matrix of estimator $\mu^{[n+1]}$ evaluated with the control $u^{[n]}$ is approximated as

$$(\mathrm{M}_{\mu^{[n+1]}})_{j_1,j_2} = \frac{1}{\sigma_\mathrm{d}^2}\sum_{k=1}^{K} \alpha_k\ \mathrm{s}_{\mu^{[n+1]},j_1}^{k,\ell,[n]\top}\ \Psi_s^\top\Psi_s\ \mathrm{s}_{\mu^{[n+1]},j_2}^{k,\ell,[n]}$$

or, using the weighting matrix W,

$$(\mathrm{M}_{\mu^{[n+1]}})_{j_1,j_2} = \frac{1}{\sigma_\mathrm{d}^2}\sum_{k=1}^{K} \alpha_k\ \mathrm{s}_{\mu^{[n+1]},j_1}^{k,\ell,[n]\top}\ \mathrm{W}^\ell\ \mathrm{s}_{\mu^{[n+1]},j_2}^{k,\ell,[n]},$$

where $\mathrm{W}^\ell = \Psi_s^\top \mathrm{W}\Psi_s$.

Pre-saving the matrix $\Psi_s^\top\Psi_s$ (or W^ℓ) $\in \mathbb{R}^{d\times d}$, this evaluation is independent of dimension N. Every time we need to evaluate the Fisher's information matrix for parameter $\mu^{[n+1]}$ and a general control function u, we will first evaluate the ROM approximation of the state variable $y_{\mu^{[n+1]}}$ (in the RB built in phase two) and then evaluate the ROM approximation of the sensitivity variables $s_{\mu^{[n+1]},j}$ for $j = 1,\dots,d$ (in the RB built in the intermediate step).

6. NUMERICAL EXAMPLES

We consider examples in a one-dimensional spatial interval $\Omega = (0, L) = (0, 4)$ with $H = L^2(\Omega)$ and $V = H^1(\Omega)$. In both cases the initial value is $y_\circ(x) \equiv 1$ and the time horizon is $T = 2$. The chosen initial control is $u(t) = \frac{1}{2}\cos(10t) \in \mathcal{U}_\mathsf{ad} = \{u \in L^2(0,T) \mid -3 \le u(t) \le 3,\ \forall t \in (0,T)\} \subset \mathcal{U} = L^2(0,T)$, and data is always evaluated with the formula (28), where $\mathrm{y}_{\mu^*}^{k,[n]}$ is evaluated with a FOM solver and $\sigma_\mathrm{d}^2 = 10^{-3}$. The initial reference parameter $\hat\mu$ in (3) is the middle point of $\mathcal{P}_\mathsf{ad}$, and at any following iteration $n > 1$ the reference parameter is the parameter $\mu^{[n-1]}$ found in the previous iteration. The constant σ in (3) is fixed to 10^{-8}.

In the discretized setting, the control $u = u(t)$ is a step function and it is determined by the vector $\mathrm{u} = (\mathrm{u}_k) \in \mathbb{R}^K$ with $u(t_k) = \mathrm{u}_k$ for $k \in \{1,\dots,K\}$. Furthermore, in the numerical example the optimal input optimization problem

$$\mathrm{u}^{[n]} = \arg\min\big\{\phi(\mathrm{u}) \,|\, \mathrm{u} \in \mathrm{U}_\mathsf{ad}\big\}$$
$$\mathrm{U}_\mathsf{ad} = \big\{\mathrm{u} \in \mathbb{R}^K \mid -3 \le \mathrm{u}_k \le 3 \text{ for } k = 1,\dots,K\big\}$$

is solved using the function `fmin_l_bfgs_b` from the Python library `scipy.optimize` without specifying the gradient of $\phi(u)$ and approximating it numerically. The overall algorithm stops when $\|u^{[n+1]} - u^{[n]}\|_2 \le \varepsilon_u = 10^{-5}$.

In both experiments the FOM approximation is based on quadratic finite elements on 800 nodes and the time interval $[0, T]$ is divided into $K = 201$ steps, hence $N = 1601$ and $\Delta t = 0.01$.

Here follows a list of all numerical parameters used in the Trust-Region RB algorithm:

$$\begin{aligned} &\beta_1 = 0.95 && \beta_2 = 0.75 \\ &\beta_3 = 0.5 && \delta_0 = 1 \\ &\varepsilon_{rel} = 10^{-7} && \varepsilon_{sub} = 10^{-8} \\ &\varepsilon_{tr} = 10^{-5} && \tau_g = 10^{-3} \\ &\tau_{grad} = 10^{-2}. \end{aligned}$$

In the next tables we are going to analyze the number ℓ_y, ℓ_p of bases generated by the TR optimization method (respectively for the state and adjoint variables), the error $\mathsf{err}^* = \|\mu^{[n]} - \mu^*\|_2$ and $\phi(u^{[n]}) = \min_u \phi(u)$, where the optimal solutions $\mu^{[n]}$ and $u^{[n]}$ are computed by the strategy explained in Section 5.

Run 1 (2 parameters). We consider $d = 2$ parameters, $\mu \in \mathcal{P}_\mathsf{ad} = [0.24, 3.4] \times [0.11, 5.0]$ and an equation in strong form

$$\begin{cases} y_t(x,t) - \mu_1 y_{xx}(x,t) + \frac{1}{2}y(x,t) = 0 \\ y_x(0,t) = 0, \qquad \mu_1 y_x(1,t) = \mu_2 u(t) \\ y(x,0) = y_\circ(x) \end{cases}$$

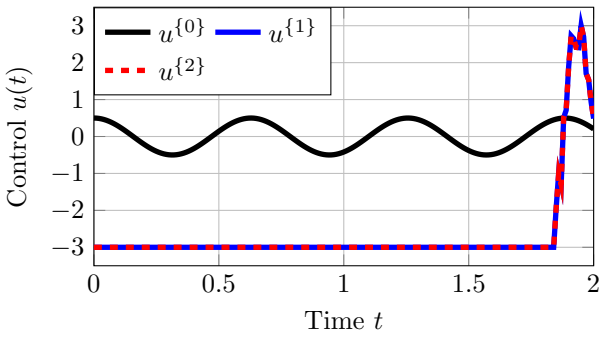
so that $a_\mu(y,\varphi) = \mu_1 \int_\Omega y'(x)\varphi'(x)\,\mathrm{d}x + \frac{1}{2}\int_\Omega y(x)\varphi(x)dx$ and $\langle f_\mu(t;u),\varphi\rangle_{V',V} = \mu_2 u(t)\varphi(L)$. The true parameter is $\mu^* = (1,2)$ and the initial parameter is $\mu^{[1]} = (3.4, 0.11)$.

Table 1. Run 1.

	Starting values	$n=2$	$n=3$
ℓ_y, ℓ_p		12, 30	18, 50
err*	3.05	3.14e-05	1.02e-06
Second phase time		11 s	9 s
$\phi(\mathrm{u}^{[n]})$	4.5e-06	1.8e-09	1.8e-09
Third phase time		288 s	31 s

We can observe how the second phase converges very fast to a parameter very close to the true parameter. Furthermore, the third phase reaches the "best" control in just one iteration. With this control the second phase in the next iteration finds a more accurate parameter and then the third phase does not find a better control, therefore stopping. In the next graph the initial control and the best controls for each iteration are plotted.

Results of of Run 1.



Run 2 (4 parameters) Let $d = 4$ and $\mathcal{P}_{\mathsf{ad}} = [0.24, 3.4] \times [0.11, 5] \times [0.013, 4] \times [0.97, 2.22]$ and

$$a_\mu(y,\varphi) = \mu_1 \int_0^{1.5} y'(x)\varphi'(x)\,\mathrm{d}x + \mu_2 \int_{1.5}^{3} y'(x)\varphi'(x)\,\mathrm{d}x + \mu_3 \int_3^4 y'(x)\varphi'(x)dx + \tfrac{1}{2}\int_\Omega y(x)\varphi(x)\,\mathrm{d}x$$

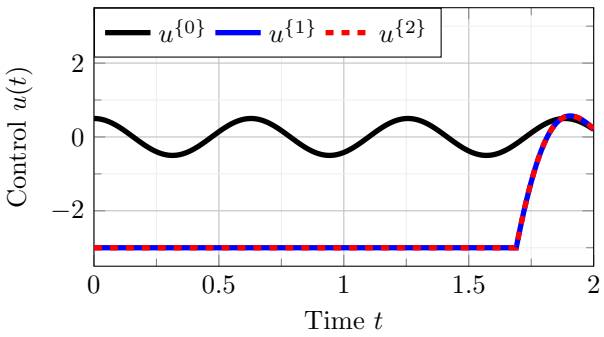
and $\langle f_\mu(t;u),\varphi\rangle_{V',V} = \mu_4 u(t)\varphi(L)$. The real parameter is $\mu^* = (1, 1.3, 0.8, 2)$ and the initial parameter is $(3, 5, 0.1, 2)$. The result are showed in the next table.

Table 2. Run 2.

	Starting values	$n=2$	$n=3$
ℓ_y, ℓ_p		24, 30	30, 40
err*	4.26	3.23	6.9e-05
Second phase time		180 s	20 s
$\phi(\mathrm{u}^{[n]})$	19	1.3e-06	2e-07
Third phase time		540 s	15 s

In this example we can see how computational times and errors rise with bigger sizes of the parameter space. Let us observe that the TR algorithm works way faster than a standard weak greedy and we can appreciate the full potential of such algorithm when applied to higher dimensions. With the first control the algorithm fails to approximate the true parameter, but as soon as a new control is generated, the trust-region approximation gives a good estimator. In the next plot we can see the control function generated.

Numerical example of Run 2.



We want to point out that in both experiments there is a correlation between the time variable and how influential the control function at such time variable is: the first time steps are more important and have a bigger impact on the uncertainty of an experiment. In a manner of speaking, it does not change much if the control function is constant at value -3 or if it goes at $+3$ in the last time steps, since these time steps do not have a big impact on the Fisher's information matrix.

7. CONCLUSION

In this work we have considered an algorithm for the optimal input design of a parameter-dependent evolution problem. Constructing the algorithm on a bi-level optimization framework, the idea of the creation and the enrichment of a basis on-the-go is preferred to an offline-online computation.

Starting from the parabolic problems in our numerical examples, extensions can include non-linearities in the parameters, where for example it is not trivial evaluating a-posteriori error estimates for the ROM. In the same way, the a-posteriori error estimates we use are strongly based on the coercivity of the bilinear form, hence it would be of interest analyzing non-coercive problems.

Another possible extension is the addition of an algebraic state in the evolution system, which is typical, for example, in lithium-ion battery models. In that case the differential state (i.e. the ion concentration) is not observable and measurements are possible only on the algebraic state (the potential).

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