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Goal-oriented model adaptivity for viscous incompressible flows

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Abstract In van Opstal et al. (Comput Mech 50:779–788, 2012) airbag inflation simulations were performed where the flow was approximated by Stokes flow. Inside the intricately folded initial geometry the Stokes assumption is argued to hold. This linearity assumption leads to a boundary-integral representation, the key to bypassing mesh generation and remeshing. It therefore enables very large displacements with near-contact. However, such a coarse assumption cannot hold throughout the domain, where it breaks down one needs to revert to the original model. The present work formalizes this idea. A model adaptive approach is proposed, in which the coarse model (a Stokes boundary-integral equation) is locally replaced by the original high-fidelity model (Navier–Stokes) based on a-posteriori estimates of the error in a quantity of interest. This adaptive modeling framework aims at taking away the burden and heuristics of manually partitioning the domain while providing new insight into the physics. We elucidate how challenges pertaining to model disparity can be addressed. Essentially, the solution in the interior of the

coarse model domain is reconstructed as a post-processing step. We furthermore present a two-dimensional numerical experiments to show that the error estimator is reliable.

Keywords Finite element · Boundary element · Adaptivity

1 Introduction

In many applications, a mathematical model that adequately describes the physical processes involved is unfortunately intractable with respect to current computer resources or discretization techniques. The idea is then to replace this fine model by a simpler model, also referred to as the coarse model, in some subregions of the computational domain where it is deemed sufficient. Approximations by means of a surrogate model based on the coupling of multiple models using a domain decomposition-type approach is already quite well established and desirable for several reasons: (1) in the case where the fine model is nonlinear, it may be advantageous to replace it by a linear model to avoid using an iterative solver [11]; (2) in the case that the coarse model can be equivalently recast into a boundary integral formulation, the dimension of the computational domain can simply be reduced by one [5, 32]; (3) finally, in the case of multiscale simulations, one may selectively reduce the number of degrees of freedom by considering a coarse-scale model instead of the full fine-scale model [2, 21].

Our ultimate interest lies in the analysis of inflatable structures such as airbags. Robust mesh generation and simulation of a realistic stowed configuration is very challenging due to the complex geometry. A rational, a priori partitioning of the domain, e.g. to control the error incurred by local application of the coarse model, is generally non-trivial. In order to treat this class of problems and circumvent associated

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issues, two-scale models were developed in [19,29,30] by approximating the complex flow problem with a linearized boundary integral formulation. The approximations required to enable application of the boundary-integral formulation are not applicable in the inflated part of the domain and should therefore only be used on a subdomain. The coarse model (which plays the role of a sub-grid scale model in the geometrically complex subdomain) can however be coupled to the base fluid model defined on the rest of the domain. To explore model-adaptivity based on a posteriori error estimates in this context, we focus on a simpler model problem that avoids auxiliary complications such as moving domains [28] and time-dependence.

A natural question that arises when using an approximate model on a subdomain is: Which partitioning is optimal? i.e., which partitioning yields a sufficiently accurate solution at minimal cost? To define what is actually meant by an accurate solution, one needs to define a measure for accuracy: In many cases, a user has a very restricted interest in the solution, which can be formulated as a functional of the solution, the *goal functional*. In terms of the error in the goal functional, we want to assess the modeling error that arises from using an approximate model on a certain subdomain. Also, we would like to know how to choose this subdomain in an optimal way. Goal-oriented model adaptivity [3,17,24] provides a tractable framework in which such questions can be addressed. This framework has been applied to, e.g. heterogeneous materials [18], flow problems [22], atomistic-to-continuum problems [2], free-surface flows [20], turbulence modeling [13] and flows in arteries or rivers [9].

In this work we use a domain decomposition approach, with a Stokes boundary integral equation and the Navier–Stokes equations in weak form governing complementary parts of the domain. Furthermore the error in terms of a goal functional with respect to a full Navier–Stokes flow is investigated. This work can be conceived of as an extension of earlier work on domain decomposition for incompressible flow, cf. [10,11], and coupling of boundary integral and partial differential equations, eg. [5], to model adaptivity.

This paper is organized as follows. In Sect. 2, a monolithic formulation for the multiphysics problem is presented. A posteriori estimation of the modeling error and an adaptive strategy are presented in Sect. 3. In Sect. 4, first, in Sect. 4.1, the discretization and adaptive algorithm are detailed; then, in Sect. 4.2, the numerical results are presented. We conclude with a discussion in Sect. 5.

2 A sharp interface multi-model problem

Consider a bounded, open domain $\Omega \subset \mathbb{R}^2$ with Lipschitz boundary, partitioned into two open subdomains Ω^N and Ω^S as shown in Fig. 1. We will often use the index $m \in \{N, S\}$

Fig. 1 Schematic of domain-decomposition approach for model adaptivity

to refer to the Navier–Stokes and Stokes models, respectively. We assume a partitioning of the domain such that $\overline{\Omega^N} \cup \overline{\Omega^S} = \overline{\Omega}$, $\Omega^N \cap \Omega^S = \emptyset$ and such that Ω^m are also Lipschitz domains, so that we can define Sobolev spaces and their traces on them, as well as their outward unit normals $\mathbf{n}^m$ (almost everywhere). The boundary $\partial\Omega$ is partitioned into $\partial\Omega_D$ and $\partial\Omega_N$, along which Dirichlet ($\mathbf{g}$) and Neumann ($\mathbf{h}$) data are prescribed. For simplicity we assume $\partial\Omega_N \cap \partial\Omega^S$ to be empty, although the approach can be extended. In this section we consider the partitioning, and hence the interface between these subdomains, $\Sigma := \partial\Omega^N \cap \partial\Omega^S$, to be pre-defined. Consider the steady incompressible Navier–Stokes equations on Ω^N in strong form

$$\mathbf{u}^N \cdot \nabla \mathbf{u}^N - \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}^N, p^N) = \mathbf{0} \quad \text{in } \Omega^N, \quad (1a)$$

$$\nabla \cdot \mathbf{u}^N = 0 \quad \text{in } \Omega^N, \quad (1b)$$

$$\mathbf{u}^N = \mathbf{g} \quad \text{on } \partial\Omega_D \cap \partial\Omega^N, \quad (1c)$$

$$\boldsymbol{\sigma}(\mathbf{u}^N, p^N) \cdot \mathbf{n}^N = \mathbf{h} \quad \text{on } \partial\Omega_N \cap \partial\Omega^N; \quad (1d)$$

and the Stokes equations on Ω^S

$$-\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}^S, p^S) = \mathbf{0} \quad \text{in } \Omega^S, \quad (2a)$$

$$\nabla \cdot \mathbf{u}^S = 0 \quad \text{in } \Omega^S, \quad (2b)$$

$$\mathbf{u}^S = \mathbf{g} \quad \text{on } \partial\Omega_D \cap \partial\Omega^S; \quad (2c)$$

and suitable transmission conditions on the interface:

$$\mathbf{u}^S = \mathbf{u}^N \quad \text{on } \Sigma, \quad (3a)$$

$$\mathbf{t}^S + \mathbf{t}^N = \mathbf{0} \quad \text{on } \Sigma. \quad (3b)$$

with $\mathbf{t}^m := \boldsymbol{\sigma}(\mathbf{u}^m, p^m) \mathbf{n}^m$ the traction acting on the body Ω^m . We define the global fields $\mathbf{u}$ and p as

$$\mathbf{u} := \begin{cases} \mathbf{u}^N, & \text{in } \Omega^N \\ \mathbf{u}^S, & \text{in } \Omega^S \end{cases}, \quad p := \begin{cases} p^N, & \text{in } \Omega^N \\ p^S, & \text{in } \Omega^S \end{cases}, \quad (4)$$

where we leave the definition of $(\mathbf{u}, p)$ on Σ undefined for now. The fluid is Newtonian, i.e., $\sigma_{ij}(\mathbf{u}, p) := -p\delta_{ij} + (u_{i,j} + u_{j,i})/\text{Re}$, with Re the Reynolds number. We derive

a formulation based on [10]. To this end we introduce some notation and define test and trial spaces. The usual Hilbert Sobolev space with index k is denoted $H^k(\Omega)$. Its associated inner product and derived norm are denoted by $(\cdot, \cdot)_{k,\Omega}$ and $\|\cdot\|_{k,\Omega}$, respectively. We identify $H^0(\Omega)$ as $L^2(\Omega)$. We denote by

$$\gamma^{\partial\Omega} : H^1(\Omega) \rightarrow H^{1/2}(\partial\Omega) : \gamma^{\partial\Omega}(\mathbf{u}) = \mathbf{u} \quad \text{on } \partial\Omega \quad (5)$$

(in the distributional sense) the standard *trace operator*, and by $\ell^{\partial\Omega} : H^{1/2}(\partial\Omega) \rightarrow H^1(\Omega)$ a suitable right inverse, referred to as the *lifting operator*. Both exist, and are linear and bounded, see [15]. We have introduced $H^{1/2}(\partial\Omega)$ to denote the image of the trace operator. We denote the space of bounded linear functionals on $H^{1/2}(\partial\Omega)$ by $H^{-1/2}(\partial\Omega)$. The space $H^{1/2}(\omega)$, with $\omega \subset \partial\Omega$, is the restriction of functions in $H^{1/2}(\partial\Omega)$ to ω . In particular, we have, cf. e.g. [23],

$$H_{00}^{1/2}(\Sigma) := \{\mathbf{u} \in H^{1/2}(\Sigma) : \text{the zero extension of } \mathbf{u} \text{ to all of } \partial\Omega \text{ is in } H^{1/2}(\partial\Omega)\}. \quad (6)$$

The space $H^{-1/2}(\omega)$ is then defined as the dual space of $H_{00}^{1/2}(\omega)$, and the duality pairing between them is denoted by $\langle \cdot, \cdot \rangle_{-1/2,\omega}$.

The velocity $\mathbf{u}^N$ resides in $\ell^{\partial\Omega_D}(\mathbf{g}) + V$, with

$$V := \{\mathbf{v} \in H^1(\Omega^N) : \mathbf{v} = \mathbf{0} \text{ on } \partial\Omega_D \cap \partial\Omega^N\}, \quad (7)$$

equipped with the norm $\|\cdot\|_{1,\Omega^N}$. The pressure resides in the space

$$Q := \left\{ p \in L^2(\Omega^N) : \int_{\Omega^N} p = 0 \right\} \quad (8)$$

equipped with the usual L^2 -norm $\|\cdot\|_{0,\Omega^N}$. We multiply Eq. (1) by test functions $\mathbf{v} \in V$ and $q \in Q$ and integrate by parts to obtain:

$$\begin{aligned} & (\mathbf{u} \cdot \nabla \mathbf{u}, \mathbf{v})_{0,\Omega^N} + \text{Re}^{-1}(\nabla \mathbf{u}, \nabla \mathbf{v})_{0,\Omega^N} - (p, \nabla \cdot \mathbf{v})_{0,\Omega^N} \\ & - (q, \nabla \cdot \mathbf{u})_{0,\Omega^N} = \text{Re}^{-1}(\mathbf{n} \cdot \nabla \mathbf{u}, \mathbf{v})_{0,\partial\Omega^N} - (p\mathbf{n}, \mathbf{v})_{0,\partial\Omega^N}. \end{aligned}$$

On Ω^S , we solve a boundary integral equation equivalent to (2), which engenders a map between the Dirichlet $\gamma^{\partial\Omega^S} \mathbf{u}^S$ and Neumann $\mathbf{t}^S$ data. The traction $\mathbf{t}^S$ resides in $T := H^{-1/2}(\partial\Omega^S)$. The normal component of $\mathbf{t}^S$, which is in the kernel of the single-layer boundary integral operator, is constrained by a Lagrange multiplier as in [30]. Testing the boundary integral equation and its constraint against arbitrary $\boldsymbol{\psi}$ and μ , we arrive at

$$\begin{aligned} & \langle \boldsymbol{\psi}, \mathbf{V} \mathbf{t}^S \rangle_{-1/2,\partial\Omega^S} + \mu \langle \mathbf{t}^S, \mathbf{n}^S \rangle_{-1/2,\partial\Omega^S} + \lambda \langle \boldsymbol{\psi}, \mathbf{n}^S \rangle_{-1/2,\partial\Omega^S} \\ & = \langle \boldsymbol{\psi}, \gamma^{\partial\Omega^S} \mathbf{u}^S/2 + \mathbf{K} \gamma^{\partial\Omega^S} \mathbf{u}^S \rangle_{-1/2,\partial\Omega^S}, \end{aligned}$$

with boundary integral operators

$$\begin{aligned} \mathbf{V} \boldsymbol{\psi} &:= \frac{1}{4\pi \text{Re}} \oint_{\partial\Omega^S} \left(\boldsymbol{\psi}(\mathbf{y}) \log \frac{1}{r} + \frac{\mathbf{x} - \mathbf{y}}{r^2} (\mathbf{x} - \mathbf{y}) \cdot \boldsymbol{\psi}(\mathbf{y}) \right) d\mathbf{y} \\ \mathbf{K} \boldsymbol{\phi} &:= \frac{3}{4\pi} \oint_{\partial\Omega^S} \frac{\mathbf{x} - \mathbf{y}}{r^4} (\mathbf{x} - \mathbf{y}) \cdot \boldsymbol{\phi}(\mathbf{y}) (\mathbf{x} - \mathbf{y}) \cdot \mathbf{n}(\mathbf{y}) d\mathbf{y} \end{aligned}$$

cf. e.g. [14,26].

Inserting boundary and transmission conditions and introducing the bi- and trilinear forms

$$a(\mathbf{u}, \mathbf{v}) := \text{Re}^{-1}(\nabla \mathbf{u}, \nabla \mathbf{v})_{0,\Omega^N}, \quad (9a)$$

$$b(\mathbf{u}, p) := -(\nabla \cdot \mathbf{u}, p)_{0,\Omega^N}, \quad (9b)$$

$$c(\mathbf{u}, \mathbf{v}, \mathbf{w}) := (\mathbf{u} \cdot \nabla \mathbf{v}, \mathbf{w})_{0,\Omega^N}, \quad (9c)$$

$$d(\mathbf{t}, \boldsymbol{\psi}) := \langle \boldsymbol{\psi}, \mathbf{V} \mathbf{t} \rangle_{-1/2,\partial\Omega^S}, \quad (9d)$$

$$e_\omega(\mathbf{u}, \boldsymbol{\psi}) := \langle \boldsymbol{\psi}, \gamma^\omega \mathbf{u}/2 + \mathbf{K} \gamma^\omega \mathbf{u} \rangle_{-1/2,\omega}, \quad (9e)$$

$$f(\mu, \boldsymbol{\psi}) := \mu \langle \boldsymbol{\psi}, \mathbf{n}^S \rangle_{-1/2,\partial\Omega^S}, \quad (9f)$$

we arrive at the following weak formulation of the coupled Stokes/Navier–Stokes system:

Given $\mathbf{g} \in H^{1/2}(\partial\Omega_D)$ and $\mathbf{h} \in H^{-1/2}(\partial\Omega_N)$, find $(\mathbf{u}^N, p^N, \mathbf{t}^S, \lambda) \in (\ell^{\partial\Omega}(\mathbf{g}) + V) \times Q \times T \times \mathbb{R}$ such that:

$$\begin{aligned} & c(\mathbf{u}, \mathbf{u}, \mathbf{v}) + a(\mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) + b(\mathbf{u}, q) + d(\boldsymbol{\psi}, \mathbf{t}^S) \\ & - e_\Sigma(\boldsymbol{\psi}, \gamma^\Sigma \mathbf{u}^N) + f(\mu, \mathbf{t}^S) + f(\lambda, \boldsymbol{\psi}) \\ & = e_{\partial\Omega^S \cap \partial\Omega_D}(\boldsymbol{\psi}, \mathbf{g}) \\ & + (\mathbf{h}, \mathbf{v})_{0,\partial\Omega_N} \quad \forall (\mathbf{v}, q, \boldsymbol{\psi}, \mu) \in V \times Q \times T \times \mathbb{R}. \end{aligned} \quad (10)$$

We introduce the condensed notation

$$\mathcal{T} := \{\mathbf{g}, \mathbf{h}\} \text{ as in (10)}$$

$$\begin{aligned} N((\mathbf{u}, p, \mathbf{t}, \lambda); (\mathbf{v}, q, \boldsymbol{\psi}, \mu)) &:= c^N(\mathbf{u}, \mathbf{u}, \mathbf{v}) + a(\mathbf{u}, \mathbf{v}) \\ &+ b(\mathbf{v}, p) + b(\mathbf{u}, q) + d(\boldsymbol{\psi}, \mathbf{t}) - e_\Sigma(\boldsymbol{\psi}, \gamma^\Sigma \mathbf{u}) \\ &+ f(\mu, \mathbf{t}^S) + f(\lambda, \boldsymbol{\psi}) \end{aligned}$$

$$F((\mathbf{v}, q, \boldsymbol{\psi}, \mu)) := (\mathbf{h}, \mathbf{v})_{0,\partial\Omega_N} + e_{\partial\Omega^S \cap \partial\Omega_D}(\boldsymbol{\psi}, \mathbf{g})$$

such that (10) is equivalent to

Given $\mathcal{T}$, find $(\mathbf{u}^N, p^N, \mathbf{t}^S, \lambda) \in V \times Q \times T \times \mathbb{R}$ such that:

$$\begin{aligned} N((\mathbf{u}^N, p^N, \mathbf{t}^S, \lambda); (\mathbf{v}, q, \boldsymbol{\psi}, \mu)) &= F((\mathbf{v}, q, \boldsymbol{\psi}, \mu)) \\ \forall (\mathbf{v}, q, \boldsymbol{\psi}, \mu) &\in V \times Q \times T \times \mathbb{R}. \end{aligned} \quad (11)$$

To evaluate residuals of the base model in the interior of Ω^S , a reconstruction is required, based on the data $(\gamma^{\partial\Omega^S} \mathbf{u}^S, \mathbf{t}^S)$. This is furnished by the representation formulae, cf. e.g. [26]:

$$\mathbf{u}^S := \mathbf{V} \mathbf{t}^S - \mathbf{K} \gamma^{\partial\Omega^S} \mathbf{u}^S, \quad (12a)$$

$$p^S := \mathbf{V}^p \mathbf{t}^S + 2\mathbf{K}^p \gamma^{\partial\Omega^S} \mathbf{u}^S \quad (12b)$$

with operators

$$\begin{aligned} \mathbf{V}^p \boldsymbol{\psi} &:= \frac{1}{2\pi \operatorname{Re}} \oint_{\partial\Omega^S} \frac{(\mathbf{x} - \mathbf{y}) \cdot \boldsymbol{\psi}(\mathbf{y})}{r^2} d\mathbf{y} \\ \mathbf{K}^p \boldsymbol{\phi} &:= \frac{1}{2\pi} \oint_{\partial\Omega^S} \left(\frac{-\mathbf{n}(\mathbf{y}) \cdot \boldsymbol{\phi}(\mathbf{y})}{r^2} + 2(\mathbf{x} - \mathbf{y}) \right. \\ &\quad \left. \cdot \mathbf{n}(\mathbf{y}) \frac{(\mathbf{x} - \mathbf{y}) \cdot \boldsymbol{\phi}(\mathbf{y})}{r^4} \right) d\mathbf{y}. \end{aligned}$$

3 A posteriori error estimation and adaptivity

In this section, we shall consider that one is not necessarily interested in the full solution $(\mathbf{u}, p)$ of the base model, but rather in some (differentiable) functional $J((\mathbf{u}, p))$, the *goal quantity*. This functional should, of course, also be evaluated at the solution $(\mathbf{u}^N, p^N, \mathbf{t}^S, \lambda)$ of the surrogate problem (11), made possible through (4) and (12). In this discussion, it is assumed that the subdomain associated with J is a subset of Ω^N , in order to avoid introducing terms and test functions on the interior of the BEM subdomain in the so-called dual problem (17). The generalization to arbitrary decompositions Σ and appropriate linearizations of J , is left as future work. Examples of possible goal quantities are:

1. The vorticity in subregion $\omega \subset \Omega$:

$$J((\mathbf{u}, p)) = \int_{\omega} \operatorname{curl} \mathbf{u} = \int_{\omega} u_{x,y} - u_{y,x} \quad (13)$$

2. The $\mathbf{v}$ -weighted traction $\mathbf{t}$, for some $\mathbf{v} \in H^{1/2}(\partial\Omega)$:¹

$$\begin{aligned} J((\mathbf{u}, p)) &= \oint_{\partial\Omega} \mathbf{t}(\mathbf{u}, p) \cdot \mathbf{v} = F\left(\left(\ell^{\partial\Omega}(\mathbf{v}), 0\right)\right) \\ &\quad - N_{\Sigma}\left((\mathbf{u}, p), \left(\ell^{\partial\Omega}(\mathbf{v}), 0\right)\right), \end{aligned}$$

with $\gamma^{\partial\Omega}$ as in (5), where the last equality follows by interpreting the boundary integral as a $H^{-1/2}(\partial\Omega) \times H^{1/2}(\Omega)$ duality pairing such that the functional is bounded.

3. Kinetic energy in some subdomain $\omega \subset \Omega$ (the functional is in this case nonlinear):

$$J((\mathbf{u}, p)) = \frac{1}{2} \|\mathbf{u}\|_{0,\omega}^2$$

4. Average or mollified versions of pointwise values, as in [22].

It is often unnecessary to solve the Navier–Stokes equations on the entire domain Ω to achieve an acceptable accuracy in the goal quantity. In fact, one may often replace the Navier–Stokes equations by the Stokes equations, on a subdomain (when the convective term is small with respect to the diffusive term, for example). Application of the Stokes model on a subdomain is particularly beneficial if that subdomain has a complicated shape or undergoes large displacements, as the boundary element approximation of the Stokes problem bypasses the construction of a volume grid. Goal-oriented model adaptivity provides a systematic way to arrive at an optimal computational model. In this section we present the methodology, based on [17,22]. In this discussion, the single quote $(\cdot)'$ denotes the Fréchet derivative of a functional, the existence of which is assumed.

3.1 Estimation of the error in a goal quantity

Consider the nonlinear *fine* model.

Given $\mathcal{Y}$, find $(\mathbf{u}_1, p_1) \in (\ell^{\partial\Omega^D}(\mathbf{g}) + V_1) \times Q_1$ such that:

$$\begin{aligned} N_1((\mathbf{u}_1, p_1, \mathbf{0}, 0); (\mathbf{v}, q, \mathbf{0}, 0)) &= F((\mathbf{v}, q, \mathbf{0}, 0)) \\ \forall (\mathbf{v}, q) &\in V \times Q, \end{aligned} \quad (14)$$

where the subscript 1 denotes the partitioning $\Omega^N = \Omega$ so that $\Omega^S = \emptyset$, and the spaces V_1 and Q_1 are defined accordingly. The residual at an approximation $(\mathbf{u}_0, p_0)$, reconstructed on Ω^S as explained above, is given by

$$\begin{aligned} \mathcal{R}((\mathbf{u}_0, p_0); (\mathbf{v}, q)) &:= F((\mathbf{v}, q, \mathbf{0}, 0)) \\ &\quad - N_1((\mathbf{u}_0, p_0, \mathbf{0}, 0); (\mathbf{v}, q, \mathbf{0}, 0)), \end{aligned} \quad (15)$$

where we note that the last two components of the solution are irrelevant since the solution has been reconstructed on Ω^S . We recall that the reconstruction inside Ω^S is entirely dependent on the boundary data, so that no mesh is required here.² For consistency in notation, these components are set to zero. We obtain this approximation by solving a mixed-model problem, the *primal problem*:

Given $\mathcal{Y}$, find $(\mathbf{u}_0^N, p_0^N, \mathbf{t}_0^S, \lambda_0) \in V_0 \times Q_0 \times T_0 \times \mathbb{R}$ such that:

$$\begin{aligned} N_0((\mathbf{u}_0^N, p_0^N, \mathbf{t}_0^S, \lambda); (\mathbf{v}, q, \boldsymbol{\psi}, \mu)) &= F((\mathbf{v}, q, \boldsymbol{\psi}, \mu)) \\ \forall (\mathbf{v}, q, \boldsymbol{\psi}, \mu) &\in V_0 \times Q_0 \times T_0 \times \mathbb{R}, \end{aligned} \quad (16)$$

¹ This is similar to a residual evaluation at a function with support on (part of) $\partial\Omega_D$, see also [27].

² Except possibly locally if one chooses to define the test function $(\mathbf{v}, q)$ using a mesh.

where the subscript 0 denotes the domain partitioning pertaining to the primal problem. Recall that in this discussion J is restricted to Ω^N . This restricted goal is denoted by $J_0 : V_0 \times Q_0 \rightarrow \mathbb{R}$. A potentially different domain partitioning $\tilde{\Sigma}$ is considered for the dual (or adjoint) problem such that $\Omega_0^N \subseteq \tilde{\Omega}^N \subseteq \Omega_1^N \equiv \Omega$. This *dual problem* is given by

$$\begin{aligned} & \text{Find } (\tilde{z}^N, \tilde{\zeta}^N, \tilde{y}^S, \tilde{x}) \in \tilde{V} \times \tilde{Q} \times \tilde{T} \times \mathbb{R} \text{ such that:} \\ & \tilde{N}' \left((\tilde{u}_0^N, 0, \mathbf{0}, 0); (v, q, \psi, \mu), (\tilde{z}^N, \tilde{\zeta}^N, \tilde{y}^S, \tilde{x}) \right) \\ & = J'_0 \left((u_0^N, p_0^N); (v, q) \right) \\ & \forall (v, q, \psi, \mu) \in \tilde{V} \times \tilde{Q} \times \tilde{T} \times \mathbb{R}. \end{aligned} \quad (17)$$

Note that, in the present case of Stokes/Navier–Stokes coupling, the linearization N' depends only on the velocity (apart from convection in Ω^N the system is linear), hence, we only need to reconstruct $V_0 \ni u_0^N \rightarrow \tilde{u}_0^N := u_0|_{\tilde{\Omega}^N} \in \tilde{V}$. Therefore, as before, the subsequent components are set to zero.

It is generally intractable to solve the exact dual ($\tilde{\Omega}^N := \Omega$). Sometimes the adjoint equation of the forward problem (16) is employed ($\tilde{\Omega}^N := \Omega_0^N$), as explained in [3]. Alternatively, an enriched problem (s.t. $\tilde{\Omega}^N \supsetneq \Omega_0^N$) can be considered, where Ω^N is enlarged by extending the interface Σ into Ω^S , see for instance [2].

If the *modeling error* is denoted by $(e, e) = (u_1 - u_0, p_1 - p_0)$, and the error in the dual solution by $(\epsilon, \epsilon) = (z_1 - \tilde{z}, \zeta_1 - \tilde{\zeta})$, the error in the goal can be approximated as

As shown in theorem 2 of [17], the error of any approximation (u_0, p_0) can be represented as

$$J((u_1, p_1)) - J((u_0, p_0)) = \mathcal{R}((u_0, p_0); (\tilde{z}, \tilde{\zeta})) + r, \quad (18)$$

with integral remainder terms

$$\begin{aligned} r = & -\frac{1}{2} \int_0^1 Q''((u_0 + se, p_0 + se); (e, e), (e, e)) ds \\ & + \frac{1}{2} \int_0^1 N''((u_0 + se, p_0 + se); (e, e), (e, e), \\ & (\tilde{z} + s\epsilon, \tilde{\zeta} + s\epsilon)) ds + \frac{1}{2} \int_0^1 \left(Q'''((u_0 + se, p_0 + se); \right. \\ & (e, e), (e, e), (e, e)) \\ & - 3N'''((u_0 + se, p_0 + se); (e, e), (e, e), (\epsilon, \epsilon)) \\ & - N'''((u_0 + se, p_0 + se); (e, e), (e, e), (e, e), \\ & \left. (\tilde{z} + s\epsilon, \tilde{\zeta} + s\epsilon)) \right) (s-1) ds \end{aligned}$$

In the following, the higher order remainder in the error representation of (19) is ignored, and the (absolute value of the) dual-weighted residual is taken as an estimate of the error: $EE := |\mathcal{R}((u_0, p_0); (\tilde{z}, \tilde{\zeta}))|$.

3.2 Model adaptivity

To establish the goal-adaptive procedure, we consider an approximation (u_1^h, p_1^h) in a finite-dimensional, conforming subspace $V_1^h \times Q_1^h \subset V_1 \times Q_1$ in which the base model problem (14) is set. The primal and dual solutions, solving (16) and (17) resp., are computed on some other space, depending on Σ_0 and $\tilde{\Sigma}$. The projections of their reconstructions in $V_1 \times Q_1$ onto $V_1^h \times Q_1^h$ are denoted (u_0^h, p_0^h) and $(\tilde{z}^h, \tilde{\zeta}^h)$, respectively. In the context of the present work, we shall only consider modeling errors and ignore discretization errors. For concurrent treatment of modeling and discretization errors, see e.g. [24,25].

We define a basis $\Phi^h := \{(\phi, \phi)_i\}_{i \in I}$ consisting of locally supported functions, such that $\text{span } \Phi^h = V_1^h \times Q_1^h$. The dual solution can now be represented by a linear combination of the elements of Φ^h as

$$(\tilde{z}^h, \tilde{\zeta}^h) = \left(\sum_{i \in I} \phi_i \hat{z}_i^h, \sum_{i \in I} \phi_i \hat{\zeta}_i^h \right) = \sum_{i \in I} (\phi, \phi)_i (\hat{z}^h, \hat{\zeta}^h)_i,$$

where the last equality simply introduces a convenient notation. Now the error estimate $R((u_0^h, p_0^h); (\tilde{z}^h, \tilde{\zeta}^h))$ can be split into basis function contributions as follows:

$$\begin{aligned} \varepsilon &:= |J((u_1^h, p_1^h)) - J((u_0^h, p_0^h))| \lesssim \sum_{i \in I} \eta_i =: \text{EB}, \quad (19) \\ \eta_i &:= |R((u_0^h, p_0^h); (\phi, \phi)_i) (\hat{z}^h, \hat{\zeta}^h)_i|, \end{aligned}$$

where $\eta_i \in \mathbb{R}$. The true error is denoted by ε and EB is the ℓ^1 norm of the indicator set. Note that EB is an upper bound for the estimate EE but not a guaranteed bound of the error in the goal on account of the higher-order remainder r of (19).

Equipped with information on the local error contributions, η_i , the second step is to enhance the mixed model, i.e. to update Σ_0 . First, a subset $K \subset I$ of contributions is marked for refinement. Some common strategies are to mark $\{\eta_k\}_{k \in K}$ for which

1. $|\eta_k| > \theta \max_{i \in I} |\eta_i|$, with $0 \leq \theta \leq 1$ (maximum algorithm),
2. η_k belongs to the fraction $0 < \theta \leq 1$ of largest contributions (fixed-fraction marking),
3. η_k belongs to a minimal set of indicators such that their sum is at least $0 < \theta \leq 1$ of the total sum of indicators (Dörfler marking) [7].

A new domain decomposition is obtained by adding the support of the marked basis functions to the fine domain:

$$\Omega^N \leftarrow \Omega^N \cup \left(\bigcup_{k \in K} \text{supp}(\phi, \phi)_k \right)$$

Commonly, the domain is tessellated into a disjoint union of elements $\kappa \in \mathcal{T}^h$ facilitating the structure for the construction of a basis and approximation space. The update of the fine-model domain Ω^N then amounts to element-wise switching the model. Note that the elements interior to Ω^S are not used in the computation by virtue of the boundary integral formulation.

4 Numerical experiments

We first present some details of the numerical method in Sect. 4.1 and then provide a numerical example in Sect. 4.2.

4.1 Discretization

Tesselations $\mathcal{T}^h$ and $\mathcal{S}^h$ are provided over Ω^N and $\partial\Omega^S$, respectively, and are chosen such that vertices coincide at the interface Σ . The velocity-pressure pair on Ω^N is approximated in the inf-sup stable vector space (cf. [4, 8]) $\mathbb{P}_{\text{bubble}}^1(\mathcal{T}^h) \times \mathbb{P}^1(\mathcal{T}^h) =: V_0^h \times Q_0^h$. The approximate traction on $\partial\Omega^S$ is sought in the conforming space $\mathbb{P}_{\text{discont}}^1(\mathcal{S}^h) =: T_0^h$.

Standard quadrature rules will fail to converge where the integrands in the BEM subproblem become singular. The integrals are evaluated analytically in these cases, as detailed in [30]. Along the remainder of the boundary, a sufficiently high quadrature rule is used, in this case 8th-order Gauss quadrature.

The model-adaptive algorithm performed in the sequel conforms to the following procedure:

0. Definition of the problem data: Σ_0, γ, J ; and some adaptivity parameters specified: TOL (the target value for the error bound), $\tilde{n}$ (the extension of $\tilde{\Sigma}$ w.r.t. Σ_0), and θ (the fraction for the marking strategy).
1. Solution of the primal problem. The discrete spaces are constructed according to Σ_0 , Newton's method is used to solve the nonlinear system.
2. Solution of the dual problem. If $\tilde{\Sigma} \neq \Sigma_0$, the approximation spaces are adapted accordingly and the primal solution reconstructed where required. Otherwise, the adjoint of the Jacobian matrix can be recycled.
3. Estimation of the error bound and contributions. The space $V_1^h \times Q_1^h$ is constructed or recycled, and the primal and dual solutions reconstructed (in this case in the whole domain, but, more generally, only in the vicinity of the fine-model domain).
4. Assessment of the adaptive scheme. If the bound drops below TOL the model-adaptive procedure is stopped; otherwise, Ω^N is extended according to the chosen marking strategy and the procedure continues at step 1.

In step 1 of the algorithm, the Stokes equations in Ω^S (in boundary-integral form) and the Navier–Stokes equations in Ω^N are coupled and solved simultaneously. Alternatively, one may opt to apply an iterative procedure to solve the coupled problem, analogous to [11].

The adaptive procedure adds steps 2–4 to a non-adaptive procedure, note that many components of step 1 can be reused, such as the assembly of a residual and a Jacobian matrix. The integer $\tilde{n}$ is the extension of the boundary for the dual problem. When $\tilde{n} = 0$, the dual problem is simply the transpose of the primal problem. If $\tilde{n} = 1$, the extension of $\Omega_0^N, \tilde{\Omega}^N$ additionally contains every element in Ω_0^S sharing a vertex with Σ_0 . For $\tilde{n} > 1$ the extension procedure is simply repeated recursively $\tilde{n}$ times.

4.2 Lid-driven cavity problem

The model-adaptive strategy is applied to the classical lid-driven cavity benchmark problem. Due to its simplicity, some basic features of the domain decomposition method and adaptive strategy can be demonstrated. The flow is confined to the unit square with a constant, unit, horizontal velocity along the top boundary and homogeneous Dirichlet conditions along the other boundaries. The Reynolds number is set to 100. The quantity of interest is the vorticity in the lower-right corner, (13) with $\omega := \{(x, y) \in \Omega : x - y \geq 0.7\}$.

A quasi-uniform triangulation $\mathcal{T}_1^h$ of the domain consisting of $4.3 \cdot 10^3$ elements is used, and it is assumed that discretization errors are sufficiently small. The tolerance on the error bound, TOL is set to 0, such that the entire model-adaptive process is traversed. The different test cases considered are summarized in Table 1. Two different marking strategies are used: the maximum and the fixed-fraction strategy. The fractions θ have been selected such that the adaptive processes span at least 10 iterations. Furthermore, increasingly enriched dual problems are compared, $\tilde{n} \in \{0, 1, 2, 3\}$, corresponding to the number of additional layers of elements in the dual problem.

First, we consider an isolated domain-decomposition problem, which is in fact one iteration of the model-adaptive procedure, cf. Fig. 2. Note that the interface Σ_0 is fairly serrated and that there are disconnected patches of elements where the FEM is used. Nevertheless, it is observed that

1. The solution is quite smooth across the interface;

Table 1 Test cases considered for the Re = 100 lid-driven cavity problem

$\tilde{n}$	0	1	2	3
Maximum ($\theta = 0.1$)	M0	M1	M2	M3
Fixed-fraction ($\theta = 0.01$)	F0	F1	F2	F3

Fig. 2 Domain decomposition and primal solution components for model iteration 4 of case F1. The border of the FEM subdomain is given in red. The *top*, *middle* and *bottom* panels correspond to the horizontal, vertical velocity components and the pressure, resp. (Color figure online)

2. The Newton iterations converge quite well, typically within 7 iterations with a tolerance of 10^{-8} .

The smoothness of the solution across the interface is a prerequisite for the domain-decomposition approach to be a valid alternative. The resolution of the traction approximation, which is at the same level as that of the serrations, does not seem to pollute the solution near the interface.

Secondly, the Newton iterations converge well, even for this challenging domain decomposition. This fact indicates the ability to tackle arbitrary domain decompositions. This, in turn, greatly eases the model adaptive procedure. From this point of view, no special care is required to ensure that subdomains remain connected, or that the interface remains smooth. However, we will comment on the ramifications of such a naive interface update later.

The monolithic solution of the FEM/BEM coupled problem is instrumental in this observed stability. In this configuration, there is considerable backflow through the interface into the FEM domain, along which Neumann conditions are defined. Thus, the FEM subproblem is by itself ill-posed, and partitioned iterations will fail. This problem does not manifest in a monolithic setting as the Dirichlet data is determined concurrently by the BEM subproblem. The authors observed that partitioned strategies possessed poor stability properties, even for simple configurations without backflow. For a partitioned approach to work, the formulation should be modified by switching the interface conditions to arrive at the mixed BEM subproblem [31], or by employing one of the stabilizations suggested in [16] for backflow divergence in the Navier–Stokes equations.

Now consider the error indicators corresponding to the primal solution of Fig. 2, visualized in Fig. 3. Note that the contributions to the error in the interior of Ω^N rapidly decrease at a small distance from the interfaces of the primal and dual problems, the last of which has been plotted. In Ω^S there are some oscillations in the indicators, due to the quality of the reconstruction. In this work a naive reconstruction based on standard Gauss quadrature schemes is employed. To better account for the near-singular behaviour of these reconstructions, a smarter quadrature, such as that proposed in [1], can be employed. This scheme can be applied to the velocity and pressure reconstructions used in this paper. We expect that this will increase the fidelity of the coarse model and the effectivity of the model-adaptive procedure.

In Fig. 4, we observe that the model-adaptive process seems relatively insensitive to specific algorithmic choices such as the refinement strategy and the number of additional element layers in the dual problem. However, a few differences are apparent. The evolution of the error bound is more monotone for higher $\tilde{n}$. It is to be expected that a dual solution from an enriched dual problem (higher $\tilde{n}$) contains more information to guide the adaptive process. The

Fig. 3 Error indicators corresponding to model iteration 4 of case F1. The border of the FEM subdomain of the dual problem is given in red. The visualization is given by $\sum_i \eta_i N_i$, i.e., each indicator is multiplied by its corresponding basis function. The top, middle and bottom panels correspond to the horizontal, vertical velocity components and the pressure, resp. (Color figure online)

Fig. 4 Evolution of the error bounds EB (solid) and estimates EE (dashed) in terms of the fraction of elements refined. Colors indicate the number of levels of enrichment of the dual problem, $\bar{n} = 0, 1, 2, 3$. Simulations M0–M3 are plotted in the upper panel, and F0–F3 in the lower panel. Values along the vertical axis have been normalized by the quantity of interest $J((u_1, p_1)) = -6.12 \cdot 10^{-1}$. (Color figure online)

slope of the error bound EB is in all cases very mild, flattening throughout a large part of the adaptive process. This was to be expected, because the convective terms are important throughout the entire domain for the lid-driven cavity problem. We re-emphasize that this problem has only been selected as a simple case to demonstrate the method.

In conclusion, Fig. 5 shows the successive domain decompositions in the model adaptive process F1. It is observed that all except the first two model refinements take place at the boundary of the previous iteration. In the first iteration, the two corner singularities are refined. A pollution error due to inaccurate approximation of these singularities is to be expected. In the second iteration, some isolated patches are

Fig. 5 Refinement history of simulation F1. Black is the initial (bottom-right corner) and white the ultimate (15th) refinement

refined in the interior, probably because of inaccuracies in the reconstruction as discussed above.

5 Conclusions

We have presented a formulation for multi-model, viscous, incompressible, steady flow based on domain decomposition, where a boundary integral representation of a surrogate model is used on a subdomain. This representation eliminates the requirement of meshing that subdomain, which avoids complex meshing and remeshing procedures when the geometry is complex, undergoes large deformations or exhibits near-self-contact. Secondly, the errors due to the introduction of a surrogate model were assessed in terms of a quantity of interest and estimated by solving a suitable dual problem. A simple but effective degree-of-freedom-wise (nodal) error indicator was presented, based on nodal components of the dual-weighted residual. The full model-adaptive procedure was applied to a lid-driven cavity problem.

It was demonstrated that the multi-model problem can be easily solved even for quite arbitrary domain decompositions with serrated edges and disconnected elements, as can arise for a general model update (i.e., refinement) strategy based on error indicators.

However, it was observed that in general the largest local error contributions lie close to the interface. Moreover, model updates where elements away from the interface were marked, generally did not drive down the bound. These two observations suggest that an approach based on shape-derivatives (cf. e.g. [6]) would be appropriate. In such an approach, a perturbation of the interface is pursued which most effectively reduces the error bound. This would simply amount to the replacement of the maximum or fixed-fraction

marking strategy by a more sophisticated one, in which only elements adjacent to the interface are considered for marking. The baseline approach pursued in the present work, viz., to compute error indicators on the entire domain, is undesirable in practice. The fundamental advantage of the adaptive FE/BE approach is that it avoids the generation of a mesh in the BE domain. A shape-derivative approach would entirely obviate this as the mesh need only be extended dynamically a few layers into Ω^S to compute the relevant indicators. An exclusive boundary representation of the flow in Ω^S then suffices for the entire model-adaptive iteration. One should be aware of the fact that the shape-derivative approach is based on the assumption that the largest error contributions are restricted to the vicinity of the interface. Whenever there is insufficient intuition of where modeling errors are high, computation of error indicators throughout Ω^S , as done in this paper, may be necessary.

Considering an enriched dual problem (in which the fine-model region of the dual problem strictly includes that of the primal problem), is observed to lead to a “more monotone” evolution of the error bound.

The proposed technique automates the non-trivial process of domain decomposition, provides estimates (and bounds to the estimate) of the modeling error, and, in addition, offers insight into the flow features relevant to a specific quantity of interest.

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