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RESEARCH ARTICLE

*Domain Decomposition and Balanced Truncation Model
Reduction for Shape Optimization of the Stokes System*

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The optimal design of structures and systems described by partial differential equations (PDEs) often gives rise to large-scale optimization problems, in particular if the underlying system of PDEs represents a multi-scale, multi-physics problem. Therefore, reduced order modeling techniques such as balanced truncation model reduction, proper orthogonal decomposition, or reduced basis methods are used to significantly decrease the computational complexity while maintaining the desired accuracy of the approximation. In this paper, we are interested in such shape optimization problems where the design issue is restricted to a relatively small portion of the computational domain. In this case, it appears to be natural to rely on a full order model only in that specific part of the domain and to use a reduced order model elsewhere. A convenient methodology to realize this idea consists in a suitable combination of domain decomposition techniques and balanced truncation model reduction. We will consider such an approach for shape optimization problems associated with the time-dependent Stokes system and derive explicit error bounds for the modeling error.

As an application in life sciences, we will be concerned with the optimal design of capillary barriers as part of a network of microchannels and reservoirs on microfluidic biochips that are used in clinical diagnostics, pharmacology, and forensics for high-throughput screening and hybridization in genomics and protein profiling in proteomics.

Keywords: shape optimization; time-dependent Stokes system; domain decomposition; balanced truncation model reduction; microfluidic biochips

AMS Subject Classification: 49Q10;65M55;76D07

1. Introduction

We study a method for the numerical solution of a class of shape optimization problems governed by the time dependent Stokes or the time dependent linearized Navier-Stokes equations, linearized around a steady state, in which only a small part of the overall domain is modified. The numerical solution of such optimization problems using gradient based optimization methods requires the solution of coupled systems of partial differential equations (PDEs) involving the forward in time governing equation and the backward in time adjoint equation. The solution of this coupled system can be very expensive, both in terms of computing time and memory.

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Our approach to reduce the computational complexity of the numerical optimization is an integration of domain decomposition and model reduction. Domain decomposition in space is used to decouple the small subproblem that corresponds to the subdomain whose shape is modified by the optimization from the fixed subdomain problem. Balanced truncation model reduction is used to replace the subproblem corresponding to the fixed subdomain by a substantially smaller problem. Domain decomposition identifies the proper connectivities between the subproblems, which are used in the balanced truncation. In principle any model reduction technique can be used, but balanced truncation provides an error bound for the quality of the reduced order subsystem. This error bound will be used to derive an error bound for the coupled shape optimization problem.

Domain decomposition and balanced truncation model reduction (DDBTMR) have been integrated for the solution of locally nonlinear systems, where the solution shows nonlinear behavior only in a relatively small subdomain of the computational domain, but is governed by a linear regime otherwise [5, 36, 37]. The papers [36, 37] contain numerical studies for the simulation of time dependent PDEs with local nonlinearities. The numerical solution of optimal control and shape optimization problems associated with linear time dependent advection-diffusion equations by DDBTMR has been recently considered in [5]. The present paper extends the approach and analysis in [5] to shape optimization problems governed by the time dependent Stokes or the time dependent linearized Navier-Stokes equations, linearized around a steady state. Although conceptually the approach in this paper is similar to the one in [5], the extension to the Stokes system requires several important changes. These are due to the presence of the incompressibility constraints and affect the model reduction, the domain decomposition, the coupling of both, and the analysis.

Section 2 of this paper is devoted to an appropriate set-up of the problem. Balanced truncation model reduction (BTMR) for the semi-discretized Stokes system is reviewed in Section 3. Section 4 introduces the domain decomposition (DD) methodology, including the specification of the optimality systems for the respective subdomain and interface problems. This is followed by the application of BTMR to the domain decomposed optimality system in Section 5. Section 6 is concerned with an a priori estimate of the modelling error which, under certain assumptions, is shown to be largely determined by the BTMR error bound. The application of DDBTMR to the shape optimization of a capillary barrier in a surface acoustic wave driven microfluidic biochip is considered in Section 7 demonstrating the feasibility of the approach for a challenging design problem in life sciences. Finally, Section 8 contains some concluding remarks as well as an outlook to possible extensions. While problems governed by the Stokes system are used to demonstrate our approach, it can be applied to problems governed by the Oseen equation or linearized Navier-Stokes equations, linearized around a steady state.

2. Shape optimization of the time-dependent Stokes system

Let $\Omega(\theta) \subset \mathbb{R}^2$ be a bounded domain that depends on design variables $\theta = (\theta_1, \dots, \theta_d)^T \in \Theta$, where $\Theta \subset \mathbb{R}^d$ is a given convex set, e.g., $\theta_i, 1 \leq i \leq d$, are the Bézier control points of a Bézier curve representation of the boundary and $\Theta := \{\theta_i \in \mathbb{R} \mid \theta_{min}^{(i)} \leq \theta_i \leq \theta_{max}^{(i)}, 1 \leq i \leq d\}$. We assume that the boundary $\partial\Omega(\theta)$ consists of an inflow boundary $\Gamma_{in}(\theta)$, an outflow boundary $\Gamma_{out}(\theta)$, and a lateral boundary $\Gamma_{lat}(\theta)$ such that $\partial\Omega(\theta) = \bar{\Gamma}_{in}(\theta) \cup \bar{\Gamma}_{out}(\theta) \cup \bar{\Gamma}_{lat}(\theta)$, $\Gamma_{in}(\theta) \cap \Gamma_{out}(\theta) \cap \Gamma_{lat}(\theta) = \emptyset$. We set $Q(\theta) := \Omega(\theta) \times (0, T)$, $\Sigma(\theta) := \partial\Omega(\theta) \times (0, T)$, $\Sigma_{in}(\theta) :=$

$\Gamma_{in}(\theta) \times (0, T), \Sigma_{lat}(\theta) := \Gamma_{lat}(\theta) \times (0, T), T > 0$, and consider shape optimization problems associated with the time-dependent Stokes system of the form

$$\inf_{\theta \in \Theta} J(\theta) \quad (1a)$$

where

$$J(\theta) := \int_0^T \int_{\Omega(\theta)} \ell(\mathbf{v}(\theta), p(\theta), x, t) \, dx \, dt, \quad (1b)$$

and where $\mathbf{v}(\theta), p(\theta)$ solve

$$\frac{\partial}{\partial t} \mathbf{v}(x, t) - \nu \Delta \mathbf{v}(x, t) + \nabla p(x, t) = \mathbf{f}(x, t), \quad (x, t) \in Q(\theta), \quad (1c)$$

$$\nabla \cdot \mathbf{v}(x, t) = 0, \quad (x, t) \in Q(\theta), \quad (1d)$$

$$\mathbf{v}(x, t) = \mathbf{v}^{in}(x, t), \quad (x, t) \in \Sigma_{in}(\theta), \quad (1e)$$

$$\mathbf{v}(x, t) = 0, \quad (x, t) \in \Sigma_{lat}(\theta), \quad (1f)$$

$$(\nabla \mathbf{v}(x, t) - p(x, t) \mathbf{I}) \mathbf{n} = 0, \quad (x, t) \in \Sigma_{out}(\theta), \quad (1g)$$

$$\mathbf{v}(x, 0) = \mathbf{v}^{(0)}(x), \quad x \in \Omega(\theta). \quad (1h)$$

Here, $\mathbf{v} = \mathbf{v}(x, t) = (v_1(x, t), v_2(x, t))^T$ and $p = p(x, t)$ stand for the velocity and the pressure, $\mathbf{f} = \mathbf{f}(x, t)$ is a given forcing term, \mathbf{v}^{in} denotes a prescribed normal velocity on $\Sigma_{in}(\theta)$, $\mathbf{v}^{(0)} = \mathbf{v}^{(0)}(x), x \in \Omega(\theta)$, is the velocity distribution at initial time $t = 0$, satisfying $\nabla \cdot \mathbf{v}^{(0)} = 0$, $\nu > 0$ refers to the viscosity of the fluid, and \mathbf{t}, \mathbf{n} are the unit tangential and unit exterior normal vector on $\partial\Omega(\theta)$. Moreover, the integrand $\ell(\cdot)$ in the objective functional J is a given function of the velocity, the pressure, and the independent variables x, t .

For the spatial discretization of the time-dependent Stokes system we use one of the many standard methods [16], such as the classical P2-P1 Taylor Hood element, or methods with discontinuous pressure discretizations. We will discuss this in more detail in Section 4. We assume that the simplicial triangulation \mathcal{T}_h of the spatial domain $\Omega(\theta)$ is geometrically conforming and aligns with $\Gamma_{in}(\theta), \Gamma_{lat}(\theta)$ and $\Gamma_{out}(\theta)$. This leads to the semi-discrete optimization problem

$$\inf_{\theta \in \Theta} J(\theta) \quad (2a)$$

where

$$J(\theta) := \int_0^T \ell(\mathbf{v}(\theta), \mathbf{p}(\theta), x, t, \theta) \, dt, \quad (2b)$$

and where $\mathbf{v}(\theta), \mathbf{p}(\theta)$ solve

$$\mathbf{E}(\theta) \frac{d}{dt} \begin{pmatrix} \mathbf{v}(t) \\ \mathbf{p}(t) \end{pmatrix} + \mathbf{S}(\theta) \begin{pmatrix} \mathbf{v}(t) \\ \mathbf{p}(t) \end{pmatrix} = \begin{pmatrix} \mathbf{g}_1(\theta)(t) \\ \mathbf{g}_2(\theta)(t) \end{pmatrix}, \quad t \in (0, T], \quad (2c)$$

$$\mathbf{M}(\theta) \mathbf{v}(0) = \mathbf{v}^{(0)}(\theta), \quad (2d)$$

$$-\mathbf{B}(\theta)\mathbf{M}^{-1}\mathbf{v}^{(0)}(\theta) + \mathbf{g}_2(\theta)(0) = \mathbf{0}. \quad (2e)$$

Here, the integrand $\ell(\cdot)$ in (2b) results from the spatial discretization of the inner integral of the objective functional in (1b). The block matrix $\mathbf{E}(\theta)$ and the discrete Stokes operator $\mathbf{S}(\theta)$ in (2c) are given by

$$\mathbf{E}(\theta) := \begin{pmatrix} \mathbf{M}(\theta) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathbf{S}(\theta) := \begin{pmatrix} \mathbf{A}(\theta) & \mathbf{B}^T(\theta) \\ \mathbf{B}(\theta) & \mathbf{0} \end{pmatrix}, \quad (3)$$

where $\mathbf{M}(\theta) \in \mathbb{R}^{n \times n}$, $\mathbf{A}(\theta) \in \mathbb{R}^{n \times n}$ and $\mathbf{B}(\theta) \in \mathbb{R}^{m \times n}$ are the lumped mass matrix, the stiffness matrix, and the matrix representation of the discrete divergence operator. The vector $\mathbf{g}_2(\theta)(t) \in \mathbb{R}^m$ in (2c) stems from the semi-discretization of the incompressibility condition due to the boundary condition at the inflow boundary and $\mathbf{v}^{(0)}(\theta)$ is the initial velocity satisfying the discrete incompressibility condition (2e). We note that the data of the semi-discrete problem depend on the design variable θ due to the dependence of the spatial domain on θ .

The Oseen equation and the linearized Navier-Stokes equations, linearized around a steady state, also lead to systems of the type (2c)–(3). The existence and uniqueness of a solution $(\mathbf{v}, \mathbf{p}) \in L^2((0, T); \mathbb{R}^n) \times L^2((0, T); \mathbb{R}^m / (\text{Ker } \mathbf{B}^T))$ of the semi-discretized equations (2c), (2d) as well as its continuous dependence on the data of the problem is a consequence of the following result which will also play a prominent role with regard to the application of BTMR and the derivation of upper estimates for the modeling error. The following result applies to the semi discretized Stokes system, but also to class of problems governed by the Oseen equations or the linearized Navier-Stokes equations.

THEOREM 2.1 *Let $\mathbf{A}, \mathbf{M} \in \mathbb{R}^{n \times n}$, $\mathbf{B} \in \mathbb{R}^{m \times n}$, $m < n$, be matrices with the following properties:*

- (i) \mathbf{M} is symmetric positive definite.
- (ii) \mathbf{A} is positive definite (not necessarily symmetric) on $\text{Ker } \mathbf{B}$, i.e., there exists a constant $\alpha > 0$ such that

$$\mathbf{v}^T \mathbf{A} \mathbf{v} \geq \alpha \|\mathbf{v}\|^2, \quad \mathbf{v} \in \text{Ker } \mathbf{B}. \quad (4)$$

- (iii) \mathbf{B} has full row rank m .

Consider the initial value problem

$$\mathbf{E} \frac{d}{dt} \begin{pmatrix} \mathbf{v}(t) \\ \mathbf{p}(t) \end{pmatrix} + \mathbf{S} \begin{pmatrix} \mathbf{v}(t) \\ \mathbf{p}(t) \end{pmatrix} = \begin{pmatrix} \mathbf{g}_1(t) \\ \mathbf{g}_2(t) \end{pmatrix}, \quad t \in (0, T], \quad (5a)$$

$$\mathbf{M} \mathbf{v}(0) = \mathbf{v}^{(0)}, \quad (5b)$$

where \mathbf{E}, \mathbf{S} are as in (3) and $\mathbf{g}_1 \in C([0, T]; \mathbb{R}^n)$, $\mathbf{g}_2, d\mathbf{g}_2/dt \in C([0, T]; \mathbb{R}^m)$ and $\mathbf{v}^{(0)} \in \mathbb{R}^n$ satisfies

$$-\mathbf{B} \mathbf{M}^{-1} \mathbf{v}^{(0)} + \mathbf{g}_2(0) = \mathbf{0}. \quad (6)$$

Under the assumptions (i), (ii) and (iii), the initial value problem (5a), (5b) has a unique solution $(\mathbf{v}, \mathbf{p}) \in C([0, T]; \mathbb{R}^n) \times C([0, T]; \mathbb{R}^m / (\text{Ker } \mathbf{B}^T))$, and there exist

constants $C_1 \geq 0, C_2 \geq 0$, depending on $\mathbf{A}, \mathbf{B}, \mathbf{M}$ such that

$$\begin{aligned} \|\mathbf{v}\|_{L^2} &\leq C_1 \|\mathbf{v}^{(0)}\| + C_2 (\|\mathbf{g}_1\|_{L^2} + \|\mathbf{g}_2\|_{L^2}), \\ \|\mathbf{p}\|_{L^2} &\leq C_1 \|\mathbf{v}^{(0)}\| + C_2 \left(\|\mathbf{g}_1\|_{L^2} + \|\mathbf{g}_2\|_{L^2} + \left\| \frac{d}{dt} \mathbf{g}_2 \right\|_{L^2} \right). \end{aligned}$$

Proof We set $\mathbf{\Pi} := \mathbf{I} - \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}$. Since $\mathbf{\Pi}^2 = \mathbf{\Pi}$, $\mathbf{\Pi}\mathbf{M} = \mathbf{M}\mathbf{\Pi}^T$, $\text{null}(\mathbf{\Pi}) = \text{range}(\mathbf{B}^T)$ and $\text{range}(\mathbf{\Pi}) = \text{null}(\mathbf{B}\mathbf{M}^{-1})$, i.e., $\mathbf{\Pi}$ is an oblique projector.

We split $\mathbf{v}(t) = \mathbf{v}_H(t) + \mathbf{v}_P(t)$ and $\mathbf{v}^{(0)} = \mathbf{\Pi}\mathbf{v}^{(0)} + \mathbf{v}_P^{(0)}$, where

$$\begin{aligned} \mathbf{v}_H(t) &\in \text{Ker } \mathbf{B} \quad , \quad \mathbf{v}_P(t) := \mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{g}_2(t), \\ \mathbf{v}_P^{(0)} &= \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{g}_2(0). \end{aligned} \quad (7)$$

We note that $\mathbf{v}_P(t)$ and $\mathbf{v}_P^{(0)}$ are particular solutions of the second equation in (5a) and of (6), respectively. Then, the initial value problem (5a),(5b) can be transformed to

$$\mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^T \frac{d}{dt} \mathbf{v}_H(t) = -\mathbf{\Pi}\mathbf{A}\mathbf{\Pi}^T \mathbf{v}_H(t) + \mathbf{\Pi}\tilde{\mathbf{g}}(t) \quad , \quad t \in (0, T], \quad (8a)$$

$$\mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^T \mathbf{v}_H(0) = \mathbf{v}_H^{(0)}, \quad (8b)$$

where $\mathbf{v}_H^{(0)} = \mathbf{\Pi} \mathbf{v}^{(0)}$ and $\tilde{\mathbf{g}} \in \mathbb{R}^n$ is given by

$$\tilde{\mathbf{g}}(t) := \mathbf{g}_1(t) - \mathbf{A}\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{g}_2(t). \quad (9)$$

Moreover, $\mathbf{p}(t) \in \mathbb{R}^m / (\text{Ker } \mathbf{B}^T)$ can be recovered according to

$$\mathbf{p}(t) = (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1} \left(\mathbf{B}\mathbf{M}^{-1} \left(-\mathbf{A}\mathbf{v}_H(t) + \tilde{\mathbf{g}}(t) \right) - \frac{d}{dt} \mathbf{g}_2(t) \right). \quad (10)$$

In view of (i),(ii), the matrices $\overline{\mathbf{M}} := \mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^T$ and $\overline{\mathbf{A}} := \mathbf{\Pi}\mathbf{A}\mathbf{\Pi}^T$ are symmetric positive definite on $\text{Ker } \mathbf{B}$ and satisfy

$$-\mathbf{v}^T \overline{\mathbf{A}} \mathbf{v} \leq -\alpha \mathbf{v}^T \overline{\mathbf{M}} \mathbf{v} \quad , \quad \mathbf{v} \in \text{Ker } \mathbf{B}.$$

Then, Lemma 5 in [5] implies

$$\|\mathbf{v}_H\|_{L^2} \leq \frac{\sqrt{2} \|\overline{\mathbf{M}}^{-1/2}\| \|\overline{\mathbf{M}}^{1/2}\|}{\sqrt{\alpha}} \|\mathbf{v}_H^{(0)}\| + \frac{2 \|\overline{\mathbf{M}}^{-1}\|}{\alpha} \|\tilde{\mathbf{g}}\|_{L^2}. \quad (11)$$

We conclude due to (7),(10) and (11). \blacksquare

3. Balanced truncation model reduction for Stokes-type systems

Balanced truncation model reduction is a particular model reduction technique that seeks to replace a large-scale system of differential or difference equations by a system of substantially lower dimension that has nearly the same response characteristics, that preserves asymptotic stability and that provides an error bound on the discrepancy between the outputs of the full and reduced order system

[7, 9, 15, 18, 28, 40]. Originally, balanced truncation model reduction was developed for systems of ordinary differential equations (ODEs). Recently it has been extended to descriptor systems. An overview of balanced truncation model reduction for descriptor systems can be found in [26]. Balanced truncation model reduction for semidiscretized Stokes and linearized Navier-Stokes systems is studied in [21, 32, 35]. We summarize the basic ideas for a system that is closely related to the optimality system arising in control and shape optimization problems governed by the semidiscretized Stokes or linearized Navier-Stokes equations. Our presentation follows [21]. We consider

$$\mathbf{M} \frac{d}{dt} \mathbf{v}(t) = -\mathbf{A} \mathbf{v}(t) - \mathbf{B}^T \mathbf{p}(t) + \mathbf{K} \mathbf{u}(t), \quad t \in (0, T), \quad (12a)$$

$$0 = -\mathbf{B} \mathbf{v}(t) + \mathbf{L} \mathbf{u}(t), \quad t \in (0, T) \quad (12b)$$

$$\mathbf{z}(t) = \mathbf{C} \mathbf{v}(t) + \mathbf{F} \mathbf{p}(t) + \mathbf{D} \mathbf{u}(t), \quad t \in (0, T), \quad (12c)$$

$$\mathbf{M} \mathbf{v}(0) = \mathbf{v}^{(0)}, \quad (12d)$$

$$\mathbf{B} \mathbf{M}^{-1} \mathbf{v}^{(0)} = \mathbf{L} \mathbf{u}(0), \quad (12e)$$

and

$$-\mathbf{M} \frac{d}{dt} \boldsymbol{\lambda}(t) = -\mathbf{A}^T \boldsymbol{\lambda}(t) - \mathbf{B}^T \boldsymbol{\kappa}(t) + \mathbf{C}^T \mathbf{w}(t), \quad t \in (0, T), \quad (13a)$$

$$0 = -\mathbf{B} \boldsymbol{\lambda}(t) + \mathbf{F}^T \mathbf{w}(t), \quad t \in (0, T), \quad (13b)$$

$$\mathbf{q}(t) = \mathbf{K}^T \boldsymbol{\lambda}(t) + \mathbf{L}^T \boldsymbol{\kappa}(t) + \mathbf{D}^T \mathbf{w}(t), \quad t \in (0, T), \quad (13c)$$

$$\mathbf{M} \boldsymbol{\lambda}(T) = \boldsymbol{\lambda}^{(T)}, \quad (13d)$$

$$\mathbf{B} \mathbf{M}^{-1} \boldsymbol{\lambda}^{(T)} = \mathbf{F}^T \mathbf{w}(T), \quad (13e)$$

where $\mathbf{M} \in \mathbb{R}^{n_v \times n_v}$ is a symmetric positive definite matrix, $\mathbf{A} \in \mathbb{R}^{n_v \times n_v}$, $\mathbf{B} \in \mathbb{R}^{n_p \times n_v}$, $n_p < n_v$, is a matrix with rank n_p , $\mathbf{K} \in \mathbb{R}^{n_v \times n_g}$, $\mathbf{L} \in \mathbb{R}^{n_p \times n_g}$, $\mathbf{C} \in \mathbb{R}^{n_z \times n_v}$, $\mathbf{F} \in \mathbb{R}^{n_z \times n_p}$, and $\mathbf{D} \in \mathbb{R}^{n_z \times n_g}$. The terms $\mathbf{D} \mathbf{u}(t)$ and $\mathbf{D}^T \mathbf{w}(t)$ are ‘feed through terms’ in the output equations. The system (13) is the adjoint system corresponding to (12). Conditions (12e) and (13e) ensure the compatibility of the inputs \mathbf{u} and \mathbf{w} with the initial and final values [13].

In addition to the assumptions above, we assume that the generalized eigenvalues of the pair (\mathbf{A}, \mathbf{M}) have positive real part. This assumption is needed to apply balanced truncation model reduction.

The numerical method discussed in [21] for computing reduced order models using balanced truncation is applied to the system (12,13) directly. However, it is derived by eliminating the variables \mathbf{p} and $\boldsymbol{\kappa}$ via projection. This leads to dynamical systems governed by ODEs to which standard balanced truncation can be applied. The application of balanced truncation to the projected system of ODEs is then translated into an approach that applies directly to (12,13). Since the transformation of (12,13) into a system of ODEs is also important for the later application of balanced truncation in optimization contexts, we summarize the main steps. Details can be found in [21].

As in the proof of Theorem 2.1 we choose $\mathbf{v}(t) = \mathbf{v}_H(t) + \mathbf{v}_P(t)$, where

$$\mathbf{v}_P(t) = \mathbf{M}^{-1} \mathbf{B}^T (\mathbf{B} \mathbf{M}^{-1} \mathbf{B}^T)^{-1} \mathbf{L} \mathbf{u}(t) \quad (14)$$

is a particular solution of (12b) and $\mathbf{v}_H(t)$ satisfies $\mathbf{0} = \mathbf{B}\mathbf{v}_H(t)$. If we insert $\mathbf{v}(t) = \mathbf{v}_H(t) + \mathbf{v}_P(t)$, (14) into (12a-c), we obtain

$$\begin{aligned} \mathbf{M} \frac{d}{dt} \mathbf{v}_H(t) &= -\mathbf{A}\mathbf{v}_H(t) - \mathbf{B}^T \mathbf{p}(t) \\ &\quad + (\mathbf{K} - \mathbf{A}\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L}) \mathbf{u}(t) \\ &\quad - \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L} \frac{d}{dt} \mathbf{u}(t), \end{aligned} \quad (15a)$$

$$\mathbf{0} = \mathbf{B}\mathbf{v}_H(t), \quad (15b)$$

$$\mathbf{z}(t) = \mathbf{C}\mathbf{v}_H(t) + \mathbf{F}\mathbf{p}(t) + (\mathbf{D} + \mathbf{C}\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L}) \mathbf{u}(t). \quad (15c)$$

Equations (15a,b) imply that

$$\begin{aligned} \mathbf{p}(t) &= -(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}\mathbf{A}\mathbf{v}_H(t) \\ &\quad + (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}(\mathbf{K} - \mathbf{A}\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L}) \mathbf{u}(t) \\ &\quad - (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L} \frac{d}{dt} \mathbf{u}(t) \end{aligned} \quad (16)$$

and $\mathbf{\Pi}^T \mathbf{v}_H(t) = \mathbf{v}_H(t)$, where

$$\mathbf{\Pi} = \mathbf{I} - \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}. \quad (17)$$

Note that $\mathbf{\Pi}^2 = \mathbf{\Pi}$, $\mathbf{\Pi}\mathbf{M} = \mathbf{M}\mathbf{\Pi}^T$, $\text{null}(\mathbf{\Pi}) = \text{range}(\mathbf{B}^T)$ and $\text{range}(\mathbf{\Pi}) = \text{null}(\mathbf{B}\mathbf{M}^{-1})$, i.e., $\mathbf{\Pi}$ is an oblique projector.

Next, we insert (16) into (15a,c), use the identity $\mathbf{\Pi}^T \mathbf{v}_H(t) = \mathbf{v}_H(t)$, and multiply the resulting equation (15a) by $\mathbf{\Pi}$. Since $\mathbf{\Pi}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L} = \mathbf{0}$ this leads to

$$\mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^T \frac{d}{dt} \mathbf{v}_H(t) = -\mathbf{\Pi}\mathbf{A}\mathbf{\Pi}^T \mathbf{v}_H(t) + \mathbf{\Pi}\tilde{\mathbf{B}}\mathbf{u}(t), \quad (18a)$$

$$\mathbf{z}(t) = \tilde{\mathbf{C}}\mathbf{\Pi}^T \mathbf{v}_H(t) + \tilde{\mathbf{D}}\mathbf{u}(t) - \mathbf{F}(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L} \frac{d}{dt} \mathbf{u}(t), \quad (18b)$$

where

$$\tilde{\mathbf{B}} = \mathbf{K} - \mathbf{A}\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L},$$

$$\tilde{\mathbf{C}} = \mathbf{C} - \mathbf{F}(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}\mathbf{A},$$

$$\tilde{\mathbf{D}} = \mathbf{D} + \mathbf{C}\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L} + \mathbf{F}(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}\tilde{\mathbf{B}}.$$

To obtain the initial condition for \mathbf{v}_H we set $\mathbf{v}^{(0)} = \mathbf{\Pi}\mathbf{v}^{(0)} + (\mathbf{I} - \mathbf{\Pi})\mathbf{v}^{(0)}$ and use (12e)

$$\begin{aligned} \mathbf{v}^{(0)} &= \mathbf{\Pi}\mathbf{v}^{(0)} + \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}\mathbf{v}^{(0)} \\ &= \mathbf{\Pi}\mathbf{v}^{(0)} + \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L}\mathbf{u}(0). \end{aligned}$$

Furthermore, we have

$$\begin{aligned}\mathbf{M}\mathbf{v}(0) &= \mathbf{M}\mathbf{v}_H(0) + \mathbf{M}\mathbf{v}_P(0) = \mathbf{M}\mathbf{\Pi}^T\mathbf{v}_H(0) + \mathbf{M}\mathbf{v}_P(0) \\ &= \mathbf{\Pi}\mathbf{M}\mathbf{v}_H(0) + \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{L}\mathbf{u}(0).\end{aligned}$$

This leads to

$$\mathbf{\Pi}\mathbf{M}\mathbf{v}_H(0) = \mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^T\mathbf{v}_H(0) = \mathbf{\Pi}\mathbf{v}^{(0)} \quad (=: \mathbf{v}_H^{(0)}). \quad (18c)$$

We can proceed in the same way to transform (13). We set $\boldsymbol{\lambda} = \boldsymbol{\lambda}_H(t) + \boldsymbol{\lambda}_P(t)$ where $\boldsymbol{\lambda}_P(t) = \mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T\mathbf{w}(t)$. The equations (13) can be transformed into

$$\begin{aligned}-\mathbf{M}\frac{d}{dt}\boldsymbol{\lambda}_H(t) &= -\mathbf{A}^T\boldsymbol{\lambda}_H(t) - \mathbf{B}^T\boldsymbol{\kappa}(t) \\ &\quad + (\mathbf{C}^T - \mathbf{A}^T\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T)\mathbf{w}(t) \\ &\quad + \mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T\frac{d}{dt}\mathbf{w}(t)\end{aligned} \quad (19a)$$

$$\mathbf{0} = \mathbf{B}\boldsymbol{\lambda}_H(t), \quad (19b)$$

$$\mathbf{q}(t) = \mathbf{K}^T\boldsymbol{\lambda}_H(t) + \mathbf{L}^T\boldsymbol{\kappa}(t) + (\mathbf{D}^T + \mathbf{K}^T\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T)\mathbf{w}(t). \quad (19c)$$

Equations (19a,b) imply that

$$\begin{aligned}\boldsymbol{\kappa}(t) &= -(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}\mathbf{A}^T\boldsymbol{\lambda}_H(t) \\ &\quad + (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{B}\mathbf{M}^{-1}(\mathbf{C}^T - \mathbf{A}^T\mathbf{M}^{-1}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T)\mathbf{w}(t) \\ &\quad + (\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T\frac{d}{dt}\mathbf{w}(t)\end{aligned} \quad (20)$$

and $\mathbf{\Pi}^T\boldsymbol{\lambda}_H(t) = \boldsymbol{\lambda}_H(t)$, where $\mathbf{\Pi}$ is given as before.

Next, we insert (20) into (19a,c), use the identity $\mathbf{\Pi}^T\boldsymbol{\lambda}_H(t) = \boldsymbol{\lambda}_H(t)$, and multiply the resulting equation (19a) by $\mathbf{\Pi}$. Since $\mathbf{\Pi}\mathbf{B}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T = \mathbf{0}$ this leads to

$$-\mathbf{\Pi}\mathbf{M}\mathbf{\Pi}^T\frac{d}{dt}\boldsymbol{\lambda}_H(t) = -\mathbf{\Pi}\mathbf{A}^T\mathbf{\Pi}^T\boldsymbol{\lambda}_H(t) + \mathbf{\Pi}\tilde{\mathbf{C}}^T\mathbf{w}(t), \quad (21a)$$

$$\mathbf{q}(t) = \tilde{\mathbf{B}}^T\mathbf{\Pi}^T\boldsymbol{\lambda}_H(t) + \tilde{\mathbf{D}}^T\mathbf{w}(t) + \mathbf{L}^T(\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^T)^{-1}\mathbf{F}^T\frac{d}{dt}\mathbf{w}(t), \quad (21b)$$

$$\mathbf{M}\boldsymbol{\lambda}_H(T) = \mathbf{\Pi}\boldsymbol{\lambda}^{(T)}, \quad (21c)$$

where $\tilde{\mathbf{B}}$, $\tilde{\mathbf{C}}$ and $\tilde{\mathbf{D}}$ are given as before.

For model reduction purposes we view \mathbf{u} and $\frac{d}{dt}\mathbf{u}$ as inputs into (18) and \mathbf{w} and $\frac{d}{dt}\mathbf{w}$ as inputs into (21). The terms involving \mathbf{u} and \mathbf{w} in (18b) and (21b) are ‘feed through’ terms, since inputs are directly fed to the outputs \mathbf{z} and \mathbf{q} respectively. These terms are not reduced. Note that the transformed system (21) is the adjoint system corresponding to (18).

The systems (18) and (21) are almost in the form to which standard balanced truncation model reduction can be applied. Since $\mathbf{\Pi}$ has a non-trivial null-space,

the dynamical systems in (18) and (21) have to be solved for \mathbf{v}_H with $\mathbf{\Pi}^T \mathbf{v}_H = \mathbf{v}_H$ and $\boldsymbol{\lambda}_H$ with $\mathbf{\Pi}^T \boldsymbol{\lambda}_H = \boldsymbol{\lambda}_H$. This can be made explicit by expressing

$$\mathbf{\Pi} = \boldsymbol{\Theta}_l \boldsymbol{\Theta}_r^T \quad (22a)$$

with $\boldsymbol{\Theta}_l, \boldsymbol{\Theta}_r \in \mathbb{R}^{n_v \times (n_v - n_p)}$ satisfying

$$\boldsymbol{\Theta}_l^T \boldsymbol{\Theta}_r = \mathbf{I}. \quad (22b)$$

Substituting this decomposition into (18) shows that $\tilde{\mathbf{v}}_H = \boldsymbol{\Theta}_l^T \mathbf{v}_H \in \mathbb{R}^{n_v - n_p}$ must satisfy

$$\boldsymbol{\Theta}_r^T \mathbf{M} \boldsymbol{\Theta}_r \frac{d}{dt} \tilde{\mathbf{v}}_H(t) = -\boldsymbol{\Theta}_r^T \mathbf{A} \boldsymbol{\Theta}_r \tilde{\mathbf{v}}_H(t) + \boldsymbol{\Theta}_r^T \tilde{\mathbf{B}} \mathbf{u}(t), \quad (23a)$$

$$\mathbf{z}(t) = \tilde{\mathbf{C}} \boldsymbol{\Theta}_r \frac{d}{dt} \tilde{\mathbf{v}}_H(t) + \tilde{\mathbf{D}} \mathbf{u}(t) - \mathbf{F}(\mathbf{B} \mathbf{M}^{-1} \mathbf{B}^T)^{-1} \mathbf{L} \frac{d}{dt} \mathbf{u}(t). \quad (23b)$$

An analogous substitution is applied in (21). Standard balanced truncation model reduction can now be applied to the system (23) and the corresponding adjoint system derived from (21). The projection matrices computed by balanced truncation for (23) and the corresponding adjoint system derived from (21) can then be transformed into projection matrices for the systems (18) and (21).

Balanced truncation model reduction generates projection matrices $\mathbf{V}, \mathbf{W} \in \mathbb{R}^{n_v \times k}$ with $k \ll n_v$ such that

$$\mathbf{V} = \mathbf{\Pi}^T \mathbf{V}, \mathbf{W} = \mathbf{\Pi}^T \mathbf{W}, \text{ and } \mathbf{W}^T \mathbf{M} \mathbf{V} = \mathbf{I}.$$

The reduced order model for (18) is obtained by replacing $\mathbf{v}_H(t)$ in (18) by $\mathbf{V} \hat{\mathbf{v}}(t)$ and multiplying the resulting equation by \mathbf{W}^T . This gives

$$\frac{d}{dt} \hat{\mathbf{v}}(t) = -\mathbf{W}^T \mathbf{A} \mathbf{V} \hat{\mathbf{v}}(t) + \mathbf{W}^T \tilde{\mathbf{B}} \mathbf{u}(t), \quad (24a)$$

$$\hat{\mathbf{z}}(t) = \tilde{\mathbf{C}} \mathbf{V} \hat{\mathbf{v}}(t) + \tilde{\mathbf{D}} \mathbf{u}(t) - \mathbf{F}(\mathbf{B} \mathbf{M}^{-1} \mathbf{B}^T)^{-1} \mathbf{L} \frac{d}{dt} \mathbf{u}(t), \quad (24b)$$

$$\hat{\mathbf{v}}(t) = \mathbf{W}^T \mathbf{\Pi} \mathbf{v}^{(0)}. \quad (24c)$$

Similarly, the reduced order model for (21) is obtained by replacing $\boldsymbol{\lambda}_H(t)$ in (21) by $\mathbf{W} \hat{\boldsymbol{\lambda}}(t)$ and multiplying the resulting equation by \mathbf{V}^T . This gives

$$-\frac{d}{dt} \hat{\boldsymbol{\lambda}}(t) = -\mathbf{V}^T \mathbf{A}^T \mathbf{W} \hat{\boldsymbol{\lambda}}(t) + \mathbf{V}^T \tilde{\mathbf{C}}^T \mathbf{w}(t), \quad (25a)$$

$$\hat{\mathbf{q}}(t) = \tilde{\mathbf{B}}^T \mathbf{W} \hat{\boldsymbol{\lambda}}(t) + \tilde{\mathbf{D}}^T \mathbf{w}(t) + \mathbf{L}^T (\mathbf{B} \mathbf{M}^{-1} \mathbf{B}^T)^{-1} \mathbf{F}^T \frac{d}{dt} \mathbf{w}(t), \quad (25b)$$

$$\hat{\boldsymbol{\lambda}}(t) = \mathbf{V}^T \mathbf{\Pi} \boldsymbol{\lambda}^{(T)}. \quad (25c)$$

We can show that $\mathbf{W}^T \mathbf{A} \mathbf{V}$ is stable see [21, Sec. 7] for details. Furthermore if $\mathbf{v}_H(0) = \boldsymbol{\lambda}_H(T) = \mathbf{0}$, then for any given inputs \mathbf{u}, \mathbf{w} we have

$$\|\mathbf{z} - \hat{\mathbf{z}}\|_{L^2} \leq 2 \|\mathbf{u}\|_{L^2} (\sigma_{k+1} + \dots + \sigma_n), \quad (26a)$$

$$\|\mathbf{q} - \hat{\mathbf{q}}\|_{L^2} \leq 2 \|\mathbf{w}\|_{L^2} (\sigma_{k+1} + \dots + \sigma_n). \quad (26b)$$

Remark 1 Inhomogeneous initial conditions can be handled by modifying the balanced truncation model reduction as discussed in [8].

4. Domain decomposition

We consider a decomposition of $\Omega(\theta)$ into subdomains $\Omega_1, \Omega_2(\theta)$ such that

$$\overline{\Omega}(\theta) = \overline{\Omega}_1 \cup \overline{\Omega}_2(\theta) \quad , \quad \Omega_1 \cap \Omega_2(\theta) = \emptyset \quad , \quad \Gamma := \overline{\Omega}_1 \cap \overline{\Omega}_2(\theta), \quad (27)$$

where Γ stands for the interfaces between the subdomains. The domain decomposition is motivated by such PDE constrained optimization problems where the optimal design issues focus on a relatively small portion of the domain, namely the subdomain $\Omega_2(\theta)$. Consequently, only that subdomain is supposed to depend on the design variables θ , whereas Ω_1 is independent of θ . In practice, the subdomains Ω_1 and $\Omega_2(\theta)$ can be further subdivided. Multiple subdomains can be incorporated into our approach, but to keep the presentation simple we consider the two subdomain case.

We assume that the objective functional can be split accordingly

$$J(\theta) := J_1(\mathbf{v}, p) + J_2(\mathbf{v}(\theta), p(\theta), \theta). \quad (28)$$

Here, $J_1(\mathbf{v}, p)$ is given in terms of observation operators $C : \mathbf{L}^2((0, T); \mathbf{V}) \rightarrow L^2((0, T); (L^2(\Omega_1)^q))$, $F : L^2((0, T); L_0^2(\Omega)) \rightarrow L^2((0, T); (L^2(\Omega_1)^q))$ and a feed-through operator $D : \mathbf{L}^2((0, T); \mathbf{L}^2(\Omega)) \rightarrow L^2((0, T); (L^2(\Omega_1)^q))$, $q \in \mathbb{N}$. For a given function $\mathbf{d} \in L^2((0, T); (L^2(\Omega_1)^q))$, we define

$$J_1(\mathbf{v}, p) := \int_0^T \int_{\Omega_1} |C\mathbf{v} + Fp + D\mathbf{u} - \mathbf{d}|^2 dx dt. \quad (29)$$

On the other hand, $J_2(\mathbf{v}, p, \theta)$ is supposed to be as in (1b) with $\Omega(\theta)$ replaced by $\Omega_2(\theta)$.

We consider geometrically conforming simplicial triangulations $\mathcal{T}_h(\Omega(\theta))$ that align with the decomposition in the sense that their restrictions to $\Omega_1, \Omega_2(\theta)$ represent geometrically conforming triangulations $\mathcal{T}_h(\Omega_1), \mathcal{T}_h(\Omega_2(\theta))$. The semi-discretization in space of the Stokes equation in the domain decomposition context requires some care. See, e.g., [2, 11, 24, 29–31, 38, 39]. For semi-discretization in space, we may use stable discontinuous pressure elements such as nonconforming P2-P0 or P1-P0 elements [14] or spectral elements [29, 39]. The subsequent analysis also applies, if we use continuous pressure elements such as the Taylor-Hood P2-P1 element or the mini-element [10, 12], provided the incompressibility condition on the interface $\Gamma(\theta)$ is not discretized and hence, we do not explicitly consider the semi-discrete pressure on the interface $\Gamma(\theta)$ (cf., e.g., [31]).

The discretization needs to be such that the coupled problem is solvable, i.e., the local subproblems corresponding to the subdomains Ω_1 and $\Omega_2(\theta)$ as well as those corresponding to the interface are solvable. The global problem (2c)–(2e) has a unique solution $(\mathbf{v}, \mathbf{p}) \in L^2((0, T); \mathbb{R}^n) \times L^2((0, T); \mathbb{R}^m / (\text{Ker } \mathbf{B}^T))$. Some of the local problems associated with the subdomain Ω_1 or $\Omega_2(\theta)$ correspond to Stokes subdomain problems with Dirichlet boundary conditions only. Consequently, for these subproblems the pressure is only unique up to a constant. To ensure that the subdomain solution is the restriction of the solution of

(2c)–(2e) to the subdomain, we split the subdomain pressures into a constant and a subdomain pressure with zero spatial average. The latter is determined uniquely as the solution of the subdomain problem, whereas the constant is determined through the coupled problems. This split is not necessary for subdomains with an outflow condition, where the local pressure is unique. However, to simplify the presentation, we assume that the split has to be made for both subdomains.

The velocities are discretized using

$$v_h(x, t) = \sum_{j=1}^n \mathbf{v}_j(t) \phi_j(x),$$

where $\phi_j(t)$, $j = 1, \dots, n_1$ have support in $\bar{\Omega}_1$, $\phi_j(t)$, $j = n_1 + 1, \dots, n_1 + n_2$ have support in $\bar{\Omega}_2$, and $\phi_j(t)$, $j = n_1 + n_2 + 1, \dots, n = n_1 + n_2 + n_\Gamma$ are the remaining basis functions, which are associated with the interface. The semidiscretized pressure $p_h(x, t)$ is the sum of subdomain pressures $p_{h,i}(x, t)$, $i = 1, 2$ with zero average on the subdomain, $\int_{\Omega_j} p_{h,i}(x, t) dx = 0$, $i = 1, 2$, and constant pressures $p_{0,i}(t)$, $i = 1, 2$, for each subdomain. We have

$$p_h(x, t) = \sum_{j=1}^2 p_{0,j}(t) \chi_{\bar{\Omega}_j}(x) + \sum_{j=1}^{m-2} p_j(t) \psi_j(x),$$

where $\chi_{\mathcal{S}}$ denotes the characteristic function of a set $\mathcal{S} \subset \Omega$, $\psi_j(t)$, $j = 1, \dots, m_1$ are basis functions that have support in $\bar{\Omega}_1$, and $\psi_j(t)$, $j = m_1 + 1, \dots, m-2 = m_1 + m_2$ have support in $\bar{\Omega}_2$. We require that

$$\int_{\Omega_j} \sum_{j=1}^{m_1} p_j(t) \psi_j(x) dx = \int_{\Omega_j} \sum_{j=1}^{m_2} p_{m_1+j}(t) \psi_{m_1+j}(x) dx = 0.$$

Thus, we have velocities $\mathbf{v}_1(t) \in \mathbb{R}^{n_1}$, $\mathbf{v}_2(t) \in \mathbb{R}^{n_2}$, $\mathbf{v}_\Gamma(t) \in \mathbb{R}^{n_\Gamma}$ associated with Ω_1 , $\Omega_2(\theta)$, and $\Gamma(\theta)$, respectively. We set $\mathbf{v}(t) = (\mathbf{v}_1(t), \mathbf{v}_2(t), \mathbf{v}_\Gamma(t))^T$. The pressures associated with Ω_1 , $\Omega_2(\theta)$ are $\mathbf{p}_1(t) \in \mathbb{R}^{m_1}$, $\mathbf{p}_2(t) \in \mathbb{R}^{m_2}$. Additionally, we have constants $p_{0,1}(t), p_{0,2}(t) \in \mathbb{R}$. We set $\mathbf{p}_0(t) = (p_{0,1}(t), p_{0,2}(t))^T$ and $\mathbf{p}(t) = (\mathbf{p}_1(t), \mathbf{p}_2(t), \mathbf{p}_0(t))^T$. Finally, we define the state variables

$$\mathbf{x}(t) := (\mathbf{v}_1, \mathbf{p}_1, \mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0)^T, \quad t \in [0, T]. \quad (30)$$

With this discretization and partitioning of variables, the matrices $\mathbf{A}(\theta)$ and $\mathbf{B}(\theta)$ can be partitioned as follows

$$\mathbf{A}(\theta) = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{0} & \mathbf{A}_{1\Gamma} \\ \mathbf{0} & \mathbf{A}_{22}(\theta) & \mathbf{A}_{2\Gamma}(\theta) \\ \mathbf{A}_{1\Gamma}^T & \mathbf{A}_{2\Gamma}^T(\theta) & \mathbf{A}_{\Gamma\Gamma}(\theta) \end{pmatrix}, \quad \mathbf{B}(\theta) = \begin{pmatrix} \mathbf{B}_{11} & \mathbf{0} & \mathbf{B}_{1\Gamma} \\ \mathbf{0} & \mathbf{B}_{22}(\theta) & \mathbf{B}_{2\Gamma}(\theta) \\ \mathbf{0} & \mathbf{0} & \mathbf{B}_0(\theta) \end{pmatrix}. \quad (31)$$

Here, $\mathbf{A}_{11} \in \mathbb{R}^{n_1 \times n_1}$, $\mathbf{A}_{22}(\theta) \in \mathbb{R}^{n_2 \times n_2}$, $\mathbf{A}_{\Gamma\Gamma}(\theta) \in \mathbb{R}^{n_\Gamma \times n_\Gamma}$, $\mathbf{A}_{i\Gamma}(\theta) \in \mathbb{R}^{n_i \times n_\Gamma}$, $1 \leq i \leq 2$, and $\mathbf{B}_{11} \in \mathbb{R}^{m_1 \times m_1}$, $\mathbf{B}_{22}(\theta) \in \mathbb{R}^{m_2 \times m_2}$, $\mathbf{B}_{i\Gamma}(\theta) \in \mathbb{R}^{m_i \times n_\Gamma}$, $1 \leq i \leq 2$, $\mathbf{B}_0(\theta) \in \mathbb{R}^{2 \times n_\Gamma}$. Likewise, the matrices $\mathbf{K}(\theta)$, $\mathbf{L}(\theta)$ and the lumped mass matrix $\mathbf{M}(\theta)$ admit the decompositions

$$\mathbf{K}(\theta) = (\mathbf{K}_1, \mathbf{K}_2(\theta), \mathbf{K}_\Gamma(\theta))^T \quad \mathbf{L}(\theta) = (\mathbf{L}_1, \mathbf{L}_2(\theta), \mathbf{L}_0(\theta))^T, \quad (32a)$$

$$\mathbf{M}(\theta) = \mathbf{blockdiag}(\mathbf{M}_1, \mathbf{M}_2(\theta), \mathbf{M}_\Gamma(\theta)), \quad (32b)$$

where $\mathbf{K}_i(\theta) \in \mathbb{R}^{n_i \times k}$, $\mathbf{L}_i(\theta) \in \mathbb{R}^{m_i \times k}$, $1 \leq i \leq 2$, $\mathbf{K}_\Gamma(\theta) \in \mathbb{R}^{n_\Gamma \times k}$, $\mathbf{L}_\Gamma(\theta) \in \mathbb{R}^{2 \times k}$ and $\mathbf{M}_1 \in \mathbb{R}^{n_1 \times n_1}$, $\mathbf{M}_2(\theta) \in \mathbb{R}^{n_2 \times n_2}$, $\mathbf{M}_\Gamma(\theta) \in \mathbb{R}^{n_\Gamma \times n_\Gamma}$. We set

$$\mathbf{E}(\theta) = \begin{pmatrix} \mathbf{E}_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{E}_2(\theta) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{E}_\Gamma(\theta) \end{pmatrix}, \quad \mathbf{S}(\theta) = \begin{pmatrix} \mathbf{S}_1 & \mathbf{0} & \mathbf{S}_{1\Gamma} \\ \mathbf{0} & \mathbf{S}_2(\theta) & \mathbf{S}_{2\Gamma}(\theta) \\ \mathbf{S}_{1\Gamma}^T & \mathbf{S}_{2,\Gamma}^T(\theta) & \mathbf{S}_\Gamma(\theta) \end{pmatrix}, \quad (33)$$

where

$$\mathbf{E}_1 = \begin{pmatrix} \mathbf{M}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathbf{E}_2(\theta) = \begin{pmatrix} \mathbf{M}_2(\theta) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathbf{E}_\Gamma(\theta) = \begin{pmatrix} \mathbf{M}_\Gamma(\theta) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad (34a)$$

$$\mathbf{S}_1 = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{B}_{11}^T \\ \mathbf{B}_{11} & \mathbf{0} \end{pmatrix}, \quad \mathbf{S}_2(\theta) = \begin{pmatrix} \mathbf{A}_{22}(\theta) & \mathbf{B}_{22}^T(\theta) \\ \mathbf{B}_{22}(\theta) & \mathbf{0} \end{pmatrix}, \quad (34b)$$

$$\mathbf{S}_\Gamma(\theta) = \begin{pmatrix} \mathbf{A}_{\Gamma\Gamma}(\theta) & \mathbf{B}_0^T(\theta) \\ \mathbf{B}_0(\theta) & \mathbf{0} \end{pmatrix}, \quad \mathbf{S}_{i\Gamma}(\theta) = \begin{pmatrix} \mathbf{A}_{i\Gamma}(\theta) & \mathbf{0} \\ \mathbf{B}_{i\Gamma}(\theta) & \mathbf{0} \end{pmatrix}, \quad 1 \leq i \leq 2, \quad (34c)$$

and

$$\mathbf{N}(\theta) = (\mathbf{K}_1 \mid \mathbf{L}_1 \mid \mathbf{K}_2(\theta) \mid \mathbf{L}_2(\theta) \mid \mathbf{K}_\Gamma(\theta) \mid \mathbf{L}_0(\theta))^T. \quad (35)$$

We further denote by $\mathbf{C}_1 \in \mathbb{R}^{q \times n_1}$, $\mathbf{F}_1 \in \mathbb{R}^{q \times m_1}$, $\mathbf{D}_1 \in \mathbb{R}^{q \times n_1}$, $\mathbf{d}(t) \in \mathbb{R}^q$, $t \in (0, T)$, the matrices and the vector and by $\ell(\mathbf{v}_2, \mathbf{v}_\Gamma, \mathbf{p}_2, \mathbf{p}_0, t, \theta)$ the functional resulting from the semi-discretization of the inner integrals in J_2 . We set

$$J(\theta) := J_1(\mathbf{v}_1, \mathbf{p}_1, \mathbf{p}_0) + J_2(\mathbf{v}_2(\theta), \mathbf{v}_\Gamma(\theta), \mathbf{p}_2(\theta), \mathbf{p}_0(\theta), \theta) \quad (36)$$

where J_1 and J_2 are given by

$$J_1(\mathbf{v}_1, \mathbf{p}_1, \mathbf{p}_0) = \frac{1}{2} \int_0^T |\mathbf{C}_1 \mathbf{v}_1(t) + \mathbf{F}_1 \mathbf{p}_1(t) + \mathbf{F}_0 \mathbf{p}_0(t) + \mathbf{D}_1 \mathbf{u}(t) - \mathbf{d}(t)|^2 dt, \quad (37a)$$

$$J_2(\mathbf{v}_2, \mathbf{v}_\Gamma, \mathbf{p}_2, \mathbf{p}_0, \theta) = \int_0^T \ell(\mathbf{v}_2, \mathbf{v}_\Gamma, \mathbf{p}_2, \mathbf{p}_0, t, \theta) dt. \quad (37b)$$

The semi-discretized, domain decomposed shape optimization problem can be formulated according to

$$\inf_{\theta \in \Theta} J(\theta) \quad (38a)$$

where $\mathbf{x} = (\mathbf{v}_1, \mathbf{p}_1, \mathbf{v}_2(\theta), \mathbf{p}_2(\theta), \mathbf{v}_\Gamma(\theta), \mathbf{p}_0(\theta))^T$ solves

$$\mathbf{P}(\theta) \mathbf{x}(t) := \mathbf{E}(\theta) \frac{d}{dt} \mathbf{x}(t) + \mathbf{S}(\theta) \mathbf{x}(t) = \mathbf{N}(\theta) \mathbf{u}(t), \quad t \in (0, T], \quad (38b)$$

$$\mathbf{M}(\theta) \mathbf{v}(0) = \mathbf{v}^{(0)}(\theta). \quad (38c)$$

Remark 1 If the Stokes equations are replaced by the Oseen equations or the linearized Navier-Stokes equations, linearized around a steady state, we also arrive

at a semi-discretized, domain decomposed shape optimization problem that is essentially of the type (38). In this case, the matrix $\mathbf{A}(\theta)$ and consequently, the matrix $\mathbf{S}(\theta)$, are no longer symmetric. However, this nonsymmetry can be easily incorporated and the discussion in this and the following sections can be easily extended to classes of problems governed by the Oseen equation and the linearized Navier-Stokes equations.

Introducing Lagrange multipliers $\boldsymbol{\lambda}(t) \in \mathbb{R}^n$, $\boldsymbol{\kappa}(t) \in \mathbb{R}^m$, $t \in [0, T]$, that are partitioned accordingly, and setting

$$\boldsymbol{\mu}(t) = (\boldsymbol{\lambda}_1(t), \boldsymbol{\kappa}_1(t), \boldsymbol{\lambda}_2(t), \boldsymbol{\kappa}_2(t), \boldsymbol{\lambda}_\Gamma(t), \boldsymbol{\kappa}_0(t))^T,$$

the Lagrangian associated with (38a)-(38c) is given by

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\mu}, \theta) := J(\mathbf{v}, \mathbf{p}, \theta) + \int_0^T \boldsymbol{\mu}(t)^T (\mathbf{P}(\theta)\mathbf{x}(t) - \mathbf{N}(\theta)\mathbf{u}(t)) dt, \quad (39)$$

and the optimality conditions read

$$\nabla_{\mathbf{x}}\mathcal{L}(\mathbf{x}, \boldsymbol{\mu}, \theta) = 0, \quad \nabla_{\boldsymbol{\mu}}\mathcal{L}(\mathbf{x}, \boldsymbol{\mu}, \theta) = 0, \quad \nabla_{\theta}\mathcal{L}(\mathbf{x}, \boldsymbol{\mu}, \theta)^T(\tilde{\theta} - \theta) \geq 0, \quad \tilde{\theta} \in \Theta. \quad (40)$$

It is obvious that due to the special structure of the decomposed optimization problems, the optimality conditions (40) can be split into a coupled system of optimality conditions associated with the subdomains Ω_1 , $\Omega_2(\theta)$, and the interface $\Gamma(\theta)$.

(i) Optimality system associated with subdomain Ω_1 :

$$\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} - \mathbf{S}_{1\Gamma} \begin{pmatrix} \mathbf{v}_\Gamma(t) \\ \mathbf{p}_0(t) \end{pmatrix} + \begin{pmatrix} \mathbf{K}_1 \\ \mathbf{L}_1 \end{pmatrix} \mathbf{u}(t), \quad (41a)$$

$$\mathbf{z}_1(t) = \mathbf{C}_1 \mathbf{v}_1(t) + \mathbf{F}_1 \mathbf{p}_1(t) + \mathbf{F}_0 \mathbf{p}_0(t) + \mathbf{D}_1 \mathbf{u}(t) - \mathbf{d}(t), \quad (41b)$$

$$\mathbf{M}_1 \mathbf{v}_1(0) = \mathbf{v}_1^{(0)}, \quad (41c)$$

$$\mathbf{L}_1 \mathbf{u}(0) = \mathbf{B}_{11} \mathbf{M}_1^{-1} \mathbf{v}_1^{(0)} + \mathbf{B}_{1\Gamma} \mathbf{M}_\Gamma^{-1} \mathbf{v}_\Gamma^{(0)}(\theta), \quad (41d)$$

and

$$-\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} - \mathbf{S}_{1\Gamma} \begin{pmatrix} \boldsymbol{\lambda}_\Gamma(t) \\ \boldsymbol{\kappa}_0(t) \end{pmatrix} - \begin{pmatrix} \mathbf{C}_1^T \\ \mathbf{F}_1^T \end{pmatrix} \mathbf{z}_1(t), \quad (42a)$$

$$\mathbf{M}_1 \boldsymbol{\lambda}_1(T) = \boldsymbol{\lambda}_1^{(T)}, \quad (42b)$$

$$\mathbf{F}_1^T \mathbf{z}_1(T) = -\mathbf{B}_{11} \mathbf{M}_1^{-1} \boldsymbol{\lambda}_1^{(T)} - \mathbf{B}_{1\Gamma} \mathbf{M}_\Gamma(\theta)^{-1} \boldsymbol{\lambda}_\Gamma^{(T)}(\theta). \quad (42c)$$

(ii) Optimality system associated with subdomain $\Omega_2(\theta)$:

$$\mathbf{E}_2(\theta) \frac{d}{dt} \begin{pmatrix} \mathbf{v}_2(t) \\ \mathbf{p}_2(t) \end{pmatrix} = -\mathbf{S}_2(\theta) \begin{pmatrix} \mathbf{v}_2(t) \\ \mathbf{p}_2(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}(\theta) \begin{pmatrix} \mathbf{v}_\Gamma(t) \\ \mathbf{p}_0(t) \end{pmatrix} + \begin{pmatrix} \mathbf{K}_2(\theta) \\ \mathbf{L}_2(\theta) \end{pmatrix} \mathbf{u}(t), \quad (43a)$$

$$\mathbf{M}_2(\theta) \mathbf{v}_2(0) = \mathbf{v}_2^{(0)}(\theta), \quad (43b)$$

$$\mathbf{L}_2(\theta) \mathbf{u}(0) = \mathbf{B}_{22}(\theta) \mathbf{M}_2(\theta)^{-1} \mathbf{v}_2^{(0)}(\theta) + \mathbf{B}_{2\Gamma}(\theta) \mathbf{M}_\Gamma(\theta)^{-1} \mathbf{v}_\Gamma^{(0)}(\theta), \quad (43c)$$

and

$$-\mathbf{E}_2(\theta) \frac{d}{dt} \begin{pmatrix} \boldsymbol{\lambda}_2(t) \\ \boldsymbol{\kappa}_2(t) \end{pmatrix} = -\mathbf{S}_2(\theta) \begin{pmatrix} \boldsymbol{\lambda}_2(t) \\ \boldsymbol{\kappa}_2(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}(\theta) \begin{pmatrix} \boldsymbol{\lambda}_\Gamma(t) \\ \boldsymbol{\kappa}_0(t) \end{pmatrix} - \begin{pmatrix} \nabla_{\mathbf{v}_2} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta) \\ \nabla_{\mathbf{p}_2} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta) \end{pmatrix}, \quad (44a)$$

$$\mathbf{M}_2(\theta) \boldsymbol{\lambda}_2(T) = \boldsymbol{\lambda}_2^{(T)}(\theta), \quad (44b)$$

$$\begin{aligned} \nabla_{\mathbf{p}_2} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta) &= -\mathbf{B}_{22}(\theta) \mathbf{M}_2(\theta)^{-1} \boldsymbol{\lambda}_2^{(T)}(\theta) \\ &\quad - \mathbf{B}_{2\Gamma}(\theta) \mathbf{M}_\Gamma(\theta)^{-1} \boldsymbol{\lambda}_\Gamma^{(T)}(\theta). \end{aligned} \quad (44c)$$

(iii) Optimality system associated with the interface $\Gamma(\theta)$:

$$\mathbf{E}_\Gamma(\theta) \frac{d}{dt} \begin{pmatrix} \mathbf{v}_\Gamma(t) \\ \mathbf{p}_0(t) \end{pmatrix} = -\mathbf{S}_\Gamma(\theta) \begin{pmatrix} \mathbf{v}_\Gamma(t) \\ \mathbf{p}_0(t) \end{pmatrix} - \mathbf{S}_{1\Gamma}^T \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}^T(\theta) \begin{pmatrix} \mathbf{v}_2(t) \\ \mathbf{p}_2(t) \end{pmatrix} + \begin{pmatrix} \mathbf{K}_\Gamma(\theta) \\ \mathbf{L}_0(\theta) \end{pmatrix} \mathbf{u}(t), \quad (45a)$$

$$\mathbf{M}_\Gamma(\theta) \mathbf{v}_\Gamma(0) = \mathbf{v}_\Gamma^{(0)}(\theta), \quad (45b)$$

$$\mathbf{L}_0(\theta) \mathbf{u}(0) = \mathbf{B}_0(\theta) \mathbf{M}_\Gamma(\theta)^{-1} \mathbf{v}_\Gamma^{(0)}(\theta), \quad (45c)$$

and

$$-\mathbf{E}_\Gamma(\theta) \begin{pmatrix} \boldsymbol{\lambda}_\Gamma(t) \\ \boldsymbol{\kappa}_0(t) \end{pmatrix} = -\mathbf{S}_\Gamma(\theta) \begin{pmatrix} \boldsymbol{\lambda}_\Gamma(t) \\ \boldsymbol{\kappa}_0(t) \end{pmatrix} - \mathbf{S}_{1\Gamma}^T \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}^T(\theta) \begin{pmatrix} \boldsymbol{\lambda}_2(t) \\ \boldsymbol{\kappa}_2(t) \end{pmatrix} - \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_0^T \end{pmatrix} \mathbf{z}_1, \quad (46a)$$

$$-\begin{pmatrix} \nabla_{\mathbf{v}_\Gamma} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta) \\ \nabla_{\mathbf{p}_0} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta) \end{pmatrix} - \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_0^T \end{pmatrix} \mathbf{z}_1, \quad (46b)$$

$$\mathbf{M}_\Gamma(\theta) \boldsymbol{\lambda}_\Gamma(T) = \boldsymbol{\lambda}_\Gamma^{(T)}(\theta), \quad (46b)$$

$$\nabla_{\mathbf{p}_0} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta) + \mathbf{F}_0^T \mathbf{z}_1 = -\mathbf{B}_0(\theta) \mathbf{M}_\Gamma(\theta)^{-1} \boldsymbol{\lambda}_\Gamma^{(T)}(\theta). \quad (46c)$$

The equations (41)-(46) have to be complemented by the variational inequality

$$\begin{aligned} & \int_0^T \nabla_{\theta} \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_{\Gamma}, \mathbf{p}_0, t, \theta)^T (\tilde{\theta} - \theta) dt \\ & + \int_0^T \begin{pmatrix} \boldsymbol{\mu}_2(t) \\ \boldsymbol{\mu}_{\Gamma}(t) \end{pmatrix}^T \begin{pmatrix} (D_{\theta} \mathbf{P}_2(\theta)(\tilde{\theta} - \theta)) \mathbf{x}_2(t) - (D_{\theta} \mathbf{N}_2(\theta)(\tilde{\theta} - \theta)) \mathbf{u}(t) \\ (D_{\theta} \mathbf{P}_{\Gamma}(\theta)(\tilde{\theta} - \theta)) \mathbf{x}_{\Gamma}(t) - (D_{\theta} \mathbf{N}_{\Gamma}(\theta)(\tilde{\theta} - \theta)) \mathbf{u}(t) \end{pmatrix} dt \geq 0 \end{aligned} \quad (47)$$

for all $\tilde{\theta} \in \Theta$.

Remark 2 Since we are faced with implicit Hessenberg index 2 differential-algebraic systems, the final values $\boldsymbol{\lambda}_1^{(T)}$, $\boldsymbol{\lambda}_2^{(T)}(\theta)$ and $\boldsymbol{\lambda}_{\Gamma}^{(T)}(\theta)$ are in general nonzero and have to be computed as outlined in [13]. It seems that for most examples considered in the flow control literature (see, e.g., [1, 20, 27]) the problem structure is such that $\boldsymbol{\lambda}_1^{(T)} = \mathbf{0}$, $\boldsymbol{\lambda}_2^{(T)}(\theta) = \mathbf{0}$ and $\boldsymbol{\lambda}_{\Gamma}^{(T)}(\theta) = \mathbf{0}$. For a flow control problem in which the adjoint has a nonzero final time value see, e.g., [34].

5. Balanced truncation model reduction of the domain decomposed optimality system

We construct a reduced order model for the optimality system (41)-(47) by applying balanced truncation only to the optimality system (41),(42) associated with the fixed subdomain Ω_1 . To do this, we have to examine (41)-(47) to see how the subsystems (41),(42) interact with the remaining subsystems. This leads to

$$\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} - \mathbf{S}_{1\Gamma} \begin{pmatrix} \mathbf{v}_{\Gamma}(t) \\ \mathbf{p}_0(t) \end{pmatrix} + \begin{pmatrix} \mathbf{K}_1 \\ \mathbf{L}_1 \end{pmatrix} \mathbf{u}(t), \quad (48a)$$

$$\mathbf{z}_1(t) = \mathbf{C}_1 \mathbf{v}_1(t) + \mathbf{F}_1 \mathbf{p}_1(t) + \mathbf{F}_0 \mathbf{p}_0(t) + \mathbf{D}_1 \mathbf{u}(t) - \mathbf{d}(t), \quad (48b)$$

$$\begin{pmatrix} \mathbf{z}_{v,\Gamma}(t) \\ \mathbf{z}_{p,\Gamma}(t) \end{pmatrix} = -\mathbf{S}_{1\Gamma}^T \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix}, \quad (48c)$$

$$\mathbf{M}_1 \mathbf{v}_1(0) = \mathbf{v}_1^{(0)}, \quad (48d)$$

$$\mathbf{L}_1 \mathbf{u}(0) = \mathbf{B}_{11} \mathbf{M}_1^{-1} \mathbf{v}_1^{(0)} + \mathbf{B}_{1\Gamma} \mathbf{M}_{\Gamma}(\theta)^{-1} \mathbf{v}_{\Gamma}^{(0)}(\theta), \quad (48e)$$

and

$$-\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} - \mathbf{S}_{1\Gamma} \begin{pmatrix} \boldsymbol{\lambda}_{\Gamma}(t) \\ \boldsymbol{\kappa}_0(t) \end{pmatrix} - \begin{pmatrix} \mathbf{C}_1^T \\ \mathbf{F}_1^T \end{pmatrix} \mathbf{z}_1(t), \quad (49a)$$

$$\mathbf{q}_1(t) = \mathbf{K}_1^T \boldsymbol{\lambda}_1(t) + \mathbf{L}_1^T \boldsymbol{\kappa}_1(t) - \mathbf{D}_1^T \mathbf{z}_1(t), \quad (49b)$$

$$\begin{pmatrix} \mathbf{q}_{v,\Gamma}(t) \\ \mathbf{q}_{p,\Gamma}(t) \end{pmatrix} = -\mathbf{S}_{1\Gamma}^T \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} - \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_0^T \end{pmatrix} \mathbf{z}_1, \quad (49c)$$

$$\mathbf{M}_1 \boldsymbol{\lambda}_1(T) = \boldsymbol{\lambda}_1^{(T)}, \quad (49d)$$

$$\mathbf{F}_1^T \mathbf{z}_1(T) = -\mathbf{B}_{11} \mathbf{M}_1^{-1} \boldsymbol{\lambda}_1^{(T)} - \mathbf{B}_{1\Gamma} \mathbf{M}_{\Gamma}(\theta)^{-1} \boldsymbol{\lambda}_{\Gamma}^{(T)}(\theta). \quad (49e)$$

The outputs (48c) and (49c) are inputs into the subsystems (45) and (46), respectively. The terms \mathbf{v}_{Γ} , \mathbf{p}_0 , $\boldsymbol{\lambda}_{\Gamma}$, $\boldsymbol{\kappa}_0$ are auxiliary inputs into the subsystems (48a) and

(49a). The output (49b) does not feed into any of the subsystems in (41)-(47), but is added to emphasize the fact that (48) and (49) is exactly of the form (12) and (13). An important observation is that due to the fact that pressures are discontinuous on the boundary, the second row block in $\mathbf{S}_{1\Gamma}^T$ is zero (cf., (31) and (34c)). Consequently,

$$\mathbf{z}_{p,\Gamma}(t) \equiv 0 \quad \text{and} \quad \mathbf{q}_{p,\Gamma}(t) = -\mathbf{F}_0^T \mathbf{z}_1(t). \quad (50)$$

The subsystems (48a-c) and (49a-c) can be written as

$$\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} + \begin{pmatrix} -\mathbf{A}_{1\Gamma} & \mathbf{0} & \mathbf{K}_1 \\ -\mathbf{B}_{1\Gamma} & \mathbf{0} & \mathbf{L}_1 \end{pmatrix} \begin{pmatrix} \mathbf{v}_\Gamma(t) \\ \mathbf{p}_0(t) \\ \mathbf{u}(t) \end{pmatrix}, \quad (51a)$$

$$\begin{pmatrix} \mathbf{z}_{v,\Gamma}(t) \\ \mathbf{z}_{p,\Gamma}(t) \\ \mathbf{z}_1(t) \end{pmatrix} = \begin{pmatrix} -\mathbf{A}_{1\Gamma}^T & -\mathbf{B}_{1\Gamma}^T \\ \mathbf{0} & \mathbf{0} \\ \mathbf{C}_1 & \mathbf{F}_1 \end{pmatrix} \begin{pmatrix} \mathbf{v}_1(t) \\ \mathbf{p}_1(t) \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{F}_0 \mathbf{p}_0(t) + \mathbf{D}_1 \mathbf{u}(t) - \mathbf{d}(t) \end{pmatrix} \quad (51b)$$

and

$$-\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} + \begin{pmatrix} -\mathbf{A}_{1\Gamma} & \mathbf{0} & \mathbf{C}_1^T \\ -\mathbf{B}_{1\Gamma} & \mathbf{0} & \mathbf{F}_1^T \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda}_\Gamma(t) \\ \boldsymbol{\kappa}_0(t) \\ -\mathbf{z}_1(t) \end{pmatrix}, \quad (52a)$$

$$\begin{pmatrix} \mathbf{q}_{v,\Gamma}(t) \\ \mathbf{q}_{p,\Gamma}(t) \\ \mathbf{q}_1(t) \end{pmatrix} = \begin{pmatrix} -\mathbf{A}_{1\Gamma}^T & -\mathbf{B}_{1\Gamma}^T \\ \mathbf{0} & \mathbf{0} \\ \mathbf{K}_1^T & \mathbf{L}_1^T \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda}_1(t) \\ \boldsymbol{\kappa}_1(t) \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_0^T \\ \mathbf{D}_1^T \end{pmatrix} (-\mathbf{z}_1(t)). \quad (52b)$$

To be able to apply the balanced truncation model reduction technique outlined in Section 3 we assume that $\mathbf{B}_{11} \in \mathbb{R}^{m_1 \times n_1}$ has rank m_1 , that $\mathbf{M}_{11} \in \mathbb{R}^{n_1 \times n_1}$ is symmetric positive definite, and that the generalized eigenvalues of $(\mathbf{A}_{11}, \mathbf{M}_{11})$ have positive real part. These assumptions are satisfied with a proper spatial decomposition of the problem.

If we apply the techniques introduced in Section 3 we obtain the following reduced optimality system.

(i) Reduced optimality system associated with the subdomain Ω_1 :

$$\frac{d}{dt} \widehat{\mathbf{v}}_1(t) = -\mathbf{W}^T \mathbf{A}_{11} \mathbf{V} \widehat{\mathbf{v}}_1(t) + \mathbf{W}^T \widetilde{\mathbf{B}}_1 \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \\ \mathbf{u}(t) \end{pmatrix}, \quad (53a)$$

$$\begin{pmatrix} \widehat{\mathbf{z}}_{v,\Gamma}(t) \\ \widehat{\mathbf{z}}_{p,\Gamma}(t) \\ \widehat{\mathbf{z}}_1(t) \end{pmatrix} = \widetilde{\mathbf{C}}_1 \mathbf{V} \widehat{\mathbf{v}}_1(t) + \widetilde{\mathbf{D}}_1 \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \\ \mathbf{u}(t) \end{pmatrix} - \widetilde{\mathbf{H}}_1 \frac{d}{dt} \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \\ \mathbf{u}(t) \end{pmatrix}, \quad (53b)$$

$$\widehat{\mathbf{v}}(0) = \mathbf{W}^T \boldsymbol{\Pi}_1 \mathbf{v}_1^{(0)} \quad (53c)$$

and

$$-\frac{d}{dt}\widehat{\boldsymbol{\lambda}}_1(t) = -\mathbf{V}^T \mathbf{A}_{11} \mathbf{W} \widehat{\boldsymbol{\lambda}}_1(t) + \mathbf{V}^T \widetilde{\mathbf{C}}_1^T \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \\ -\widehat{\boldsymbol{z}}_1(t) \end{pmatrix}, \quad (54a)$$

$$\begin{pmatrix} \widehat{\mathbf{q}}_{v,\Gamma}(t) \\ \widehat{\mathbf{q}}_{p,\Gamma}(t) \\ \widehat{\mathbf{q}}_1(t) \end{pmatrix} = \widetilde{\mathbf{B}}_1^T \mathbf{W} \widehat{\boldsymbol{\lambda}}_1(t) + \widetilde{\mathbf{D}}_1^T \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \\ -\widehat{\boldsymbol{z}}_1(t) \end{pmatrix} + \widetilde{\mathbf{H}}_1^T \frac{d}{dt} \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \\ -\widehat{\boldsymbol{z}}_1(t) \end{pmatrix}, \quad (54b)$$

$$\widehat{\boldsymbol{\lambda}}_1(T) = \mathbf{V}^T \boldsymbol{\Pi}_1 \boldsymbol{\lambda}_1^{(T)}. \quad (54c)$$

Here $\boldsymbol{\Pi}_1 = \mathbf{I} - \mathbf{B}_{11}^T (\mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T)^{-1} \mathbf{B}_{11} \mathbf{M}_{11}^{-1}$ and

$$\begin{aligned} \widetilde{\mathbf{B}}_1 &= (-\mathbf{A}_{1\Gamma} \mid \mathbf{0} \mid \mathbf{K}_1) - \mathbf{A}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T (\mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T)^{-1} (-\mathbf{B}_{1\Gamma} \mid \mathbf{0} \mid \mathbf{L}_1) \\ \widetilde{\mathbf{C}}_1 &= \begin{pmatrix} -\mathbf{A}_{1\Gamma}^T \\ \mathbf{0} \\ \mathbf{C}_1 \end{pmatrix} - \begin{pmatrix} -\mathbf{B}_{1\Gamma}^T \\ \mathbf{0} \\ \mathbf{F}_1 \end{pmatrix} (\mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T)^{-1} \mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{A}_{11}, \\ \widetilde{\mathbf{D}}_1 &= \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{F}_0 & \mathbf{D}_1 \end{pmatrix} + \begin{pmatrix} -\mathbf{A}_{1\Gamma}^T \\ \mathbf{0} \\ \mathbf{C}_1 \end{pmatrix} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T (\mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T)^{-1} (-\mathbf{B}_{1\Gamma} \mid \mathbf{0} \mid \mathbf{L}_1) \\ &\quad + \begin{pmatrix} -\mathbf{B}_{1\Gamma}^T \\ \mathbf{0} \\ \mathbf{F}_1 \end{pmatrix} (\mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T)^{-1} \mathbf{B}_{11} \mathbf{M}_{11}^{-1} \widetilde{\mathbf{B}}_1, \\ \widetilde{\mathbf{H}}_1 &= \begin{pmatrix} -\mathbf{B}_{1\Gamma}^T \\ \mathbf{0} \\ \mathbf{F}_1 \end{pmatrix} (\mathbf{B}_{11} \mathbf{M}_{11}^{-1} \mathbf{B}_{11}^T)^{-1} (-\mathbf{B}_{1\Gamma} \mid \mathbf{0} \mid \mathbf{L}_1). \end{aligned}$$

Note that the structure of $\widetilde{\mathbf{B}}_1$, $\widetilde{\mathbf{C}}_1$, $\widetilde{\mathbf{D}}_1$, and $\widetilde{\mathbf{H}}_1$ imply

$$\widehat{\mathbf{z}}_{p,\Gamma}(t) \equiv 0 \quad \text{and} \quad \widehat{\mathbf{q}}_{p,\Gamma}(t) \equiv 0. \quad (55)$$

The reduced optimality system associated with the subdomain Ω_1 is coupled to following optimality subsystems.

(ii) Optimality system associated with the subdomain $\Omega_2(\theta)$:

$$\begin{aligned} \mathbf{E}_2(\theta) \frac{d}{dt} \begin{pmatrix} \widehat{\mathbf{v}}_2(t) \\ \widehat{\mathbf{p}}_2(t) \end{pmatrix} &= -\mathbf{S}_2(\theta) \begin{pmatrix} \widehat{\mathbf{v}}_2(t) \\ \widehat{\mathbf{p}}_2(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}(\theta) \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \end{pmatrix} \\ &\quad + \begin{pmatrix} \mathbf{K}_2(\theta) \\ \mathbf{L}_2(\theta) \end{pmatrix} \mathbf{u}(t), \end{aligned} \quad (56a)$$

$$\mathbf{M}_2(\theta) \widehat{\mathbf{v}}_2(0) = \mathbf{v}_2^{(0)}(\theta), \quad (56b)$$

$$\mathbf{L}_2(\theta) \mathbf{u}(0) = \mathbf{B}_{22}(\theta) \mathbf{M}_2(\theta)^{-1} \mathbf{v}_2^{(0)}(\theta) + \mathbf{B}_{2\Gamma}(\theta) \mathbf{M}_\Gamma(\theta)^{-1} \mathbf{v}_\Gamma^{(0)}(\theta), \quad (56c)$$

and

$$-\mathbf{E}_2(\theta) \frac{d}{dt} \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_2(t) \\ \widehat{\boldsymbol{\kappa}}_2(t) \end{pmatrix} = -\mathbf{S}_2(\theta) \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_2(t) \\ \widehat{\boldsymbol{\kappa}}_2(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}(\theta) \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \end{pmatrix} \quad (57a)$$

$$- \begin{pmatrix} \nabla_{\widehat{\mathbf{v}}_2} \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, t, \theta) \\ \nabla_{\widehat{\mathbf{p}}_2} \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, t, \theta) \end{pmatrix},$$

$$\mathbf{M}_2(\theta) \widehat{\boldsymbol{\lambda}}_2(T) = \boldsymbol{\lambda}_2^{(T)}(\theta). \quad (57b)$$

(iii) Optimality system associated with the interface $\Gamma(\theta)$:

$$\mathbf{E}_\Gamma(\theta) \frac{d}{dt} \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \end{pmatrix} = -\mathbf{S}_\Gamma(\theta) \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \end{pmatrix} + \begin{pmatrix} \widehat{\mathbf{z}}_{v,\Gamma}(t) \\ \widehat{\mathbf{z}}_{p,\Gamma}(t) \end{pmatrix} \quad (58a)$$

$$- \mathbf{S}_{2\Gamma}^T(\theta) \begin{pmatrix} \widehat{\mathbf{v}}_2(t) \\ \widehat{\mathbf{p}}_2(t) \end{pmatrix} + \begin{pmatrix} \mathbf{K}_\Gamma(\theta) \\ \mathbf{L}_\Gamma(\theta) \end{pmatrix} \mathbf{u}(t),$$

$$\mathbf{M}_\Gamma(\theta) \widehat{\mathbf{v}}_\Gamma(0) = \mathbf{v}_\Gamma^{(0)}(\theta), \quad (58b)$$

and

$$-\mathbf{E}_\Gamma(\theta) \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \end{pmatrix} = -\mathbf{S}_\Gamma(\theta) \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \end{pmatrix} + \begin{pmatrix} \widehat{\mathbf{q}}_{v,\Gamma}(t) \\ \widehat{\mathbf{q}}_{p,\Gamma}(t) \end{pmatrix} - \mathbf{S}_{2\Gamma}^T(\theta) \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_2(t) \\ \widehat{\boldsymbol{\kappa}}_2(t) \end{pmatrix} \quad (59a)$$

$$- \begin{pmatrix} \nabla_{\widehat{\mathbf{v}}_\Gamma} \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, t, \theta) \\ \nabla_{\widehat{\mathbf{p}}_0} \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, t, \theta) \end{pmatrix},$$

$$\mathbf{M}_\Gamma(\theta) \widehat{\boldsymbol{\lambda}}_\Gamma(T) = \boldsymbol{\lambda}_\Gamma^{(T)}(\theta). \quad (59b)$$

The equations have to be complemented by the variational inequality

$$\int_0^T \nabla_\theta \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, t, \theta)^T (\tilde{\theta} - \theta) dt \quad (60)$$

$$+ \int_0^T \begin{pmatrix} \widehat{\boldsymbol{\mu}}_2(t) \\ \widehat{\boldsymbol{\lambda}}_\Gamma(t) \end{pmatrix}^T \begin{pmatrix} (D_\theta \mathbf{P}_2(\theta)(\tilde{\theta} - \theta)) \widehat{\mathbf{x}}_2(t) - (D_\theta \mathbf{N}_2(\theta)(\tilde{\theta} - \theta)) \mathbf{u}(t) \\ (D_\theta \mathbf{P}_\Gamma(\theta)(\tilde{\theta} - \theta)) \widehat{\mathbf{x}}_\Gamma(t) - (D_\theta \mathbf{N}_\Gamma(\theta)(\tilde{\theta} - \theta)) \mathbf{u}(t) \end{pmatrix} dt \geq 0, \quad \tilde{\theta} \in \Theta.$$

We have applied domain decomposition and balanced truncation model reduction to derive the reduced order optimality system (53)-(60) from the full order optimality system (41)-(47). This raises the question whether the reduced order optimality system (53)-(60) is the optimality system for a reduced order optimization problem. This is important, since numerically we solve the shape optimization problem using gradient based optimization methods rather than explicitly solving the optimality system.

THEOREM 5.1 *The reduced order optimality system (53)-(60) represents the first order necessary optimality conditions for the shape optimization problem*

$$\min \widehat{J}(\theta) \quad (61a)$$

$$s.t. \theta \in \Theta$$

where $\widehat{J}(\theta) = \widehat{J}_1(\widehat{\mathbf{v}}_1, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0) + \widehat{J}_2(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, \theta)$,

$$\widehat{J}_1(\widehat{\mathbf{v}}_1, \widehat{\mathbf{v}}_\Gamma) = \frac{1}{2} \int_0^T |\widehat{\mathbf{z}}_1|^2 dt, \quad (61b)$$

$$\widehat{J}_2(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, \theta) = \int_0^T \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0, t, \theta) dt. \quad (61c)$$

and where $\widehat{\mathbf{z}}_1$, $\widehat{\mathbf{v}} = (\widehat{\mathbf{v}}_1, \widehat{\mathbf{v}}_2, \widehat{\mathbf{v}}_\Gamma)^T$, $\widehat{\mathbf{p}} = (\widehat{\mathbf{p}}_2, \widehat{\mathbf{p}}_0)^T$, are given as the solution of (53), (56), (58).

The proof uses standard arguments and is omitted.

6. A priori estimate of the modeling error

Let $\theta^* \in \Theta$ and $\widehat{\theta}^* \in \Theta$ be local minima of the optimization problem (38) and its reduced version (61), where the states $\mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_\Gamma)^T$ and $\mathbf{p} = (\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_0)^T$ solve (41),(43),(45), and where the reduced states $\widehat{\mathbf{v}} = (\widehat{\mathbf{v}}_1, \widehat{\mathbf{v}}_2, \widehat{\mathbf{v}}_\Gamma)^T$ and $\widehat{\mathbf{p}} = (\widehat{\mathbf{p}}_2, \widehat{\mathbf{p}}_0)^T$ solve (53), (56), (58). Considering the states as implicit functions of the design variables, (38) and (61), can be simply written as

$$\inf_{\theta \in \Theta} J(\theta) \quad \text{and} \quad \inf_{\theta \in \Theta} \widehat{J}(\theta).$$

We want to derive an upper bound for the modeling error $\|\theta^* - \widehat{\theta}^*\|$ in terms of the Hankel singular values occurring in the BTMR of the optimality system for the fixed subdomain Ω_1 . Under the convexity assumption, there exists $\kappa > 0$ such that

$$\left(\nabla J(\widehat{\theta}^*) - \nabla J(\theta^*) \right)^T (\widehat{\theta}^* - \theta^*) \geq \kappa \|\widehat{\theta}^* - \theta^*\|^2, \quad (62)$$

It is easy to see that

$$\|\theta^* - \widehat{\theta}^*\| \leq \kappa^{-1} \|\nabla \widehat{J}(\widehat{\theta}^*) - \nabla J(\widehat{\theta}^*)\|, \quad (63)$$

see, e.g., [5]. Hence, we need to provide an upper bound for the right-hand side in (63). The gradients of the objective functions J and \widehat{J} can be expressed using the Lagrangian in (39) and its reduced analogue associated with (61). More precisely,

we have

$$\begin{aligned}
& \left(\nabla J(\theta) - \nabla \widehat{J}(\theta) \right)^T \tilde{\theta} \\
&= \int_0^T \left(\nabla_{\theta} \ell(\mathbf{v}_2, \mathbf{v}_{\Gamma}, \mathbf{p}_2, \mathbf{p}_0, t, \theta) - \nabla_{\theta} \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{v}}_{\Gamma}, \widehat{\mathbf{p}}_2, \widehat{\mathbf{p}}_0, t, \theta) \right)^T \tilde{\theta} dt \\
&\quad + \int_0^T \begin{pmatrix} \widehat{\boldsymbol{\mu}}_2(t) \\ \widehat{\boldsymbol{\mu}}_{\Gamma}(t) \end{pmatrix}^T \begin{pmatrix} (D_{\theta} \mathbf{P}_2(\theta) \tilde{\theta})(\mathbf{x}_2 - \widehat{\mathbf{x}}_2)(t) \\ (D_{\theta} \mathbf{P}_{\Gamma}(\theta) \tilde{\theta})(\mathbf{x}_{\Gamma} - \widehat{\mathbf{x}}_{\Gamma})(t) \end{pmatrix} dt \\
&\quad + \int_0^T \begin{pmatrix} (\boldsymbol{\mu}_2 - \widehat{\boldsymbol{\mu}}_2)(t) \\ (\boldsymbol{\mu}_{\Gamma} - \widehat{\boldsymbol{\mu}}_{\Gamma})(t) \end{pmatrix}^T \begin{pmatrix} (D_{\theta} \mathbf{P}_2(\theta) \tilde{\theta}) \mathbf{x}_2(t) - (D_{\theta} \mathbf{N}_2(\theta) \tilde{\theta}) \mathbf{u}(t) \\ (D_{\theta} \mathbf{P}_{\Gamma}(\theta) \tilde{\theta}) \mathbf{x}_{\Gamma}(t) - (D_{\theta} \mathbf{N}_{\Gamma}(\theta) \tilde{\theta}) \mathbf{u}(t) \end{pmatrix} dt
\end{aligned} \tag{64}$$

where $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_{\Gamma})^T$, with $\mathbf{x}_i = (\mathbf{v}_i, \mathbf{p}_i)^T$, $i = 1, 2$, $\mathbf{x}_{\Gamma} = (\mathbf{v}_{\Gamma}, \mathbf{p}_0)^T$, and $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\mu}_{\Gamma})^T$, with $\boldsymbol{\mu}_i = (\boldsymbol{\lambda}_i, \boldsymbol{\kappa}_i)^T$, $i = 1, 2$, $\boldsymbol{\mu}_{\Gamma} = (\boldsymbol{\lambda}_{\Gamma}, \boldsymbol{\kappa}_0)^T$ solve (41)-(46), and where $\widehat{\mathbf{x}} = (\widehat{\mathbf{x}}_1, \widehat{\mathbf{x}}_2, \widehat{\mathbf{x}}_{\Gamma})^T$ with $\widehat{\mathbf{x}}_1 = \widehat{\mathbf{v}}_1$, $\widehat{\mathbf{x}}_2 = (\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2)^T$, $\widehat{\mathbf{x}}_{\Gamma} = (\widehat{\mathbf{v}}_{\Gamma}, \widehat{\mathbf{p}}_0)^T$ and $\widehat{\boldsymbol{\mu}} = (\widehat{\boldsymbol{\mu}}_1, \widehat{\boldsymbol{\mu}}_2, \widehat{\boldsymbol{\mu}}_{\Gamma})^T$ with $\widehat{\boldsymbol{\mu}}_1 = \widehat{\boldsymbol{\lambda}}_1$, $\widehat{\boldsymbol{\mu}}_2 = (\widehat{\boldsymbol{\lambda}}_2, \widehat{\boldsymbol{\kappa}}_2)^T$, $\widehat{\boldsymbol{\mu}}_{\Gamma} = (\widehat{\boldsymbol{\lambda}}_{\Gamma}, \widehat{\boldsymbol{\kappa}}_0)^T$ solve (53)-(59).

In order to estimate (64) from above, we have to establish upper bounds for $\mathbf{x}_2 - \widehat{\mathbf{x}}_2$, $\mathbf{x}_{\Gamma} - \widehat{\mathbf{x}}_{\Gamma}$ and $\boldsymbol{\mu}_2 - \widehat{\boldsymbol{\mu}}_2$, $\boldsymbol{\mu}_{\Gamma} - \widehat{\boldsymbol{\mu}}_{\Gamma}$. This will be done in the sequel, where C will denote a generic positive constant not necessarily the same at each occurrence.

We apply the balanced truncation error bound (26) to estimate the error due to the reduction of the optimality subsystem 1. The error bound applies when $\mathbf{v}_1^{(0)} = 0$ and $\boldsymbol{\lambda}_1^{(T)} = 0$, which we will assume. This assumption can be relaxed when a modification of balanced truncation is applied. See Remark 1 in Section 3.

In order to provide an estimate of the errors in the adjoint states, we make the following assumption on the matrices $\mathbf{A}(\theta)$, $\mathbf{B}(\theta)$, $\mathbf{M}(\theta)$ defined in (31), (32b), and submatrices corresponding to subdomain 1. This assumption is satisfied with a proper spatial decomposition of the problem as described in Section 4.

(A₁) The matrix $\mathbf{B}(\theta) \in \mathbb{R}^{m \times n}$ has rank m , the matrix $\mathbf{M}(\theta) \in \mathbb{R}^{n \times n}$ is symmetric positive definite, and the generalized eigenvalues of $(\mathbf{A}(\theta), \mathbf{M}(\theta))$ have positive real part.

The matrix $\mathbf{B}_{11} \in \mathbb{R}^{m_1 \times n_1}$ has rank m_1 , the matrix $\mathbf{M}_{11} \in \mathbb{R}^{n_1 \times n_1}$ is symmetric positive definite, and the generalized eigenvalues of $(\mathbf{A}_{11}, \mathbf{M}_{11})$ have positive real part.

The first part allows the application of Theorem 2.1. The assumption on the submatrices corresponding to subdomain 1 were needed for the application of balanced truncation model reduction to the optimality subsystem (51,52).

LEMMA 6.1 *Let $\mathbf{x} = (\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_{\Gamma})^T$, where*

$$\mathbf{x}_i = (\mathbf{v}_i, \mathbf{p}_i)^T, \quad 1 \leq i \leq 2, \quad \mathbf{x}_{\Gamma} = (\mathbf{v}_{\Gamma}, \mathbf{p}_0)^T,$$

and $\widehat{\mathbf{x}} = (\widehat{\mathbf{x}}_1, \widehat{\mathbf{x}}_2, \widehat{\mathbf{x}}_{\Gamma})^T$, where

$$\widehat{\mathbf{x}}_1 = \widehat{\mathbf{v}}_1, \quad \widehat{\mathbf{x}}_2 = (\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2)^T, \quad \widehat{\mathbf{x}}_{\Gamma} = (\widehat{\mathbf{v}}_{\Gamma}, \widehat{\mathbf{p}}_0)^T.$$

*If **(A₁)** and $\mathbf{v}_1^{(0)} = 0$ hold and if \mathbf{x} and $\widehat{\mathbf{x}}$ satisfy (41), (43), (45) and (53), (56),*

(58), respectively, then there exists $C > 0$ such that

$$\left\| \begin{pmatrix} \mathbf{v}_2 - \widehat{\mathbf{v}}_2 \\ \mathbf{v}_\Gamma - \widehat{\mathbf{v}}_\Gamma \end{pmatrix} \right\|_{L^2} \leq C \left\| \begin{pmatrix} \mathbf{u} \\ \widehat{\mathbf{x}}_\Gamma \end{pmatrix} \right\|_{L^2} (\sigma_{k+1} + \dots + \sigma_n), \quad (65a)$$

$$\left\| \begin{pmatrix} \mathbf{p}_2 - \widehat{\mathbf{p}}_2 \\ \mathbf{p}_0 - \widehat{\mathbf{p}}_0 \end{pmatrix} \right\|_{L^2} \leq C \left\| \begin{pmatrix} \mathbf{u} \\ \widehat{\mathbf{x}}_\Gamma \end{pmatrix} \right\|_{L^2} (\sigma_{k+1} + \dots + \sigma_n), \quad (65b)$$

$$\left\| \begin{pmatrix} \mathbf{z}_1 - \widehat{\mathbf{z}}_1 \\ \mathbf{z}_{v,\Gamma} - \widehat{\mathbf{z}}_{v,\Gamma} \\ \mathbf{z}_{p,\Gamma} - \widehat{\mathbf{z}}_{p,\Gamma} \end{pmatrix} \right\|_{L^2} \leq C \left\| \begin{pmatrix} \mathbf{u} \\ \widehat{\mathbf{x}}_\Gamma \end{pmatrix} \right\|_{L^2} (\sigma_{k+1} + \dots + \sigma_n). \quad (65c)$$

Proof We introduce an auxiliary state $(\widetilde{\mathbf{v}}_1, \widetilde{\mathbf{p}}_1)$ as the solution of

$$\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \widetilde{\mathbf{v}}_1(t) \\ \widetilde{\mathbf{p}}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \widetilde{\mathbf{v}}_1(t) \\ \widetilde{\mathbf{p}}_1(t) \end{pmatrix} - \mathbf{S}_{1\Gamma} \begin{pmatrix} \widehat{\mathbf{v}}_\Gamma(t) \\ \widehat{\mathbf{p}}_0(t) \end{pmatrix} + \begin{pmatrix} \mathbf{K}_1 \\ \mathbf{L}_1 \end{pmatrix} \mathbf{u}(t), \quad (66a)$$

$$\widetilde{\mathbf{z}}_1(t) = \mathbf{C}_1 \widetilde{\mathbf{v}}_1(t) + \mathbf{F}_1 \widetilde{\mathbf{p}}_1(t) + \mathbf{F}_0 \widehat{\mathbf{p}}_0(t) + \mathbf{D}_1 \mathbf{u}(t) - \mathbf{d}(t), \quad (66b)$$

$$\begin{pmatrix} \widetilde{\mathbf{z}}_{v,\Gamma}(t) \\ \widetilde{\mathbf{z}}_{p,\Gamma}(t) \end{pmatrix} = -\mathbf{S}_{1\Gamma}^T \begin{pmatrix} \widetilde{\mathbf{v}}_1(t) \\ \widetilde{\mathbf{p}}_1(t) \end{pmatrix}, \quad (66c)$$

$$\mathbf{M}_1 \widetilde{\mathbf{v}}_1(0) = \mathbf{v}_1^{(0)}, \quad (66d)$$

$$\mathbf{L}_1 \mathbf{u}(0) = \mathbf{B}_{11} \mathbf{M}_1^{-1} \mathbf{v}_1^{(0)} + \mathbf{B}_{1\Gamma} \mathbf{M}_\Gamma(\theta)^{-1} \mathbf{v}_\Gamma^{(0)}(\theta). \quad (66e)$$

Note that because the second row block in $\mathbf{S}_{1\Gamma}^T$ is zero (cf. (31) and (34c)), we have

$$\widetilde{\mathbf{z}}_{p,\Gamma}(t) \equiv 0. \quad (67)$$

This auxiliary system (66) is almost identical to (48), but has inputs $\widehat{\mathbf{v}}_\Gamma, \widehat{\mathbf{p}}_0$ instead of $\mathbf{v}_\Gamma, \mathbf{p}_0$. Thus the inputs for (66) and the reduced system (53) are the same and we can apply the balanced truncation error bound (26) to this subsystem. The balanced truncation error bound for this subsystem is

$$\left\| \begin{pmatrix} \widetilde{\mathbf{z}}_1 - \widehat{\mathbf{z}}_1 \\ \widetilde{\mathbf{z}}_{v,\Gamma} - \widehat{\mathbf{z}}_{v,\Gamma} \\ \widetilde{\mathbf{z}}_{p,\Gamma} - \widehat{\mathbf{z}}_{p,\Gamma} \end{pmatrix} \right\|_{L^2} \leq 2(\sigma_{k+1} + \dots + \sigma_n) \left\| \begin{pmatrix} \mathbf{u} \\ \widehat{\mathbf{v}}_\Gamma \\ \widehat{\mathbf{p}}_0 \end{pmatrix} \right\|_{L^2}. \quad (68)$$

We set $\mathbf{e}_v = (\mathbf{v}_1 - \widetilde{\mathbf{v}}_1, \mathbf{v}_2 - \widehat{\mathbf{v}}_2, \mathbf{v}_\Gamma - \widehat{\mathbf{v}}_\Gamma)^T$ and $\mathbf{e}_p = (\mathbf{p}_1 - \widetilde{\mathbf{p}}_1, \mathbf{p}_2 - \widehat{\mathbf{p}}_2, \mathbf{p}_0 - \widehat{\mathbf{p}}_0)^T$. It follows from (41), (43), (45), (50) and (66), (56), (58), (55), (67) that $(\mathbf{e}_v, \mathbf{e}_p)^T$ satisfies the system

$$\mathbf{E}(\theta) \frac{d}{dt} \begin{pmatrix} \mathbf{e}_v(t) \\ \mathbf{e}_p(t) \end{pmatrix} = -\mathbf{S}(\theta) \begin{pmatrix} \mathbf{e}_v(t) \\ \mathbf{e}_p(t) \end{pmatrix} + \begin{pmatrix} \mathbf{g}_1(t) \\ \mathbf{0} \end{pmatrix}, \quad t \in (0, T], \quad (69a)$$

$$\mathbf{M}(\theta) \mathbf{e}_v(0) = \mathbf{0}, \quad (69b)$$

where

$$\mathbf{g}_1(t) = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \widetilde{\mathbf{z}}_{v,\Gamma} - \widehat{\mathbf{z}}_{v,\Gamma} \end{pmatrix}.$$

Applying Theorem 2.1 to (69) yields

$$\left\| \begin{pmatrix} \mathbf{v}_1 - \tilde{\mathbf{v}}_1 \\ \mathbf{v}_2 - \tilde{\mathbf{v}}_2 \\ \mathbf{v}_\Gamma - \tilde{\mathbf{v}}_\Gamma \end{pmatrix} \right\|_{L^2} \leq C \|\tilde{\mathbf{z}}_{v,\Gamma} - \hat{\mathbf{z}}_{v,\Gamma}\|_{L^2}, \quad \left\| \begin{pmatrix} \mathbf{p}_1 - \tilde{\mathbf{p}}_1 \\ \mathbf{p}_2 - \tilde{\mathbf{p}}_2 \\ \mathbf{p}_0 - \tilde{\mathbf{p}}_0 \end{pmatrix} \right\|_{L^2} \leq C \|\tilde{\mathbf{z}}_{v,\Gamma} - \hat{\mathbf{z}}_{v,\Gamma}\|_{L^2}. \quad (70)$$

The estimates (65a,b) follow from (68) and (70).

To prove (65c) we observe that (48b) and (66b) imply

$$\begin{aligned} \|\mathbf{z}_1 - \hat{\mathbf{z}}_1\|_{L^2} &= \|\mathbf{z}_1 - \tilde{\mathbf{z}}_1\|_{L^2} + \|\tilde{\mathbf{z}}_1 - \hat{\mathbf{z}}_1\|_{L^2} \\ &\leq C (\|\mathbf{v}_1 - \tilde{\mathbf{v}}_1\|_{L^2} + \|\mathbf{p}_1 - \tilde{\mathbf{p}}_1\|_{L^2} + \|\mathbf{p}_0 - \tilde{\mathbf{p}}_0\|_{L^2}) + \|\tilde{\mathbf{z}}_1 - \hat{\mathbf{z}}_1\|_{L^2} \\ &\leq C \|\tilde{\mathbf{z}}_{v,\Gamma} - \hat{\mathbf{z}}_{v,\Gamma}\|_{L^2} + \|\tilde{\mathbf{z}}_1 - \hat{\mathbf{z}}_1\|_{L^2}. \end{aligned}$$

Together with (68) this implies the first part of (65c). The second part of (65c) can be shown analogously. The third part of (65c) is trivially satisfied by (50) and (55). \blacksquare

In order to provide an estimate of the errors in the adjoint states, we make the following assumptions.

- (A₂) $\mathbf{F}_1 = \mathbf{0}$ and $\mathbf{F}_0 = \mathbf{0}$, i.e, the objective function J_1 does not depend explicitly on the pressure.
- (A₃) There exists a positive constant L_1 such that for all $\mathbf{x}_2, \mathbf{x}'_2, \mathbf{x}_\Gamma, \mathbf{x}'_\Gamma$ and all $\theta \in \Theta, t \in [0, T]$ there holds

$$\begin{aligned} \|\nabla_{\mathbf{v}} \ell(\mathbf{x}_2, \mathbf{x}_\Gamma, t, \theta) - \nabla_{\mathbf{v}} \ell(\mathbf{x}'_2, \mathbf{x}'_\Gamma, t, \theta)\| &\leq L_1 \left(\|\delta \mathbf{x}_2\|^2 + \|\delta \mathbf{x}_\Gamma\|^2 \right)^{1/2}, \\ \|\nabla_{\mathbf{p}} \ell(\mathbf{x}_2, \mathbf{x}_\Gamma, t, \theta) - \nabla_{\mathbf{p}} \ell(\mathbf{x}'_2, \mathbf{x}'_\Gamma, t, \theta)\| &\leq L_1 \left(\|\delta \mathbf{x}_2\|^2 + \|\delta \mathbf{x}_\Gamma\|^2 \right)^{1/2}, \\ \|\nabla_{\theta} \ell(\mathbf{x}_2, \mathbf{x}_\Gamma, t, \theta) - \nabla_{\theta} \ell(\mathbf{x}'_2, \mathbf{x}'_\Gamma, t, \theta)\| &\leq L_1 \left(\|\delta \mathbf{x}_2\|^2 + \|\delta \mathbf{x}_\Gamma\|^2 \right)^{1/2}, \end{aligned}$$

where $\mathbf{v} \in \{\mathbf{v}_2, \mathbf{v}_\Gamma\}, \mathbf{p} \in \{\mathbf{p}_2, \mathbf{p}_0\}$ and $\delta \mathbf{x}_2 := \mathbf{x}_2 - \mathbf{x}'_2, \delta \mathbf{x}_\Gamma := \mathbf{x}_\Gamma - \mathbf{x}'_\Gamma$.

- (A₄) There exists a positive constant C such that for all $\theta \in \Theta$ and θ' with $\|\theta'\| \leq 1$

$$\begin{aligned} \max \left(\|D_\theta \mathbf{M}_2(\theta)\theta'\|, \|D_\theta \mathbf{M}_\Gamma(\theta)\theta'\|, \|D_\theta \mathbf{S}_2(\theta)\theta'\|, \|D_\theta \mathbf{S}_\Gamma(\theta)\theta'\|, \right. \\ \left. \|D_\theta \mathbf{S}_{2\Gamma}(\theta)\theta'\|, \|D_\theta \mathbf{N}_2(\theta)\theta'\| \|D_\theta \mathbf{N}_\Gamma(\theta)\theta'\| \right) \leq C. \end{aligned}$$

LEMMA 6.2 *Let $\mathbf{x}, \hat{\mathbf{x}}$ as in Lemma 6.1 and $\boldsymbol{\mu} = (\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\mu}_\Gamma)^T$, where*

$$\boldsymbol{\mu}_i = (\boldsymbol{\lambda}_i, \boldsymbol{\kappa}_i)^T, \quad 1 \leq i \leq 2, \quad \boldsymbol{\mu}_\Gamma = (\boldsymbol{\lambda}_\Gamma, \boldsymbol{\kappa}_0)^T$$

and $\hat{\boldsymbol{\mu}} = (\hat{\boldsymbol{\mu}}_1, \hat{\boldsymbol{\mu}}_2, \hat{\boldsymbol{\mu}}_\Gamma)^T$, where

$$\hat{\boldsymbol{\mu}}_1 = \hat{\boldsymbol{\lambda}}_1, \quad \hat{\boldsymbol{\mu}}_2 = (\hat{\boldsymbol{\lambda}}_2, \hat{\boldsymbol{\kappa}}_2)^T, \quad \hat{\boldsymbol{\mu}}_\Gamma = (\hat{\boldsymbol{\lambda}}_\Gamma, \hat{\boldsymbol{\kappa}}_0)^T.$$

If (A₁) – (A₃), and $\boldsymbol{\lambda}_1^{(T)} = 0$ hold, and if $\mathbf{x}, \boldsymbol{\mu}$ and $\hat{\mathbf{x}}, \hat{\boldsymbol{\mu}}, \hat{\mathbf{z}}_1$ solve (41)-(46) and

(53)-(59), respectively, then

$$\left\| \begin{pmatrix} \lambda_2 - \widehat{\lambda}_2 \\ \lambda_\Gamma - \widehat{\lambda}_\Gamma \end{pmatrix} \right\|_{L^2} \leq C \left(\left\| \begin{pmatrix} \mathbf{u} \\ \widehat{\mathbf{x}}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \widehat{\mathbf{z}}_1 \\ \widehat{\boldsymbol{\mu}}_\Gamma \end{pmatrix} \right\|_{L^2} \right) (\sigma_{k+1} + \cdots + \sigma_n), \quad (71a)$$

$$\left\| \begin{pmatrix} \kappa_2 - \widehat{\kappa}_2 \\ \kappa_0 - \widehat{\kappa}_0 \end{pmatrix} \right\|_{L^2} \leq C \left(\left\| \begin{pmatrix} \mathbf{u} \\ \widehat{\mathbf{x}}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \widehat{\mathbf{z}}_1 \\ \widehat{\boldsymbol{\mu}}_\Gamma \end{pmatrix} \right\|_{L^2} \right) (\sigma_{k+1} + \cdots + \sigma_n). \quad (71b)$$

Proof As in the proof of Lemma 6.1, we introduce an auxiliary adjoint state $\widetilde{\boldsymbol{\mu}}_1 = (\widetilde{\boldsymbol{\lambda}}_1, \widetilde{\boldsymbol{\kappa}}_1)^T$ as the solution of

$$-\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \widetilde{\boldsymbol{\lambda}}_1(t) \\ \widetilde{\boldsymbol{\kappa}}_1(t) \end{pmatrix} = -\mathbf{S}_1 \begin{pmatrix} \widetilde{\boldsymbol{\lambda}}_1(t) \\ \widetilde{\boldsymbol{\kappa}}_1(t) \end{pmatrix} - \mathbf{S}_{1\Gamma} \begin{pmatrix} \widehat{\boldsymbol{\lambda}}_\Gamma(t) \\ \widehat{\boldsymbol{\kappa}}_0(t) \end{pmatrix} - \begin{pmatrix} \mathbf{C}_1^T \\ \mathbf{F}_1^T \end{pmatrix} \widehat{\mathbf{z}}_1(t), \quad (72a)$$

$$\widetilde{\mathbf{q}}_1(t) = \mathbf{K}_1^T \widetilde{\boldsymbol{\lambda}}_1(t) + \mathbf{L}_1^T \widetilde{\boldsymbol{\kappa}}_1(t) - \mathbf{D}_1^T \widehat{\mathbf{z}}_1(t), \quad (72b)$$

$$\begin{pmatrix} \widetilde{\mathbf{q}}_{\lambda,\Gamma}(t) \\ \widetilde{\mathbf{q}}_{\kappa,\Gamma}(t) \end{pmatrix} = -\mathbf{S}_{1\Gamma}^T \begin{pmatrix} \widetilde{\boldsymbol{\lambda}}_1(t) \\ \widetilde{\boldsymbol{\kappa}}_1(t) \end{pmatrix} - \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_0^T \end{pmatrix} \widehat{\mathbf{z}}_1(t), \quad (72c)$$

$$\mathbf{M}_1 \widetilde{\boldsymbol{\lambda}}_1(T) = \boldsymbol{\lambda}_1^{(T)}, \quad (72d)$$

$$\mathbf{F}_1^T \widehat{\mathbf{z}}_1(T) = -\mathbf{B}_{11} \mathbf{M}_1^{-1} \boldsymbol{\lambda}_1^{(T)} - \mathbf{B}_{1\Gamma} \mathbf{M}_\Gamma(\theta)^{-1} \boldsymbol{\lambda}_\Gamma^{(T)}(\theta). \quad (72e)$$

Note that due to $\mathbf{F}_1 = \mathbf{0}$ the compatibility condition (42c) implies the compatibility condition (72e).

Moreover, since the second row block in $\mathbf{S}_{1\Gamma}^T$ is zero (cf. (31) and (34c)) and $\mathbf{F}_0 = \mathbf{0}$, we have

$$\widetilde{\mathbf{q}}_{\kappa,\Gamma}(t) \equiv 0. \quad (73)$$

The inputs for (72) and the reduced system (54) are the same and we can apply the balanced truncation error bound (26) to this subsystem. The balanced truncation error bound for this subsystem is

$$\left\| \begin{pmatrix} \widetilde{\mathbf{q}}_1 - \widehat{\mathbf{q}}_1 \\ \widetilde{\mathbf{q}}_{\lambda,\Gamma} - \widehat{\mathbf{q}}_{\lambda,\Gamma} \\ \widetilde{\mathbf{q}}_{\kappa,\Gamma} - \widehat{\mathbf{q}}_{\kappa,\Gamma} \end{pmatrix} \right\|_{L^2} \leq 2(\sigma_{k+1} + \cdots + \sigma_n) \left\| \begin{pmatrix} \widehat{\mathbf{z}}_1 \\ \widehat{\boldsymbol{\lambda}}_\Gamma \\ \widehat{\boldsymbol{\kappa}}_0 \end{pmatrix} \right\|_{L^2}. \quad (74)$$

We set $\mathbf{e}_\lambda = (\boldsymbol{\lambda}_1 - \widetilde{\boldsymbol{\lambda}}_1, \boldsymbol{\lambda}_2 - \widehat{\boldsymbol{\lambda}}_2, \boldsymbol{\lambda}_\Gamma - \widehat{\boldsymbol{\lambda}}_\Gamma)^T$ and $\mathbf{e}_\kappa = (\boldsymbol{\kappa}_1 - \widetilde{\boldsymbol{\kappa}}_1, \boldsymbol{\kappa}_2 - \widehat{\boldsymbol{\kappa}}_2, \boldsymbol{\kappa}_0 - \widehat{\boldsymbol{\kappa}}_0)^T$. Observing (42),(44),(46), (55) as well as (72),(57),(59), (73) it follows that

$$-\mathbf{E}_1 \frac{d}{dt} \begin{pmatrix} \mathbf{e}_\lambda(t) \\ \mathbf{e}_\kappa(t) \end{pmatrix} = -\mathbf{S}(\theta) \begin{pmatrix} \mathbf{e}_\lambda(t) \\ \mathbf{e}_\kappa(t) \end{pmatrix} + \begin{pmatrix} \mathbf{g}_1(t) \\ \mathbf{g}_2(t) \end{pmatrix}, \quad t \in (0, T], \quad (75a)$$

$$\mathbf{M}(\theta) \mathbf{e}_\lambda(T) = \mathbf{0}, \quad (75b)$$

where

$$\mathbf{g}_1(t) = \begin{pmatrix} -\mathbf{C}_1^T(\mathbf{z}_1 - \widehat{\mathbf{z}}_1) \\ -\nabla_{\mathbf{v}_2} \ell(\mathbf{x}_2, \mathbf{x}_\Gamma, t, \theta) + \nabla_{\widehat{\mathbf{v}}_2} \ell(\widehat{\mathbf{x}}_2, \widehat{\mathbf{x}}_\Gamma, t, \theta) \\ \widetilde{\mathbf{q}}_{\lambda, \Gamma} - \widehat{\mathbf{q}}_{\lambda, \Gamma} - \nabla_{\mathbf{v}_\Gamma} \ell(\mathbf{x}_2, \mathbf{x}_\Gamma, t, \theta) + \nabla_{\widehat{\mathbf{v}}_\Gamma} \ell(\widehat{\mathbf{x}}_2, \widehat{\mathbf{x}}_\Gamma, t, \theta) \end{pmatrix},$$

$$\mathbf{g}_2(t) = \begin{pmatrix} -\mathbf{F}_1^T(\mathbf{z}_1 - \widehat{\mathbf{z}}_1) \\ \mathbf{0} \\ -\mathbf{F}_0^T(\mathbf{z}_1 - \widehat{\mathbf{z}}_1) \end{pmatrix}.$$

Applying Theorem 2.1 to (75) and assumption (\mathbf{A}_3) we obtain

$$\begin{aligned} \left\| \begin{pmatrix} \lambda_1 - \widetilde{\lambda}_1 \\ \lambda_2 - \widetilde{\lambda}_2 \\ \lambda_\Gamma - \widetilde{\lambda}_\Gamma \end{pmatrix} \right\|_{L^2} &\leq C \left(\|\mathbf{z}_1 - \widehat{\mathbf{z}}_1\|_{L^2} + \left\| \begin{pmatrix} \widetilde{\mathbf{q}}_{\lambda, \Gamma} - \widehat{\mathbf{q}}_{\lambda, \Gamma} \\ \widetilde{\mathbf{q}}_{\kappa, \Gamma} - \widehat{\mathbf{q}}_{\kappa, \Gamma} \end{pmatrix} \right\|_{L^2} \right. \\ &\quad \left. + \left\| \begin{pmatrix} \mathbf{v}_2 - \widehat{\mathbf{v}}_2 \\ \mathbf{v}_\Gamma - \widehat{\mathbf{v}}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \mathbf{p}_2 - \widehat{\mathbf{p}}_2 \\ \mathbf{p}_0 - \widehat{\mathbf{p}}_0 \end{pmatrix} \right\|_{L^2} \right). \end{aligned} \quad (76)$$

Inequality (71a) follows using (74), (76) and Lemma 6.1.

Application of Theorem 2.1 to (75) and using Assumption (\mathbf{A}_3) also yields

$$\begin{aligned} \left\| \begin{pmatrix} \kappa_1 - \widetilde{\kappa}_1 \\ \kappa_2 - \widetilde{\kappa}_2 \\ \kappa_0 - \widetilde{\kappa}_0 \end{pmatrix} \right\|_{L^2} &\leq C_1 \left(\|\mathbf{z}_1 - \widehat{\mathbf{z}}_1\|_{L^2} + \left\| \begin{pmatrix} \widetilde{\mathbf{q}}_{\lambda, \Gamma} - \widehat{\mathbf{q}}_{\lambda, \Gamma} \\ \widetilde{\mathbf{q}}_{\kappa, \Gamma} - \widehat{\mathbf{q}}_{\kappa, \Gamma} \end{pmatrix} \right\|_{L^2} \right. \\ &\quad \left. + \left\| \begin{pmatrix} \mathbf{v}_2 - \widehat{\mathbf{v}}_2 \\ \mathbf{v}_\Gamma - \widehat{\mathbf{v}}_\Gamma \end{pmatrix} \right\|_{L^2} + \left\| \begin{pmatrix} \mathbf{p}_2 - \widehat{\mathbf{p}}_2 \\ \mathbf{p}_0 - \widehat{\mathbf{p}}_0 \end{pmatrix} \right\|_{L^2} \right) \\ &\quad + C_2 \left(\left\| \frac{d}{dt} \mathbf{F}_1^T(\mathbf{z}_1 - \widehat{\mathbf{z}}_1) \right\|_{L^2} + \left\| \frac{d}{dt} \mathbf{F}_0^T(\mathbf{z}_1 - \widehat{\mathbf{z}}_1) \right\|_{L^2} \right). \end{aligned} \quad (77)$$

Since $\mathbf{F}_1 = \mathbf{0}$ and $\mathbf{F}_0 = \mathbf{0}$, inequality (71b) follows using (74), (77) and Lemma 6.1. \blacksquare

The preceding two lemmas lead to the following bound for the gradients of the objective functions for the full order and the reduced order problem.

THEOREM 6.3 *If $(\mathbf{A}_1) - (\mathbf{A}_4)$ are valid, then*

$$\|\nabla J(\theta) - \nabla \widehat{J}(\theta)\| \leq C \left(\sigma_{k+1} + \cdots + \sigma_n \right),$$

Proof The gradients $\nabla J(\theta)$ and $\nabla \widehat{J}(\theta)$ applied to an arbitrary $\widetilde{\theta}$ are given by

$$\begin{aligned} \nabla J(\theta)^T \widetilde{\theta} &= \int_0^T \nabla_\theta \ell(\mathbf{v}_2, \mathbf{p}_2, \mathbf{v}_\Gamma, \mathbf{p}_0, t, \theta)^T \widetilde{\theta} dt \\ &\quad + \int_0^T \begin{pmatrix} \boldsymbol{\mu}_2(t) \\ \boldsymbol{\lambda}_\Gamma(t) \end{pmatrix}^T \left(\begin{pmatrix} (D_\theta \mathbf{P}_2(\theta) \widetilde{\theta}) \mathbf{x}_2(t) - (D_\theta \mathbf{N}_2(\theta) \widetilde{\theta}) \mathbf{u}(t) \\ (D_\theta \mathbf{P}_\Gamma(\theta) \widetilde{\theta}) \mathbf{x}_\Gamma(t) - (D_\theta \mathbf{N}_\Gamma(\theta) \widetilde{\theta}) \mathbf{u}(t) \end{pmatrix} \right) dt, \end{aligned}$$

$$\begin{aligned} \nabla \widehat{J}(\theta)^T \widetilde{\theta} &= \int_0^T \nabla_{\theta} \ell(\widehat{\mathbf{v}}_2, \widehat{\mathbf{p}}_2, \widehat{\mathbf{v}}_{\Gamma}, \widehat{\mathbf{p}}_0, t, \theta)^T \widetilde{\theta} dt \\ &+ \int_0^T \begin{pmatrix} \widehat{\boldsymbol{\mu}}_2(t) \\ \widehat{\boldsymbol{\lambda}}_{\Gamma}(t) \end{pmatrix}^T \begin{pmatrix} (D_{\theta} \mathbf{P}_2(\theta) \widetilde{\theta}) \widehat{\mathbf{x}}_2(t) - (D_{\theta} \mathbf{N}_2(\theta) \widetilde{\theta}) \mathbf{u}(t) \\ (D_{\theta} \mathbf{P}_{\Gamma}(\theta) \widetilde{\theta}) \widehat{\mathbf{x}}_{\Gamma}(t) - (D_{\theta} \mathbf{N}_{\Gamma}(\theta) \widetilde{\theta}) \mathbf{u}(t) \end{pmatrix} dt. \end{aligned}$$

The estimate now follows from Lemmas 6.1 and 6.2 and Assumption **(A₃)**. \blacksquare

Under the convexity assumption (62) the bound (63) combined with Theorem 6.3 gives the desired bound for the error in the solutions computed using the full and the reduced order model.

COROLLARY 6.4 *If the assumptions of Theorem 6.3 hold and the convexity assumption (62) is valid, then there exists $C > 0$ such that*

$$\|\theta^* - \widehat{\theta}^*\| \leq C(\sigma_{k+1} + \cdots + \sigma_n).$$

7. Shape optimization of capillary barriers in microfluidic biochips

Surface acoustic wave driven microfluidic biochips are used in clinical diagnostics, pharmacology, and forensics for sequencing and hybridization in genomics, protein profiling in proteomics, and cell analysis in cytometry. The idea is to transport, for instance, DNA or proteins along a network of microchannels to a reservoir where a chemical analysis is carried out. The fluid flow is steered by piezoelectrically generated surface acoustic waves. The performance of these biochips can be significantly improved by an optimal design of the walls of the microchannels and the capillary barriers between the channels and the reservoirs. This amounts to the solution of a PDE constrained shape optimization problem, where the underlying PDEs represent a multiscale, multiphysics problem as given by the equations of piezoelectricity coupled with the compressible Navier-Stokes equations. The multiscale character of the induced fluid flow is taken care of by homogenization so that the resulting flow pattern, called acoustic streaming, can be described by Stokes flow. We refer to [3, 4, 6, 17] for details.

We consider Stokes flow in a network of microchannels and reservoirs on top of a microfluidic biochip with capillary barriers between the channels and the reservoirs that are designed to guarantee a precise filling of the reservoirs with the DNA or protein probes. The objective is twofold: Firstly, we want to design the walls of the barriers in such a way that a desired velocity profile \mathbf{v}^d is attained and secondly, we want to minimize the vorticity $\nabla \times \mathbf{v}$ in some specific part of the network.

The computational domain $\Omega \subset \mathbb{R}^2$ is displayed in Figure 1. It is decomposed into subdomains $\Omega_1 = \Omega \setminus \Omega_2$, and $\Omega_2 = \{1.5, 2.5\} \times \{9, 10\}$. The boundary $\partial\Omega$ is decomposed into $\Gamma_{\text{in}} = \{0\} \times (9, 10)$, $\Gamma_{\text{out}} = \{10\} \times (0, 1)$, and $\Gamma_{\text{lat}} = \partial\Omega \setminus (\Gamma_{\text{in}} \cup \Gamma_{\text{out}})$. The data of the problem is chosen as follows. Assume $\mathbf{f} = 0$ in $\Omega \times (0, T)$, a Poiseuille velocity profile $\mathbf{v}_{\text{in}}((x_1, x_2), t) = 4(x_2 - 9)(10 - x_2)(1 - \frac{0.8}{15}t)\sin(t)$ on $\Gamma_{\text{in}} \times (0, T)$, outflow boundary conditions on $\Gamma_{\text{out}} \times (0, T)$, and no-slip conditions on $\Gamma_{\text{lat}} \times (0, T)$. The objective is to design the shape of the top $\Gamma_{2,T}$ and the bottom $\Gamma_{2,B}$ of $\partial\Omega_2$ in such a way that a prescribed velocity profile \mathbf{v}^d is achieved in $\Omega_2 \times (0, T)$ and the vorticity is minimized in Ω_{obs} (four bulb shaped structures in Figure 1). We use a parametrization $\Omega_2(\theta)$ of Ω_2 by means of the Bézier control points $\theta \in \mathbb{R}^k$, $k = k_T + k_B$, of Bézier curve representations of $\Gamma_{2,T}$ and $\Gamma_{2,B}$, where

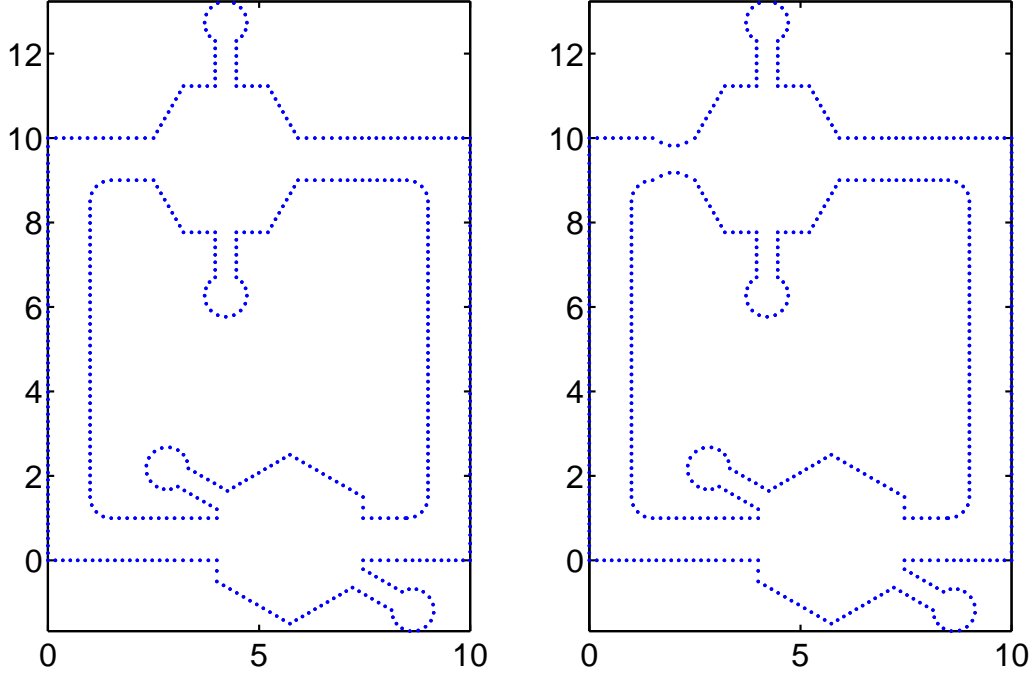


Figure 1. The reference domain Ω_{ref} (left) and the optimal domain (right).

k_T and k_B refer to the number of control points for $\Gamma_{2,T}$ and $\Gamma_{2,B}$, respectively. The shape optimization problem amounts to the minimization of

$$J(\theta) = \int_0^T \int_{\Omega_{\text{obs}}} |\nabla \times \mathbf{v}(x, t)|^2 dx dt + \int_0^T \int_{\Omega_2(\theta)} |\mathbf{v}(x, t) - \mathbf{v}^d(x, t)|^2 dx dt$$

subject to the Stokes equations

$$\begin{aligned} \mathbf{v}_t(x, t) - \mu \Delta \mathbf{v}(x, t) + \nabla p(x, t) &= \mathbf{f}(x, t), & \text{in } \Omega(\theta) \times (0, T), \\ \nabla \cdot \mathbf{v}(x, t) &= 0, & \text{in } \Omega(\theta) \times (0, T), \\ \mathbf{v}(x, t) &= \mathbf{v}_{\text{in}}(x, t) & \text{on } \Gamma_{\text{in}} \times (0, T), \\ \mathbf{v}(x, t) &= \mathbf{0} & \text{on } \Gamma_{\text{lat}} \times (0, T), \\ (\mu \nabla \mathbf{v}(x, t) - p(x, t) \mathbf{I}) \mathbf{n} &= 0 & \text{on } \Gamma_{\text{out}} \times (0, T), \\ \mathbf{v}(x, 0) &= \mathbf{0} & \text{in } \Omega(\theta). \end{aligned}$$

and design parameter constraints

$$\theta^{\min} \leq \theta \leq \theta^{\max},$$

where $\mu = 1/50$ and $T = 15$. The bounds $\theta^{\min}, \theta^{\max}$ on the design parameters are chosen such that the design constraints are never active in this example. We use $k_T = 6, k_B = 6$ Bézier control points to specify the top and the bottom boundary of the variable subdomain $\Omega_2(\theta)$ with the respective first and last control points being fixed. The desired velocity \mathbf{v}^d is computed by specifying the optimal parameter θ^* and solving the state equation on $\Omega(\theta^*)$. The optimal domain $\Omega(\theta^*)$ is shown in Figure 1.

We consider a geometrically conforming simplicial triangulation $\mathcal{T}_h(\Omega)$ of the

reference that aligns with the decomposition of Ω into the subdomains Ω_1 and Ω_2 as well as the respective boundaries. The discretization in space is taken care of by P2-P1 Taylor-Hood elements. For $D \subseteq \bar{\Omega}$, we denote by $\mathcal{N}_{\mathbf{v},h}(D), \mathcal{N}_p,h(D)$ the set of velocity and pressure nodal points in D . We use the domain decomposition methodology as before and set $N_{\mathbf{v},dof}^{(\nu)} = \text{card}(\mathcal{N}_{\mathbf{v},h}(\bar{\Omega}_\nu \setminus \Gamma_{I,\mathbf{v}}))$, $\nu = 1, 2$, and $N_{dof}^{\Gamma_{I,\mathbf{v}}} := \text{card}(\mathcal{N}_{\mathbf{v},h}(\Gamma_{I,\mathbf{v}}))$ so that $N_{\mathbf{v},dof} = N_{\mathbf{v},dof}^{(1)} + N_{\mathbf{v},dof}^{(2)} + N_{\mathbf{v},dof}^{\Gamma_{I,\mathbf{v}}}$ is the total number of velocity degrees of freedom. Similarly, $N_{p,dof} = N_{p,dof}^{(1)} + N_{p,dof}^{(2)}$ is the total number of pressure degrees of freedom.

We use automatic differentiation [19, 33] to compute the derivatives with respect to the design variables θ . The semi-discretized optimization problems are solved using a projected BFGS method with Armijo line search [23]. The optimization algorithm is terminated when the norm of projected gradient is less than $\epsilon = 10^{-4}$. The results in Figure 1(right) and Figure 2-4 and Table 2 were generated using the finest grid i.e., grid 4 with $N_{\mathbf{v},dof} = 16806$. We will explain them as we go along.

We use the multishift ADI method [21] to solve the projected Lyapunov equations. We use four shifts in the ADI method which were computed as in [21]. Figure 2 shows the largest Hankel singular values. For the model reduction, we select those Hankel singular values σ_j , with $\sigma_j \geq 10^{-3}\sigma_1$. The threshold $10^{-3}\sigma_1$ is indicated by the solid line in Figure 2 (left). In this case only twenty-nine Hankel singular values and corresponding singular vectors determine the reduced order model for the velocities in Ω_1 .

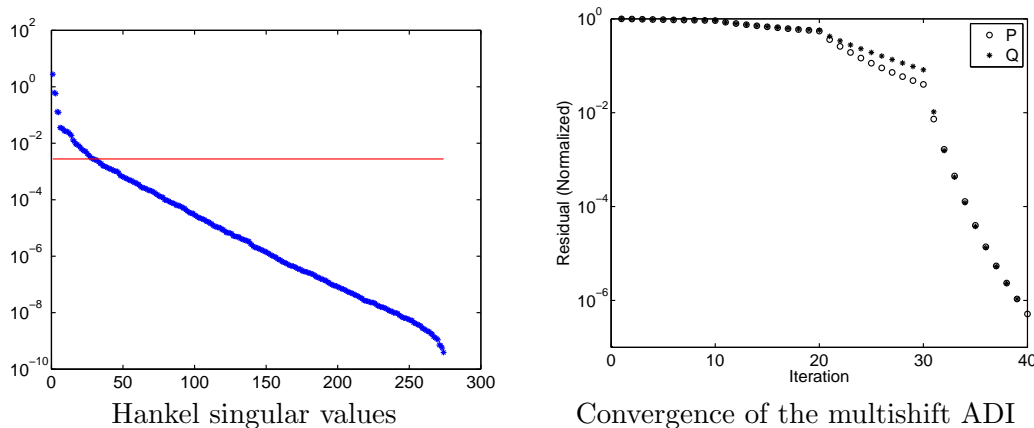


Figure 2. The left plot shows the largest Hankel singular values and the threshold $10^{-3}\sigma_1$. The right plot shows normalized residuals [21] generated by the multishift ADI for the approximate solution of the controllability Lyapunov equation (\circ) and of the observability Lyapunov equation ($*$)

In order to test our model reduction routine we compare full and the reduced order semidiscretized integrand

$$\ell(\theta_0, t) = \int_{\Omega_{\text{obs}}} |\nabla \times \mathbf{v}(x, t)|^2 dx + \int_{\Omega_2(\theta_0)} |\mathbf{v}(x, t) - \mathbf{v}^d(x, t)|^2 dx$$

as a function of time t for the initial value of the design parameter θ_0 . Note $J(\theta) = \int_0^T \ell(\theta) dt$. Figure 3 displays the results obtained. The full and reduced order models are both in excellent agreement, which is expected given the theoretical a priori error bound for the balanced truncation model reduction.

Table 1 displays the sizes of the reduced and the full order problems (in Degrees of Freedom (DoF)) for an initial coarse grid and three levels of refinement. We

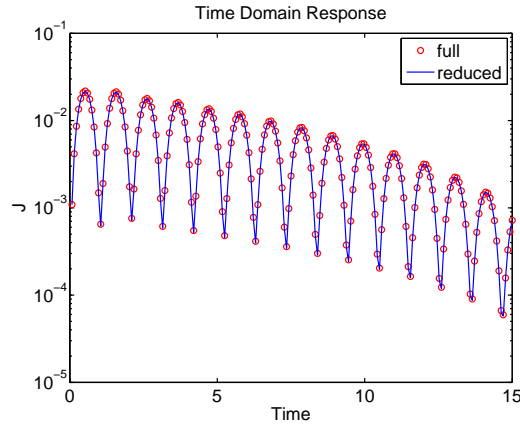


Figure 3. Time response for the full (circle) and the reduced (solid line) integrand $\ell(\theta_0)$ for the initial configuration (= reference domain) Figure 1(left).

observe that the size of the reduced order model is nearly independent of the grid size.

grid number	m	$N_{\mathbf{v},dof}^{(1)}$	$N_{\hat{\mathbf{v}},dof}^{(1)}$	$N_{\mathbf{v},dof}$	$N_{\hat{\mathbf{v}},dof}$
1	149	4752	23	4862	133
2	313	7410	25	7568	183
3	361	11474	26	11700	252
4	537	16472	29	16806	363

Table 1. The number m of observations in Ω_1 , the numbers $N_{\mathbf{v},dof}^{(1)}, N_{\hat{\mathbf{v}},dof}^{(1)}$ of velocity DoF in Ω_1 (full and reduced order), and the numbers $N_{\mathbf{v},dof}, N_{\hat{\mathbf{v}},dof}$ of velocity DoF in Ω (full and reduced order) for four discretizations.

The optimal shape parameters θ^* and $\hat{\theta}^*$ computed by minimizing the full and the reduced order model, respectively, are shown in Table 2. For the finest grid problem, the error between full and the reduced order model solutions is $\|\theta^* - \hat{\theta}^*\|_2 = 8.0751 \cdot 10^{-3}$.

θ^*	(9.8987, 9.7510, 9.7496, 9.8994, 9.0991, 9.2499, 9.2504, 9.0989)
$\hat{\theta}^*$	(9.9026, 9.7498, 9.7484, 9.9021, 9.0940, 9.2514, 9.2511, 9.0956)

Table 2. Optimal shape parameters θ^* and $\hat{\theta}^*$ (rounded to 5 digits) computed by minimizing the full and the reduced order model

The convergence histories of the projected BFGS algorithm applied to the full and the reduced order problems are shown in Figure 4. Except for the final iterations, the convergence behavior of the optimization algorithm applied to the full and the reduced order problems is nearly identical.

All the computations were performed in Matlab version 7.7.0.471 (R2008b) on a machine with 2.66 GHz Intel(R) Core(TM)2 Duo processor running Linux OS Fedora 8.

8. Conclusions

We have integrated domain decomposition and balanced truncation model reduction for the numerical solution of a class of shape optimization problems governed

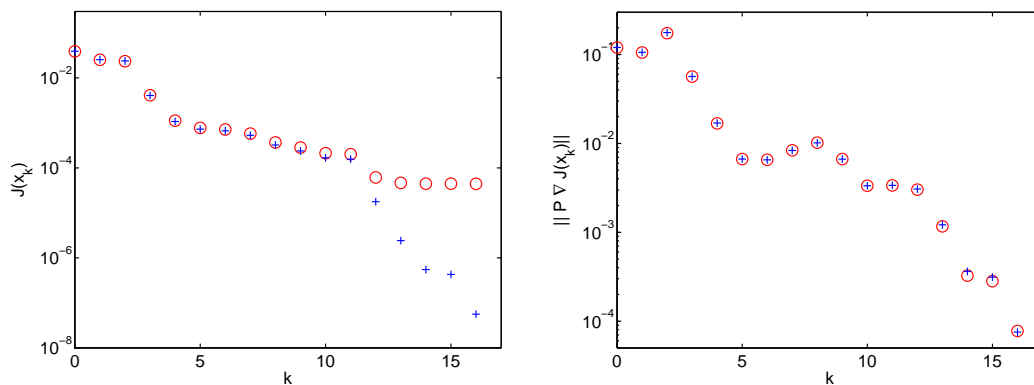


Figure 4. The convergence histories of the projected BFGS algorithm applied to the full and the reduced order problems. The left figure shows the convergence history of the objective functionals for the full (+) and reduced (o) order model. The right figure shows the convergence history of the projected gradients for the full (+) and reduced (o) order model.

by the Stokes equations. This approach can be applied when only small part of the overall domain can be modified by the optimization. Our approach leads to a reduced optimization problem with the same structure as the original one, but of potentially much smaller dimension. We have derived an estimate for the error between the solution of the original optimization problem and the solution of the reduced problem. The estimate is largely determined by the balanced truncation error estimate. The approach can be easily extended to shape optimization problems governed by the Oseen equations or the linearized Navier-Stokes equations, linearized around suitable steady flows.

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