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Flux evaluation in primal and dual boundary-coupled problems

by

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Abstract A crucial aspect in boundary-coupled problems such as fluid-structure interaction pertains to the evaluation of fluxes. In boundary-coupled problems, the flux evaluation appears implicitly in the formulation and, consequently, improper flux evaluation can lead to instability. Finite-element approximations of primal and dual problems corresponding to improper formulations can therefore be non-convergent or display suboptimal convergence rates. In this paper, we consider the main aspects of flux evaluation in finite-element approximations of boundary-coupled problems. Based on a model problem, we consider various formulations and illustrate the implications for corresponding primal and dual problems. In addition, we discuss the extension to free-boundary problems, fluid-structure interaction, and electro-osmosis applications.

Keywords Fluid-structure interaction, dual problems, flux extraction, electro-osmosis, free-boundary problems, goal-oriented adaptivity

1 Introduction

The computational simulation of boundary-coupled problems is of fundamental importance in many engineering and scientific disciplines. Important examples include (thermal) fluid-solid interaction, e.g., in aerospace engineering [1] and in biomechanics [2], electro-mechanical and electro-mechanical-fluidic interactions in, notably, micro-electro-mechanical systems (MEMS) [3], electro-osmosis and, generally, free-boundary problems [4], in which an auxiliary free-boundary condition can be interpreted as a separate subsystem.

In all such applications, the evaluation of *fluxes* (or *tractions*), i.e., the value of a certain derivative of a function at the boundary of a domain, or a function thereof, appears. The evaluation of fluxes is a standard operation in many single field computations as well. However, as opposed to single-field problems, where the flux evaluation typically appears *explicitly* as a post-processing operation, in boundary-

coupled problems the flux evaluation generally appears *implicitly* in the formulation. The implicit appearance of the flux evaluation in coupled problems has severe consequences: if the flux is evaluated incorrectly, then the corresponding formulation of the coupled problem is unstable. For numerical methods, this can in turn impede convergence or lead to suboptimal convergence rates. Dual (adjoint) problems corresponding to such formulations, e.g., in optimization or goal-adaptive-refinement procedures [5; 6], can exhibit incompressible behavior. In contrast, if the flux is incorrectly evaluated as a post-processing operation, this will generally have no significant consequences, unless the solution displays singularities in the vicinity of the boundary, e.g., near re-entrant corners.

Trace theory, including the treatment of fluxes in computational procedures, is in principle well established; see, e.g., [7]. Nevertheless, the aspect of flux evaluation and its pertinence to boundary-coupled problems are commonly unnoticed, or only observed in the form of the aforementioned problems.

In this paper, we consider the main aspects of flux evaluation in computational procedures for boundary-coupled problems. We illustrate the various formulations and implications on the basis of a simple model problem. In addition, we consider the properties of dual problems corresponding to the various formulations, to demonstrate the essential differences that occur in such dual problems on account of different flux treatments. To elucidate that the structure of the model problem is generic, we consider the analogy with various boundary-coupled problems, viz., free-boundary problems, fluid-structure interaction, and electro-osmosis.

The content of this paper is organized as follows: Section 2 presents the statement of the model problem. In section 3, we consider trace evaluation as a post-processing operation and we demonstrate the effect of singularities on the various trace formulations. Section 4 is concerned with an exposition on the coupled problem and dual problems corresponding to various trace evaluations. Section 5 treats the extension of the model problem to three distinct classes of boundary-coupled problems, viz., free-boundary problems, fluid-structure interaction and electro-osmosis. Section 6 provides some concluding remarks.

2 Problem statement

We consider a bounded domain $\Omega \subset \mathbb{R}^d$ ($d \in \{2, 3\}$) with boundary $\partial\Omega$. The boundary is composed of two complementary parts, Γ_D and Γ_N . The model problem of concern in this paper is the *flux-extraction* problem: Find $u : \Omega \rightarrow \mathbb{R}$ and

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$\alpha : \Gamma_D \rightarrow \mathbb{R}$ such that

$$-\Delta u = f \quad \text{in } \Omega \quad (1a)$$

$$u = g \quad \text{on } \Gamma_D \quad (1b)$$

$$\partial_n u = h \quad \text{on } \Gamma_N \quad (1c)$$

$$\alpha = \partial_n u \quad \text{on } \Gamma_D \quad (1d)$$

where $f : \Omega \rightarrow \mathbb{R}$, $g : \Gamma_D \rightarrow \mathbb{R}$ and $h : \Gamma_N \rightarrow \mathbb{R}$ represent exogenous data. Problem (1) is referred to as the flux-extraction problem, because α represents the flux, $\partial_n u$, of the solution u to the boundary-value problem (1a)–(1c). Evidently, $\partial_n u$ ($=: \alpha$) can be extracted from the solution of (1a)–(1c) by means of a post-processing operation. However, if α is retained as a separate variable, then (1) constitutes a boundary-coupled problem, in which the boundary-value problem in (1a)–(1c) is coupled at Γ_D to the identity (1d).

To display the generic properties of (1), we consider the canonical weak formulation of (1a)–(1c). Let $H^1(\Omega)$ denote the collection of square-integrable functions with square-integrable derivatives, and let $H_{0,\Gamma_D}^1(\Omega)$ denote the sub-class of these functions that vanish on Γ_D . The canonical weak formulation of (1a)–(1c) is:

$$u \in \ell_g + H_{0,\Gamma_D}^1(\Omega) : \quad a(u, v) = b(v) \quad \forall v \in H_{0,\Gamma_D}^1(\Omega) \quad (2)$$

where $\ell_{(\cdot)}$ denotes a linear operator, referred to as a *lift operator*, which assigns to any function (\cdot) on Γ_D a function in $H^1(\Omega)$ that coincides with (\cdot) at Γ_D . Furthermore, the bilinear form $a : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}$ and the linear form $b : H^1(\Omega) \rightarrow \mathbb{R}$ are given by

$$a(u, v) = \int_{\Omega} [\nabla u, \nabla v], \quad b(v) = \int_{\Omega} f v + \int_{\Gamma_N} h v \quad (3)$$

where $[\cdot, \cdot]$ denotes tensor contraction. For any suitable function λ on the boundary Γ_D and sufficiently smooth u , the pairing of λ with the flux satisfies

$$\begin{aligned} \int_{\Gamma_D} \lambda \alpha &= \oint_{\partial \Omega} \ell_{\lambda} \partial_n u - \int_{\Gamma_N} \ell_{\lambda} \partial_n u \\ &= \int_{\Omega} \ell_{\lambda} \Delta u + \int_{\Omega} [\nabla u, \nabla \ell_{\lambda}] - \int_{\Gamma_N} \ell_{\lambda} \partial_n u \\ &= \int_{\Omega} [\nabla u, \nabla \ell_{\lambda}] - \int_{\Omega} \ell_{\lambda} f - \int_{\Gamma_N} \ell_{\lambda} h \\ &= a(u, \ell_{\lambda}) - b(\ell_{\lambda}) \end{aligned} \quad (4)$$

The second identity results from integration by parts. The third identity follows from (1a) and (1c). It is important to note that the flux (or *Neumann* or *natural*) boundary condition (1c) appears in the weak formulation (2) in the form $\int_{\Gamma_N} h v$. Analogously, if problem (1a)–(1c) is coupled at the boundary Γ_D to an auxiliary problem and continuity of the flux between the two problems is imposed, this results in a *flux functional* of the form (4) in the right member of the auxiliary problem, with λ corresponding to the (trace of the) test function of the auxiliary problem. According to (4), this flux functional can be evaluated by pairing the *residual functional* corresponding to the solution u of the boundary-value problem (1a)–(1c), viz., $a(u, \cdot) - b(\cdot)$, with the lifted test function ℓ_{λ} . It is to be noted that ℓ_{λ} does not belong to the space $H_{0,\Gamma_D}^1(\Omega)$ of test functions in (2), because ℓ_{λ} is non-zero at Γ_D .

The structure of the above model problem is generic in that boundary-coupled problems are generally connected by continuity of fluxes. This continuity condition leads to a flux

functional in one of the two subproblems, which can be expressed by pairing the residual functional of the other subproblem with a lifted test function, analogous to (4). Section 5.2 elaborates this analogy for a fluid-structure-interaction problem; see also [8; 9].

The left- and right-most expressions in (4) encode two distinct forms of flux evaluation, referred to as *direct flux evaluation* and *flux extraction* (or *variationally-consistent flux evaluation*). To appreciate the fundamental distinction between these two forms of flux evaluation, it is to be noted that the sequence of identities (4) only hold for sufficiently smooth u . The integrals in the ultimate and penultimate expressions are finite whenever $u \in H^1(\Omega)$, while the preceding expressions are finite if, in addition, $\Delta u \in L^2(\Omega)$ and $\partial_n u \in L^2(\partial \Omega)$. Therefore, for arbitrary admissible λ , flux extraction corresponds to a bounded functional (on $H^1(\Omega)$), while direct flux evaluation does not. Essentially, this implies that, in contrast to flux extraction, direct flux evaluation is an inadmissible operation.

3 Posterior flux evaluation

To illustrate the differences between direct flux evaluation and flux extraction in numerical procedures, we consider two model problems, derived from (1). Both model problems are set in \mathbb{R}^2 and are of Dirichlet type, i.e., $d = 2$ and $\Gamma_N = \emptyset$. In the first model problem, the domain $\Omega = (0, 1)^2$ is a unit square and the exogenous data is selected such that $u(x, y) = \cos(\pi x) \sin(\pi y)$. We consider the functionals $j_d(u) = \int_{\Gamma_D} \lambda \partial_n u$ and $j_e(u) = a(u, \ell_{\lambda}) - b(\ell_{\lambda})$, corresponding to the left member of (4) (with $\alpha = \partial_n u$) and to the right member of (4), respectively, and

$$\lambda(x, y) = \begin{cases} 4(x - 1/2), & 1/2 \leq x < 3/4, y = 0 \\ -4(x - 1), & 3/4 \leq x \leq 1, y = 0 \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

The exact value of the flux functional is $j_{\text{ref}} = 4(\sqrt{2} - 1)/\pi$. In the second problem, $\Omega = (-1, 1)^2 \setminus ([0, 1] \times (-1, 0])$ corresponds to an L-shaped domain and the data is selected such that the exact solution be given by

$$u(x, y) = (x^2 + y^2)^{1/3} \sin((2/3) \text{atan}(y/x)) - (x^2 + y^2)/4 \quad (6)$$

Note that the solution (6) exhibits a singularity at the origin. We consider the functionals $j_d(u)$ and $j_e(u)$ corresponding to the left and right members of (4), respectively, with

$$\lambda(x, y) = \begin{cases} 2(y + 1/2)(1 - x), & 0 \leq x \leq 1, -1/2 \leq y \leq 0 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

The exact value of the functional is $j_{\text{ref}} = -3(2^{1/3} + 2)/10$. To avoid proliferation of symbols, we use the same notation to refer to objects related to the two model problems.

We consider approximations of the two model problems by means of standard piecewise-linear finite elements. The domain Ω is covered with a sequence of regular tessellations of uniform squares with sides of length $h \in 2^{-\mathbb{N}}$, which are further subdivided into four right triangles, to obtain a regular mesh of uniform triangles. Let S^h denote the standard finite-element space of continuous piecewise-linear functions on the mesh with parameter h . Moreover, we denote by S_{0,Γ_D}^h the collection of functions in S^h that vanish on Γ_D . The finite-element approximation of (2) is:

$$u^h \in \ell_g^h + S_{0,\Gamma_D}^h : \quad a(u^h, v^h) = b(v^h) \quad \forall v^h \in S_{0,\Gamma_D}^h. \quad (8)$$

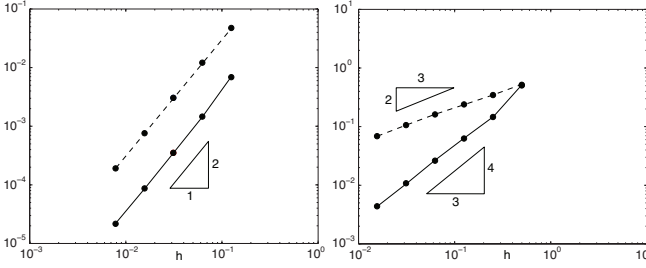


Fig. 1 Convergence of the flux functionals $j_d(u^h)$ (dashed) and $j_e(u^h)$ (solid) versus the mesh parameter h of the finite-element approximation, for model problem 1 (left) and model problem 2 (right).

where $\ell_{(\cdot)}^h$ represents a finite-element lift operator, which assigns to any function (\cdot) on Γ_D a function in S^h that coincides with the nodal-interpolant of (\cdot) at Γ_D .

Figure 1 plots the error in $j_d(u^h)$ and $j_e(u^h)$ versus h for test case 1 (left) and test case 2 (right). It can be observed that for test case 1, which possesses a smooth underlying solution, the two expressions for the flux functional exhibit the same (optimal [10]) rate of convergence, $|j_a(u^h) - j_{ref}| \leq c_a h^2$, $a \in \{d, e\}$. For proper flux extraction, however, the best constant in the error bound, c_e , is much smaller than the constant c_d pertaining to direct flux evaluation. For test case 2, which displays a singular solution, the two flux functionals provide very different convergence behavior: the error corresponding to direct flux evaluation decays only as $O(h^{2/3})$ as $h \rightarrow 0$, while the error of flux extraction decays as $O(h^{4/3})$. We refer to [11, §6.2] for an elaboration on this difference in the convergence behavior.

4 Primal and dual coupled problems

Next, we consider the finite-element approximation of the coupled flux-extraction problem (1). We restrict ourselves to a discussion of the finite-element formulations, but the analyses extend to the underlying weak formulations. We define T^h as the trace space of S^h on Γ_D i.e., the collection of functions on $\partial\Omega$ that arises by taking the boundary values at Γ_D of functions in S^h . We first consider a finite-element approximation based on the naive weak formulation:

$$(u^h, \alpha^h) \in (\ell_g^h + S_{0, \Gamma_D}^h) \times T^h : \\ a(u^h, v^h) + \int_{\Gamma_D} (\partial_n u^h - \alpha^h) \beta^h = b(v^h) \\ \forall (v^h, \beta^h) \in S_{0, \Gamma_D}^h \times T^h \quad (9)$$

with $a(\cdot, \cdot)$ and $b(\cdot)$ according to (3). Formulation (9) represents an obvious extension to the weak formulation (8) of the boundary-value problem (1a)–(1c) by a weak enforcement of the identity (1d). Formulation (9) defines α^h such that the functional $\beta^h \mapsto \int_{\Gamma_D} \alpha^h \beta^h$ corresponds to direct flux evaluation. We note in advance that the formulation is suspect, however, in view of the explicit appearance of $\partial_n u$, which represents an unbounded operator from $H_0^1(\Omega)$ to $H^{-1/2}(\Gamma_D)$; see also section 2. This implies that the final term in the left member of (9) can be unbounded for admissible u and β .

In conjunction with (9) and a linear functional of interest, $J(u, \alpha)$, we also consider the corresponding *dual problem*:

$$(w^h, \gamma^h) \in S_{0, \Gamma_D}^h \times T^h : \\ a(x^h, w^h) + \int_{\Gamma_D} (\partial_n x^h - \delta^h) \gamma^h = J(x^h, \delta^h) \\ \forall (x^h, \delta^h) \in S_{0, \Gamma_D}^h \times T^h \quad (10)$$

In comparison with the (primal) problem (9), the test and trial functions have exchanged positions in the bilinear form in the left member of the dual problem (10).

An alternative formulation of the coupled problem is provided by

$$(u^h, \alpha^h) \in (\ell_g^h + S_{0, \Gamma_D}^h) \times T^h : \\ a(u^h, v^h + \ell_{\beta^h}^h) - \int_{\Gamma_D} \alpha^h \beta^h = b(v^h + \ell_{\beta^h}^h) \\ \forall (v^h, \beta^h) \in S_{0, \Gamma_D}^h \times T^h \quad (11)$$

Formulation (11) implicitly defines α^h such that the functional $\beta^h \mapsto \int_{\Gamma_D} \alpha^h \beta^h$ corresponds to flux extraction in accordance with the final expression in (4). Note that the formulation does not explicitly involve the term $\partial_n u^h$.

To derive the associated dual problem, we first reformulate (11). To this end, we note that the space $S_{0, \Gamma_D}^h \times T^h$ is isomorphic to S^h . Given the linear lift operator $\ell_{(\cdot)}^h$, a natural isomorphism is provided by:

$$\mathcal{I} : S_{0, \Gamma_D}^h \times T^h \rightarrow S^h, \quad \mathcal{I}(v, \beta) = v + \ell_{\beta}^h \\ \mathcal{I}^{-1} : S^h \rightarrow S_{0, \Gamma_D}^h \times T^h, \quad \mathcal{I}^{-1}v = (v - \ell_{v|_{\Gamma_D}}^h, v|_{\Gamma_D})$$

where $(\cdot)|_{\Gamma_D}$ denotes the trace of (\cdot) on Γ_D . Hence, (11) can be equivalently recast as:

$$(u^h, \alpha^h) \in (\ell_g^h + S_{0, \Gamma_D}^h) \times T^h : \\ a(u^h, v^h) - \int_{\Gamma_D} \alpha^h v^h = b(v^h) \quad \forall v^h \in S^h \quad (12)$$

The dual problem, associated with problem (12) and linear functional $J(u, \alpha)$, is given by:

$$w^h \in S^h : \quad a(x^h, w^h) - \int_{\Gamma_D} \delta^h w^h = J(x^h, \delta^h) \\ \forall (x^h, \delta^h) \in S_{0, \Gamma_D}^h \times T^h \quad (13)$$

One can infer that (13) corresponds to a weak formulation of a Poisson problem for w^h with a Neumann condition on Γ_N and a Dirichlet condition on Γ_D . The naive dual (10) does not admit such an interpretation as a boundary-value problem.

To illustrate the difference between the dual formulations (10) and (13), we reconsider test case 1 from the previous section. Figure 2 plots the dual solution obtained from the naive formulation (10) (left) and from the appropriate formulation (13) (right) for a mesh with $h = 2^{-4}$. It can be observed that the dual solution of the naive formulation (10) exhibits unexpected non-smooth behavior near the boundary, as opposed to the solution of (13).

5 Extensions

To show that the structure of the model problem in Sections 2–4 is generic, we consider in this section the analogy between the model problem and three distinct classes of boundary-coupled problems, viz., free-boundary problems, fluid-structure interaction and electro-osmosis.

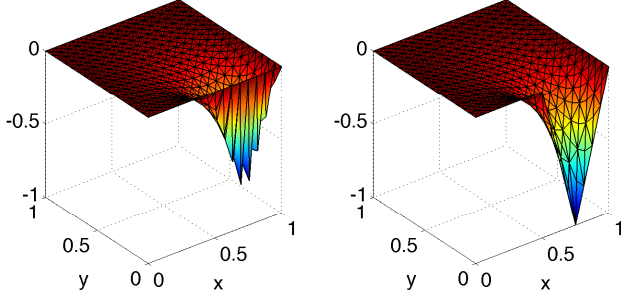


Fig. 2 The dual solution w^h computed using the unstable formulation (10) (left) and the stable formulation (13) (right) on a 1024-element mesh ($h = 2^{-4}$).

5.1 Free-boundary problems

For definiteness, we consider a model free-boundary problem referred to as the *Bernoulli free-boundary problem* [4] or *Alt-Caffarelli problem* [12]. This problem consists in finding, simultaneously, a function $u : \Omega \rightarrow \mathbb{R}$ and its domain of definition, Ω , with boundary $\partial\Omega$ consisting of a fixed part Γ_N and a variable part Γ_F (the free boundary), such that

$$-\Delta u = f \quad \text{in } \Omega \quad (14a)$$

$$\partial_n u = h \quad \text{on } \Gamma_N \quad (14b)$$

$$u = g \quad \text{on } \Gamma_F \quad (14c)$$

$$\partial_n u = h \quad \text{on } \Gamma_F \quad (14d)$$

where $f, h : \mathbb{R}^n \rightarrow \mathbb{R}$ represents sufficiently smooth data such that $h > 0$ on Γ_F . Moreover, for simplicity, we assume $g : \mathbb{R}^n \rightarrow \mathbb{R}$ to be constant. Comparing (14) with the flux-extraction problem (1), we note that (the position of) Γ_F plays a role similar to α . However, unlike (1), which is a one-way coupled problem, the free-boundary problem (14) is two-way coupled, and (14a)–(14d) must be treated simultaneously. Based on the discussion in Section 4, it is natural to consider a formulation based on (14a)–(14c) and treat (14d) using flux extraction (cf. (11)):

$$(u, \Omega) \in (\ell_g + H_{0, \Gamma_F}^1(\Omega)) \times \mathcal{O} :$$

$$a(\Omega; u, v + \ell_\beta) - b(\Omega; v + \ell_\beta) - \int_{\Gamma_F} h\beta = 0$$

$$\forall (v, \beta) \in H_{0, \Gamma_F}^1(\Omega) \times T \quad (15)$$

where \mathcal{O} is a set of admissible domains, T is a suitable space of functions on Γ_F , and $a(\cdot; \cdot, \cdot)$ and $b(\cdot; \cdot)$ are the same as in (3), except that these forms now explicitly include the dependence on the unknown domain Ω . Assuming that $H_{0, \Gamma_F}^1(\Omega) \times T$ is isomorphic to $H^1(\Omega)$, we can recast (15) as:

$$(u, \Omega) \in (\ell_g + H_{0, \Gamma_F}^1(\Omega)) \times \mathcal{O} :$$

$$a(\Omega; u, v) - b(\Omega; v) - \int_{\Gamma_F} hv = 0 \quad \forall v \in H_{0, \Gamma_F}^1(\Omega) \quad (16)$$

For nonlinear problems such as the free-boundary problem (14), the dual formulation is based on the linearized adjoint. We will show that the structure of the linearization of (14) is very similar to the model problem (1). Let us remark that the linearization of free-boundary problems is nontrivial owing to their geometric nonlinearity. One method of linearization uses techniques from shape calculus [13; 14].

Without proof, we assert that the linearization of (14) around an approximation state $(\hat{u}, \hat{\Omega})$ in compliance with

$$-\Delta \hat{u} = f \quad \text{in } \hat{\Omega}$$

$$\partial_n \hat{u} = h \quad \text{on } \Gamma_N$$

$$\hat{u} = g \quad \text{on } \hat{\Gamma}_F$$

with $\hat{\Gamma}_F$ the approximation to the free boundary corresponding to $\hat{\Omega}$, is given by:

$$-\Delta u = f \quad \text{in } \hat{\Omega} \quad (18a)$$

$$\partial_n u = h \quad \text{on } \Gamma_N \quad (18b)$$

$$u + h\alpha = g \quad \text{on } \hat{\Gamma}_F \quad (18c)$$

$$\partial_n u - c\alpha = h \quad \text{on } \hat{\Gamma}_F \quad (18d)$$

where $c = f + \partial_n h + \kappa h$ and κ denotes the additive curvature (sum of $n-1$ curvatures) of $\hat{\Gamma}_F$. Note that (18) is posed on the *fixed* domain $\hat{\Omega}$ and, instead of the unknown free-boundary, we now have an unknown boundary field $\alpha : \hat{\Gamma}_F \rightarrow \mathbb{R}$, which represents a perturbation of $\hat{\Gamma}_F$ in the normal direction.

The linearized free-boundary problem in (18) is similar to (1), in that two conditions hold on $\hat{\Gamma}_F$, involving both the state (u), the flux ($\partial_n u$) and an auxiliary variable (α). As opposed to (1), however, the auxiliary variable appears in both boundary conditions (18c) and (18d). The key aspect in the analogy to (1), however, pertains to the fact that the flux in (18d) is properly evaluated by means of flux extraction. This leads to the formulation:

$$(u, \alpha) \in (\ell_g - \ell_{h\alpha} + H_{0, \hat{\Gamma}_F}^1(\hat{\Omega})) \times \hat{T} :$$

$$a(\hat{\Omega}; u, v) - \int_{\hat{\Gamma}_F} c\alpha v = b(\hat{\Omega}; v) + \int_{\hat{\Gamma}_F} hv \quad \forall v \in H^1(\hat{\Omega}) \quad (19)$$

In (19), we have replaced the original test space $H_{0, \hat{\Gamma}_F}^1(\hat{\Omega}) \times \hat{T}$ by $H^1(\hat{\Omega})$, under the standing assumption that these two spaces are isomorphic; cf. (12) and (16).

Based on (19), the dual problem pertaining to a linear functional $J(u, \alpha)$ reads:

$$w \in H^1(\hat{\Omega}) : \quad a(\hat{\Omega}; x, w) - \int_{\hat{\Gamma}_F} c\delta w = J(x, \delta) \\ \forall (x, \delta) \in (-\ell_{h\delta} + H_{0, \hat{\Gamma}_F}^1(\hat{\Omega})) \times T \quad (20)$$

Note that the relation between u and α in the trial space in (19) can be extended to x and δ in the test space of the dual problem (20).

To facilitate the extraction of a corresponding boundary-value problem from (20), we introduce the change of variables $(x, \delta) = (\tilde{x} + \ell_{\tilde{\delta}}, -\tilde{\delta}/h)$, to recast (20) into:

$$w \in H^1(\hat{\Omega}) : \quad a(\hat{\Omega}; \tilde{x} + \ell_{\tilde{\delta}}, w) + \int_{\hat{\Gamma}_F} \frac{c}{h} \tilde{\delta} w = J(\tilde{x} + \ell_{\tilde{\delta}}, -\frac{1}{h} \tilde{\delta}) \\ \forall (\tilde{x}, \tilde{\delta}) \in H_{0, \hat{\Gamma}_F}^1(\hat{\Omega}) \times \hat{T} \quad (21)$$

The isomorphism between $H_{0, \hat{\Gamma}_F}^1(\hat{\Omega}) \times \hat{T}$ and $H^1(\hat{\Omega})$ yields

$$w \in H^1(\hat{\Omega}) :$$

$$a(\hat{\Omega}; \tilde{x}, w) + \int_{\hat{\Gamma}_F} \frac{c}{h} \tilde{x} w = J(\tilde{x}, -\frac{1}{h} \tilde{x}) \quad \forall \tilde{x} \in H^1(\hat{\Omega}) \quad (22)$$

One can infer that (22) corresponds to a weak formulation of a Poisson problem for w with a Neumann condition on Γ_N and a *Robin* condition on $\hat{\Gamma}_F$; see also [13].

5.2 Fluid–structure interaction

We next consider the analogy between the model problem (1) and a fluid–structure interaction problem, in which the incompressible Navier–Stokes equations are coupled to an elasticity problem. The incompressible Navier–Stokes equations are given by

$$\rho \mathbf{u}' + \operatorname{div} \rho \mathbf{u} \mathbf{u} + \nabla p - \nu \Delta \mathbf{u} = \mathbf{f} \quad \text{in } \Omega \quad (23a)$$

$$\operatorname{div} \mathbf{u} = 0 \quad \text{in } \Omega \quad (23b)$$

where \mathbf{u} and p denote the fluid velocity and pressure, respectively, and $(\cdot)'$ denotes the temporal derivative. Moreover, ρ and ν respectively denote the homogeneous fluid density and viscosity. The solid problem is specified on a reference domain $\bar{\Xi}$ by

$$\eta \varphi'' - \operatorname{Div} \mathbf{P}(\varphi) = \mathbf{F} \quad \text{in } \bar{\Xi} \quad (24)$$

where η denotes the structure density in the reference configuration, \mathbf{P} denotes the first Piola–Kirchhoff stress tensor, $\varphi : \bar{\Xi} \rightarrow \mathbb{R}^d$ represents the displacement field and the map $\varphi \mapsto \mathbf{P}(\varphi)$ is a constitutive relation. The actual domain corresponding to (24) is $\Xi = \bar{\Xi} + \varphi(\bar{\Xi})$ and further, we adhere to the customary notation that the divergence and gradient operators in the reference configuration are indicated by capitalized initials. The Navier–Stokes equations (23) and the elasticity problem (24) are coupled at the interface $\Gamma = \partial\Omega \cap \partial\Xi$ by the kinematic and dynamic interface conditions:

$$\mathbf{u} \circ M = \varphi' \quad \text{on } \bar{\Gamma} \quad (25a)$$

$$((p\mathbf{n} - \nu \partial_n \mathbf{u}) d\Gamma) \circ M = \mathbf{P} \mathbf{N} d\bar{\Gamma} \quad \text{on } \bar{\Gamma} \quad (25b)$$

where M denotes the map $\boldsymbol{\xi} \mapsto \boldsymbol{\xi} + \varphi(\boldsymbol{\xi})$ between the structural reference domain, $\bar{\Xi}$, and the actual domain, Ξ , and $\bar{\Gamma} = M^{-1}\Gamma$ is the representation of the interface in the reference domain. Moreover, $d\Gamma$ and $d\bar{\Gamma}$ denote the surface measures in the actual and reference domains, respectively, and \mathbf{n} and \mathbf{N} respectively denote the outward unit normal vectors on the boundaries of the fluid domain and of the structural reference domain. We suppose that the dynamic condition (25b) is imposed as a natural boundary condition on the structure subproblem. Moreover, for transparency and without loss of generality, we assume that (24) satisfies homogeneous Dirichlet boundary conditions on $\bar{\Gamma}_D = \partial\bar{\Xi} \setminus \bar{\Gamma}$. Considering a fixed time interval $(0, \tau)$, the weak formulation of (24) subject to the aforementioned boundary conditions reads:

$$\begin{aligned} \varphi : (0, \tau) &\rightarrow [H_{0, \bar{\Gamma}_D}^1(\bar{\Xi})]^d : \\ a_s(\varphi, \mathbf{w}) &= b_s \quad \forall \mathbf{w} \in [H_{0, \bar{\Gamma}_D}^1(\bar{\Xi})]^d \end{aligned}$$

everywhere in $(0, \tau)$, where

$$\begin{aligned} a_s(\varphi, \mathbf{w}) &= \int_{\bar{\Xi}} [\eta \varphi'', \mathbf{w}] + \int_{\bar{\Xi}} [\operatorname{Grad} \mathbf{w}, \mathbf{P}], \\ b_s(\mathbf{w}) &= \int_{\bar{\Xi}} [\mathbf{F}, \mathbf{w}] + \int_{\bar{\Gamma}} [((p\mathbf{n} - \nu \partial_n \mathbf{u})J) \circ M, \mathbf{w}], \end{aligned}$$

with $J = d\Gamma/d\bar{\Gamma}$. We suppose that (25a) is imposed as a Dirichlet boundary condition on the fluid subproblem (23). Furthermore, without loss of generality, we assume that (23) complies with homogeneous Neumann boundary conditions

on the complementary part of the boundary. This leads to the following weak formulation:

$$\begin{aligned} (\mathbf{u}, p) : (0, \tau) &\rightarrow (\ell_{\varphi' \circ M^{-1}} + [H_{0, \Gamma}^1(\Omega)]^d) \times L^2(\Omega) : \\ a_f(\mathbf{u}, p, \mathbf{v}, q) &= b_f(\mathbf{v}, q) \quad \forall (\mathbf{v}, q) \in [H_{0, \Gamma}^1(\Omega)]^d \times L^2(\Omega) \end{aligned}$$

everywhere in $(0, \tau)$ with

$$\begin{aligned} a_f(\mathbf{u}, p, \mathbf{v}, q) &= \int_{\Omega} [\rho \mathbf{u}', \mathbf{v}] + \int_{\Omega} [\operatorname{div} \rho \mathbf{u} \mathbf{u}, \mathbf{v}] + \nu \int_{\Omega} [\nabla \mathbf{u}, \nabla \mathbf{v}] \\ &\quad - \int_{\Omega} p \operatorname{div} \mathbf{v} - \int_{\Omega} q \operatorname{div} \mathbf{u} \\ b_f(\mathbf{v}, q) &= \int_{\Omega} [\mathbf{f}, \mathbf{v}] \end{aligned}$$

It is to be noted that the kinematic condition (25a) is imposed by means of the lift operator $\ell_{\varphi' \circ M^{-1}}$. Similar to (4), the interface contribution to the structural load functional, b_s , can be recast into:

$$\begin{aligned} \int_{\bar{\Gamma}} [((p\mathbf{n} - \nu \partial_n \mathbf{u})J) \circ M, \mathbf{w}] &= \int_{\Gamma} [p\mathbf{n} - \nu \partial_n \mathbf{u}, \mathbf{w} \circ M^{-1}] \\ &= a_f(\mathbf{u}, p, \ell_{\mathbf{w} \circ M^{-1}}, q) - b_f(\ell_{\mathbf{w} \circ M^{-1}}, q) \end{aligned} \quad (26)$$

for arbitrary q . The first identity follows from a transformation of the integral from $\bar{\Gamma}$ to Γ .

In analogy with the model problem, the coupling between the fluid and the structure occurs through a flux functional in the structure subproblem, and this flux functional is appropriately evaluated by pairing the residual functional of the fluid subproblem with a lift of the structure test function. Moreover, direct evaluation of the flux $p\mathbf{n} - \nu \partial_n \mathbf{u}$ corresponds to an unbounded operator. We refer to [15; 16] for further elaboration on traction evaluation in fluid–structure interaction.

We remark that the traction extraction encoded by the final expression in (26) actually corresponds to the continuity of the test function between the fluid and structure subsystems; see, for instance, [17]. In so-called *generalized-continuum* formulations of fluid–structure interaction, such continuity of test (and trial) functions is intrinsic.

5.3 Electro-osmosis

Finally, we consider the analogy between the model problem in (1) and electro-osmosis applications. Electro-osmosis refers to the phenomenon that a fluid in a channel moves under the effect of an electric field aligned with the channel wall, by virtue of the electric double layer (the *Debye layer*) that develops between the fluid and the channel wall. The electric field induces a force on the charged particles of the double layer, and viscous forces in the fluid in turn drive the bulk fluid in the direction of the electric field.

A standard model of electro-osmosis is the Helmholtz–Smoluchowski wall-slip model. This model assumes that the body-force term in the Navier–Stokes equations engendered by the electric double layer can be replaced by an effective slip velocity on the boundary, given by $\mathbf{u}_{\text{wall}} = (\varkappa \Psi_0 / \nu) \mathbf{E}$, with \varkappa and ν being the dielectric constant and viscosity of the fluid, respectively, Ψ_0 the electric zeta potential of the wall and \mathbf{E} the applied electric field. This approximation has been validated through both experiments and numerical simulations

[18]. The Helmholtz–Smoluchowski model of electro-osmosis translates into a boundary-coupled problem of the form:

$$-\operatorname{div}(\sigma \nabla \phi) = 0 \quad \text{in } \Omega \quad (27a)$$

$$\partial_n \phi = 0 \quad \text{on } \Gamma \quad (27b)$$

$$-\Delta \mathbf{u} + \nabla p = 0 \quad \text{in } \Omega \quad (27c)$$

$$-\operatorname{div} \mathbf{u} = 0 \quad \text{in } \Omega \quad (27d)$$

$$\mathbf{u} = -\nabla \phi \quad \text{on } \Gamma \quad (27e)$$

where σ denotes the electric conductivity of the fluid, ϕ denotes the electric potential and Γ represents the channel wall. The auxiliary boundary conditions are irrelevant for the exposition below. We refer to [19] for further details, including different formulations and an elaboration of the numerical experiments in this section.

A fundamental complication in the numerical approximation of (27) concerns the enforcement of the Dirichlet boundary condition (27e) for the fluid. A naive approach would be to impose this condition strongly in the space for \mathbf{u} . Accordingly, (27) would be condensed into the weak formulation:

$$\begin{aligned} (\phi, \mathbf{u}, p) &\in H^1(\Omega) \times (\ell_{-\nabla \phi} + H_0^1(\Omega)) \times L^2(\Omega) \\ a_f(\mathbf{u}, p, \mathbf{v}_0, q) + a_e(\phi, \psi) &= 0 \\ \forall (\psi, \mathbf{v}_0, q) &\in H^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega) \end{aligned} \quad (28)$$

where

$$\begin{aligned} a_f(\mathbf{u}, p, \mathbf{v}, q) &= \int_{\Omega} [\nabla \mathbf{u}, \nabla \mathbf{v}] - \int_{\Omega} p \operatorname{div} \mathbf{v} - \int_{\Omega} q \operatorname{div} \mathbf{u} \\ a_e(\phi, \psi) &= \int_{\Omega} \sigma [\nabla \phi, \nabla \psi] \end{aligned}$$

To elucidate the structure of (28), we modify the formulation by imposing the Dirichlet boundary condition (27e) by via a Lagrange multiplier. We then obtain the following equivalent formulation:

$$\begin{aligned} (\phi, \mathbf{u}, p) &\in H^1(\Omega) \times H^1(\Omega) \times L^2(\Omega) \\ a_f(\mathbf{u}, p, \mathbf{v}_0, q) + a_e(\phi, \psi) + \int_{\Gamma} [\mathbf{u} + \nabla \phi, \boldsymbol{\beta}] &= 0 \\ \forall (\psi, \mathbf{v}_0, q, \boldsymbol{\beta}) &\in H^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega) \times T \end{aligned} \quad (29)$$

where T represents a suitable (vector-valued) trace space on Γ . Formulation (29) conveys that the normal component of \mathbf{u} in the above formulations corresponds to a direct evaluation of the electric flux $\partial_n \phi$. In formulation (29), the direct flux evaluation is manifested by the (unbounded) functional $\boldsymbol{\beta} \mapsto \int_{\Gamma} ([\mathbf{u}, \mathbf{n}] + \partial_n \phi) [\boldsymbol{\beta}, \mathbf{n}]$. In a similar manner as for the model problem, the dual formulation of (29) (or (28)) exhibits unstable behavior; see Figure 3. We remark that the enforcement of the tangential component generally does not present a problem, by virtue of tangential integration-by-parts identities. Detailed discussion of this matter is beyond the scope of this paper; see [19].

To avoid direct flux evaluation, a formulation based on flux extraction can be considered:

$$\begin{aligned} (\phi, \mathbf{u}, p) &\in H^1(\Omega) \times H^1(\Omega) \times L^2(\Omega) \\ a_f(\mathbf{u}, p, \mathbf{v}_0, q) + a_e(\phi, \psi + \ell_{[\boldsymbol{\beta}, \mathbf{n}]}) & \\ + \int_{\Gamma} [\mathbf{u} + [\nabla \phi, \mathbf{t}] \mathbf{t}, \boldsymbol{\beta}] &= 0 \\ \forall (\psi, \mathbf{v}_0, q, \boldsymbol{\beta}) &\in H^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega) \times T \end{aligned} \quad (30)$$

Note that the test-function pair $(\mathbf{v}_0, \boldsymbol{\beta})$ can not be combined into a single test function in $H^1(\Omega)$, because \mathbf{v}_0 appears separately in (30). However, if we identify $\boldsymbol{\beta}$ with the rescaled trace of a function $\mathbf{v} \in H_0^1(\Omega)$ according to $\boldsymbol{\beta} = \frac{1}{\epsilon} \mathbf{v}|_{\Gamma}$, then we can derive the inconsistent penalty formulation:

$$\begin{aligned} (\phi_{\epsilon}, \mathbf{u}_{\epsilon}, p_{\epsilon}) &\in H^1(\Omega) \times H^1(\Omega) \times L^2(\Omega) \\ a_f(\mathbf{u}_{\epsilon}, p_{\epsilon}, \mathbf{v}, q) + a_e(\phi_{\epsilon}, \psi + \frac{1}{\epsilon} \ell_{[\mathbf{v}, \mathbf{n}]}) & \\ + \int_{\Gamma} \frac{1}{\epsilon} [\mathbf{u} + [\nabla \phi, \mathbf{t}] \mathbf{t}, \mathbf{v}] &= 0 \\ \forall (\psi, \mathbf{v}, q) &\in H^1(\Omega) \times H^1(\Omega) \times L^2(\Omega) \end{aligned} \quad (31)$$

One can show that $(\phi_{\epsilon}, \mathbf{u}_{\epsilon}, p_{\epsilon})$ converges to the solution of the electro-osmosis problem as $\epsilon \rightarrow 0$. The modified formulation (31) allows a convenient implementation of both the primal and corresponding dual problems. Essentially, formulation (31) replaces the Dirichlet condition (27e) by the mixed condition

$$(\partial_n \mathbf{u} - p \mathbf{n}) + \frac{1}{\epsilon} (\mathbf{u} + \nabla \phi) = 0 \quad (32)$$

Equation (32) corresponds to regularization of the boundary condition (27e) by means of a penalty method.

It is to be mentioned that an alternative method for the weak enforcement of Dirichlet boundary conditions is provided by Nitsche's Verfahren [20; 21]. However, Nitsche's Verfahren relies on a direct-flux-type term in the variational formulation. Accordingly, the corresponding bilinear or semilinear form is unbounded, unless the functional setting is appropriately modified.

To illustrate the difference between the dual problems corresponding to the unstable formulation (28) and the regularized formulation (31), we consider an electro-osmosis problem on the quadrangle $\Omega = (0, 5) \times (0, 1)$. The electric conductivity is set to $\sigma(x_1, x_2) = 1 + x_1$. The functional of interest that appears on the right-hand side of the dual problem is chosen here as the flow rate $J(\phi, \mathbf{u}, p) = \int_{\Gamma_O} [\mathbf{u}, \mathbf{n}]$ with $\Gamma_O = \{(x_1, x_2) \in \partial \Omega : x_1 = 5\}$. The regularization parameter is set to $\epsilon = 10^{-10}$. Simulations are performed using the `libMesh` Finite Element library [22]. Figures 3 and 4 present the dual electric fields for the unstable formulation (28) based on direct flux evaluation and the regularized formulation (31), respectively. Figure 3 illustrates that direct flux evaluation leads to oscillations in the dual electric field at the channel wall. In contrast, the dual solution obtained from the regularized formulation (31) in Figure 4 is smooth. This dual solution is appropriate for error estimation and adaptive mesh refinement; see [19].

6 Conclusion

Motivated by the fundamental importance of flux evaluation in boundary-coupled problems, we presented an analysis of flux-evaluation formulations. Based on a generic model problem, we showed that direct flux evaluation is characterized by an unbounded operator. We moreover established that proper flux extraction, corresponding to a pairing of the residual functional of the boundary-value problem with a lifted test function, does not suffer from this deficiency.

By means of numerical experiments, we showed that in finite-element approximations, direct flux evaluation and flux extraction yield a different behavior in the approximate solutions. For a problem with a regular solution, both methods exhibit the same optimal rate of convergence under mesh refinement, but the constant in the error bound is much smaller for flux extraction than for direct flux evaluation. For a problem with a singular solution, flux extraction yields a faster

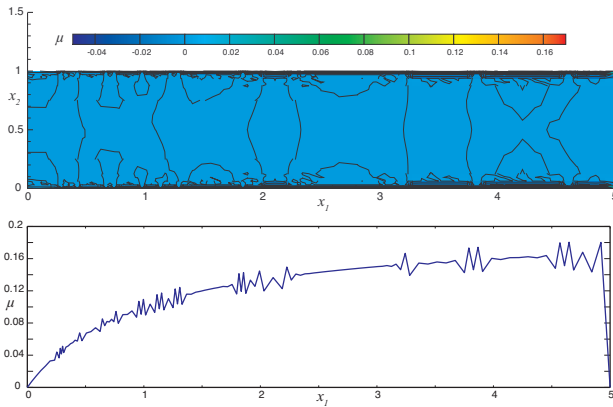


Fig. 3 Dual electric potential (μ) of the adjoint electro-osmosis problem corresponding to the formulation (28) based on direct flux evaluation (top) and its trace on the bottom boundary (bottom).

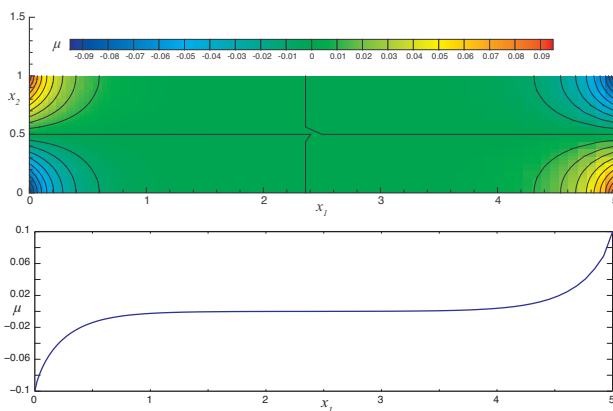


Fig. 4 Dual electric potential (μ) of the adjoint electro-osmosis problem corresponding to the regularized formulation (31) (top) and its trace on the bottom boundary (bottom).

rate of convergence: for direct flux evaluation, the error decays as $O(h^{2/3})$, while for flux extraction the error decays as $O(h^{4/3})$, as the mesh width h tends to 0.

For the model coupled problem, we showed that solutions to dual problems corresponding to the two flux-evaluation formulations behave very differently. We established that the dual problem associated with flux extraction represents a weak formulation of a well-defined boundary-value problem, as opposed to the dual problem pertaining to direct flux evaluation. In the numerical experiments, we showed that the dual solution associated with direct flux evaluation displays non-smooth behavior near the boundary, while the dual solution associated with flux extraction exhibits a smooth solution.

Finally, we considered the extension of the results for the generic model problem to three classes of boundary-coupled problems, viz., free-boundary problems, fluid-structure interaction, and electro-osmosis.

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