

1 **SHAPE OPTIMIZATION OF STOKESIAN PERISTALTIC PUMPS USING BOUNDARY
2 INTEGRAL METHODS**

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4 **Abstract.** This article presents a new boundary integral approach for finding optimal shapes of peristaltic pumps that
5 transport a viscous fluid. Formulas for computing the shape derivatives of the standard cost functionals and constraints are
6 derived. They involve evaluating physical variables (traction, pressure, etc.) on the boundary only. By employing these
7 formulas in conjunction with a boundary integral approach for solving forward and adjoint problems, we completely avoid the
8 issue of volume remeshing when updating the pump shape as the optimization proceeds. This leads to significant cost savings
9 and we demonstrate the performance on several numerical examples.

10 **Key words.** Shape sensitivity analysis, integral equations, fast algorithms

11 **1. Introduction.** Many physiological flows are realized owing to *peristalsis*, a transport mechanism
12 induced by periodic contraction waves in fluid-filled (or otherwise) tubes/vessels [12, 9, 3]. This mechanism
13 is used in engineering applications like microfluidics, organ-on-a-chip devices and MEMS devices for trans-
14 porting and mixing viscous fluids at small scale (e.g., see [27, 30, 25, 15, 32, 7]). Owing to its importance
15 in science and technological applications, numerous analytical and numerical studies were carried out in
16 the past decades to characterize the fluid dynamics of peristalsis in various physical scenarios; some recent
17 works include [26, 28, 14] for non-Newtonian flows and [5, 1, 13] for particle transport.

18 Several applications—optimal transport of drug particles in blood flow [19], understanding sperm motil-
19 ity in the reproductive tract [24], propulsion of soft micro-swimmers [8, 23]—require scalable numerical
20 methods that can handle arbitrary shape deformations. One of the challenges of existing mesh-based meth-
21 ods (e.g., finite element methods) is the high computational expense of re-meshing, needed to proceed
22 between optimization updates or in transient solution of the forward/adjoint problems. Boundary integral
23 equation (BIE) methods, on the other hand, avoid volume discretization altogether for linear partial dif-
24 ferential equations (PDEs) and are highly scalable even for moving geometry problems [22]. While BIE
25 methods have been used widely for shape optimization problems, including in linear elasticity, acoustics,
26 electrostatics, electromagnetics and heat flow (e.g., [17, 33, 2, 31, 10]), we are not aware of their application
27 to optimization of peristaltic pumps transporting simple (or complex) fluids.

28 The primary goal of this work is to derive shape sensitivity formulas that can be used in conjunction
29 with an indirect BIE method to enable fast numerical optimization routines. Our work is inspired by that
30 of Walker and Shelley [29] who considered the shape optimization of a peristaltic pump transporting a
31 Newtonian fluid at low to moderate Reynolds numbers (Re) and applied a finite element discretization.
32 Here, we restrict our attention to problems in the zero Re limit only. Following [29], we consider shapes
33 that minimize the input fluid power under constant volume and flow rate constraints. The forward problem
34 requires solving the Stokes equations in a tube with periodic flow conditions and prescribed slip on the walls
35 while the adjoint problem has a prescribed pressure drop condition across the tube. For both problems, we
36 employ the recently developed periodic BIE solver of Marple et al. [18]; the primary advantage compared
37 to classical BIE methods that rely on periodic Green’s functions is that the required slip or pressure-drop
38 conditions can be applied directly.

39 The paper is organized as follows. In Section 2, we define the shape optimization problem and the PDE
40 formulation of the forward problem in strong and weak forms. In Section 3, we derive the shape sensitivity
41 formulas for a specific objective function and the functionals required to impose the given constraints on
42 the pump shape. Using these formulas, we present a numerical optimization procedure in Section 4 based
43 on a periodic boundary integral equation formulation for the PDE solves. We present validation and shape
44 optimization results in Section 5 followed by conclusions in Section 6.

45 **2. Problem formulation.**

46 **2.1. Formulation of the wall motion.** Pumping is achieved by the channel wall shape moving
47 along the positive direction e_1 at a constant velocity c , as a traveling wave of wavelength L (the wave

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48 period therefore being $T = L/c$). The quantities L, c (and hence T) are considered as fixed in the wall
49 shape optimization process. This apparent shape motion is achieved by a suitable material motion of the
50 wall, whose material is assumed to be flexible but inextensible. Like in [29], it is convenient to introduce
51 a *wave frame* that moves along with the traveling wave, i.e. with velocity ce_1 relative to the (fixed) lab
52 frame.

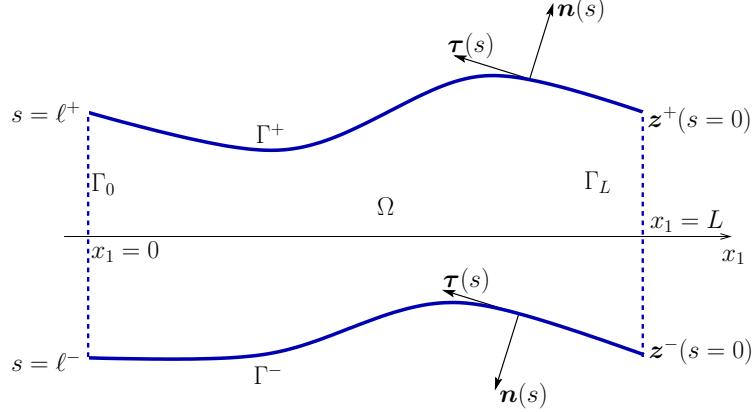


FIG. 2.1. *Channel in wave frame, 2D configuration: geometry and notation*

53 Let then Ω denote, in the wave frame, the fluid region enclosed in one wavelength of the channel (see
54 Fig. 2.1), whose boundary is $\partial\Omega = \Gamma \cup \Gamma_p$. The wall $\Gamma := \Gamma^+ \cup \Gamma^-$, which is fixed in this frame, has
55 disconnected components Γ^\pm which are not required to achieve symmetry with respect to the x_1 axis and
56 have respective lengths ℓ^\pm . The remaining contour $\Gamma_p := \Gamma_0 \cup \Gamma_L$ consists of the periodic planar end-sections
57 Γ_0 and Γ_L , respectively situated at $x_1 = 0$ and $x_1 = L$; the endpoints of Γ_L are denoted by z^\pm (Fig. 2.1).
58 Both channel walls are described as arcs $s \mapsto \mathbf{x}^\pm(s)$ with the arclength coordinate s directed “leftwards” as
59 depicted in Fig. 2.1, whereas the unit normal \mathbf{n} to $\partial\Omega$ is everywhere taken as outwards to Ω . The position
60 vector $\mathbf{x}(s)$, unit tangent $\tau(s)$, unit normal $\mathbf{n}(s)$ and curvature $\kappa(s)$ obey the Frenet formulas

61 (2.1)
$$\mathbf{x}_{,s} = \tau, \quad \tau_{,s} = \kappa \mathbf{n}, \quad \mathbf{n}_{,s} = -\kappa \tau \quad \text{on } \Gamma^+ \text{ and } \Gamma^-.$$

62 The opposite orientations of (τ, \mathbf{n}) on Γ^+ and Γ^- resulting from our choice of conventions imply opposite
63 sign conventions on the curvature, which is everywhere on Γ taken as $\kappa := \tau_{,s} \cdot \mathbf{n}$ for overall consistency.

64 In the wall frame, the wall material velocity must be tangent to Γ (wall material points being constrained
65 to remain on the surface Γ); moreover the wall material is assumed to be inextensible. In the wave frame,
66 the wall material velocities \mathbf{U} satisfying both requirements must have, on each wall, the form

67
$$\mathbf{U}(s) = U\tau(s),$$

68 where U is a constant. Moreover, in the wave frame, all wall material points travel over an entire spatial
69 period during the time interval $T = L/c$, which implies $U = cl/L$. Finally, the viscous fluid must obey a
70 no-slip condition on the wall, so that the velocity of fluid particles adjacent to $\mathbf{x}(s)$ is $\mathbf{U}(s)$. Concluding,
71 the pumping motion of the wall constrains on each wall the fluid motion through

72 (2.2)
$$\mathbf{u}(\mathbf{x}) = \mathbf{u}^D(\mathbf{x}) := \frac{\ell^\pm}{L} c \tau^\pm(\mathbf{x}), \quad \mathbf{x} \in \Gamma^\pm,$$

73 REMARK 1. The no-slip condition $\mathbf{u} = \tau$ proposed in [29], which corresponds with the present notations
74 to setting $U = c$, is inconsistent with the period $T = L/c$ of the traveling wave, unless the channel is straight
75 ($\ell^\pm = L$). This discrepancy alters the boundary condition (2.2) and hence the shape optimization problem
76 (the value of the power loss functional for given wall shape being affected in wall shape-dependent fashion).

77 **2.2. PDE formulation of forward problem.** The stationary Stokes flow in the wave frame [29]
 78 solves the governing PDE formulation

79 (2.3) (a) $\operatorname{div} \boldsymbol{\sigma}[\mathbf{u}, p] = \mathbf{0}$ in Ω (balance of momentum)
 (b) $\boldsymbol{\sigma}[\mathbf{u}, p] = -p\mathbf{I} + 2\mu\mathbf{D}[\mathbf{u}]$ in Ω (constitutive relation)
 (c) $\operatorname{div} \mathbf{u} = 0$ in Ω (incompressibility)
 (d) $\mathbf{u} = \mathbf{u}^D$ on Γ (Dirichlet BC on wall)
 (e) \mathbf{u} periodic on Γ_p

80 where \mathbf{u}, p are the velocity and pressure, $\mathbf{D}[\mathbf{u}] := (\nabla \mathbf{u} + \nabla^T \mathbf{u})/2$ is the strain rate tensor, and $\boldsymbol{\sigma}[\mathbf{u}, p]$ is the
 81 stress tensor. Equations (2.3a,b,c) respectively express the local balance of momentum (absent any body
 82 forces), the constitutive relation (μ being the dynamic viscosity) and the incompressibility condition. The
 83 prescribed wall velocity \mathbf{u}^D is given by (2.2). Problem (2.3) defines p up to an arbitrary additive constant.

84 **2.3. Weak formulation of forward problem.** In this study, flow computations rely on a boundary
 85 integral equation formulation, see Section 4.3. It is however convenient, for later establishment of shape
 86 derivative identities, to recast the forward problem (2.3) as a mixed weak formulation (e.g. [4], Chap. 6):

87 (2.4) find $\mathbf{u} \in \mathbf{V}$, $p \in \mathcal{P}$, $\mathbf{f} \in \mathcal{F}$, $\begin{cases} (a) & a(\mathbf{u}, \mathbf{v}) - b(\mathbf{v}, p) - \langle \mathbf{f}, \mathbf{v} \rangle_\Gamma = 0 & \forall \mathbf{v} \in \mathbf{V} \\ (b) & b(\mathbf{u}, q) = 0 & \forall q \in \mathcal{P} \\ (c) & \langle \mathbf{u}^D, \mathbf{g} \rangle_\Gamma - \langle \mathbf{u}, \mathbf{g} \rangle_\Gamma = 0 & \forall \mathbf{g} \in \mathcal{F} \end{cases}$

88 where $\langle \cdot, \cdot \rangle_\Gamma$ stands for the $L^2(\Gamma)$ duality product, and the bilinear forms a and b are defined by

89
$$a(\mathbf{u}, \mathbf{v}) = \int_{\Omega} 2\mu\mathbf{D}[\mathbf{u}]:\mathbf{D}[\mathbf{v}] \, dV, \quad b(\mathbf{v}, q) = \int_{\Omega} q \operatorname{div} \mathbf{v} \, dV$$

90 The function spaces in problem (2.4) are as follows: \mathbf{V} is the space of all periodic vector fields contained in
 91 $H^1(\Omega; \mathbb{R}^2)$, \mathcal{P} is the space of all $L^2(\Omega)$ functions with zero mean (i.e. obeying the constraint $\langle p, 1 \rangle_\Omega = 0$)
 92 and $\mathcal{F} = H^{-1/2}(\Gamma; \mathbb{R}^2)$. The chosen definition of \mathcal{P} caters for the fact that p would otherwise be defined only
 93 up to arbitrary additive constants. The Dirichlet boundary condition (2.3d) is (weakly) enforced explicitly
 94 through (2.4c), rather than being embedded in the velocity solution space \mathbf{V} , as this will facilitate the
 95 derivation of shape derivative identities. The unknown \mathbf{f} , which acts as the Lagrange multiplier associated
 96 with the Dirichlet boundary condition (2.3d), is in fact the force density (i.e stress vector) $\boldsymbol{\sigma}[\mathbf{u}, p] \cdot \mathbf{n}$.

97 **2.4. Formulation of optimization problem, objective functional.** We address the problem of
 98 finding the channel shape that makes peristaltic pumping most efficient, i.e., leads to minimum power loss
 99 for given mass flow rate. The power loss cost functional [29] is defined by

100 (2.5)
$$J_{PL}(\Omega) := \langle \mathbf{f}_\Omega, (\mathbf{u}^D + c\mathbf{e}_1) \rangle_\Gamma.$$

101 It is a shape functional in that its value is completely determined by the domain Ω (in a partly implicit way
 102 through \mathbf{f}_Ω). The minimization of $J_{PL}(\Omega)$, as in [29], subject to two constraints, involves two other shape
 103 functionals:

104 (a) The channel volume per wavelength has a prescribed value V_0 :

105 (2.6)
$$C_V(\Omega) := |\Omega| - V_0 = 0$$

106 (b) The mass flow rate per wavelength $Q(\Omega)$ has a prescribed value Q_0 . Expressing this constraint in the
 107 wave frame gives:

108 (2.7)
$$C_Q(\Omega) := Q(\Omega) - Q_0 = 0 \quad \text{with} \quad Q(\Omega) = \frac{1}{L} \int_{\Omega} (\mathbf{u}_\Omega + c\mathbf{e}_1) \cdot \mathbf{e}_1 \, dV.$$

109 **REMARK 2.** The power loss functional $J_{PL}(\Omega)$ is insensitive to modification of p by an additive constant.
 110 This is seen, for instance, by combining (2.4a) with $\mathbf{v} = \mathbf{u} + c\mathbf{e}_1$ and (2.4b) with $q = p$, which yields

111
$$J_{PL}(\Omega) = \langle \mathbf{f}_\Omega, (\mathbf{u}^D + c\mathbf{e}_1) \rangle_\Gamma = a(\mathbf{u}_\Omega, \mathbf{u}_\Omega).$$

112 **3. Shape sensitivities.** In this section, we review available shape derivative concepts that address
 113 our needs. Rigorous expositions of shape sensitivity theory can be found in [6, Chaps. 8,9] or [11, Chap.
 114 5].

115 **3.1. Shape sensitivity analysis: an overview.** Let $\Omega_{\text{all}} \subset \mathbb{R}^2$ denote a fixed domain chosen so that
 116 $\Omega \Subset \Omega_{\text{all}}$ always holds for the shape optimization problem of interest. Shape changes are described with
 117 the help of *transformation velocity* fields, i.e. vector fields $\boldsymbol{\theta} : \Omega_{\text{all}} \rightarrow \mathbb{R}^2$ such that $\boldsymbol{\theta} = \mathbf{0}$ in a neighborhood
 118 $\partial\Omega_{\text{all}}$. Then, shape perturbations of domains $\Omega \Subset \Omega_{\text{all}}$ can be mathematically described using a pseudo-time
 119 η and a geometrical transform of the form

$$120 \quad (3.1) \quad x \in \Omega_{\text{all}} \mapsto x^\eta = x + \eta \theta(x),$$

121 which defines a parametrized family of domains $\Omega_\eta(\boldsymbol{\theta}) := (\mathbf{I} + \eta\boldsymbol{\theta})(\Omega)$ for any given “initial” domain $\Omega \Subset \Omega_{\text{all}}$.
 122 The affine format (3.1) is sufficient for defining the first-order derivatives at $\eta = 0$ used in this work.

123 **Assumptions on shape transformations, admissible shapes.** The set \mathcal{O} of admissible shapes for
 124 the fluid region Ω in a channel period (in the wave frame) is defined as

$$125 \quad (3.2) \quad \mathcal{O} = \{\Omega \subset \Omega_{\text{all}}, \Omega \text{ is periodic and simply connected, } |\Omega| = V_0, Q(\Omega) = Q_0\}.$$

126 Accordingly, let the space Θ of admissible transformation velocities be defined as

$$^{127} \quad (3.3) \quad \Theta = \{ \boldsymbol{\theta} \in W^{1,\infty}(\Omega_{\text{all}}) \text{ such that } \begin{array}{l} \text{(i) } \boldsymbol{\theta}|_{\Gamma_0} = \boldsymbol{\theta}|_{\Gamma_L}, \text{ (ii) } \boldsymbol{\theta} \cdot \mathbf{e}_1 = 0 \text{ on } \Gamma_0, \text{ (iii) } \boldsymbol{\theta}(z^-) = \mathbf{0} \end{array} \},$$

ensuring that the shape perturbations (i) are periodic, (ii) prevent any deformation of the end sections Γ_p^\pm along the axial direction, and (iii) prevent vertical rigid translations of the channel domain. The provision $\boldsymbol{\theta} \in W_0^{1,\infty}(\Omega_{\text{all}})$ ensures that (a) there exists $\eta_0 > 0$ such that $\Omega_\eta(\boldsymbol{\theta}) \Subset \Omega_{\text{all}}$ for any $\eta \in [0, \eta_0]$, and (b) the weak formulation for the shape derivative of the forward solution is well defined if the latter belongs to the standard solution space. Note that the volume and flow rate constraints (2.6), (2.7) are not embedded in $\boldsymbol{\Theta}$; they will be accounted for via a Lagrangian.

134 **Material derivatives.** In what follows, all derivatives are implicitly taken at some given configuration
 135 Ω , i.e. at initial "time" $\eta = 0$. The "initial" material derivative $\dot{\mathbf{a}}$ of some (scalar or tensor-valued) field
 136 variable $\mathbf{a}(\mathbf{x}, \eta)$ is defined as

$$\dot{\mathbf{a}}(\mathbf{x}) = \lim_{\eta \rightarrow 0} \frac{1}{\eta} [\mathbf{a}(\mathbf{x}^\eta, \eta) - \mathbf{a}(\mathbf{x}, 0)] \quad \mathbf{x} \in \Omega,$$

138 and the material derivative of gradients and divergences of tensor fields are given by

$$(a) \quad (\nabla a)^* = \nabla \dot{a} - \nabla a \cdot \nabla \theta, \quad (b) \quad (\operatorname{div} a)^* = \operatorname{div} \dot{a} - \nabla a : \nabla \theta$$

140 Likewise, the first-order “initial” derivative J' of a shape functional $J : \mathcal{O} \rightarrow \mathbb{R}$ is defined as

$$\langle J'(\Omega), \theta \rangle = \lim_{\eta \rightarrow 0} \frac{1}{\eta} (J(\Omega_\eta(\theta)) - J(\Omega)).$$

142 **Material differentiation of integrals.** Consider, for given transformation velocity field $\theta \in \Theta$, generic
143 domain and contour integrals

$$144 \quad (3.4) \quad \text{(a)} \quad I_V(\eta) = \int_{\Omega_\eta(\boldsymbol{\theta})} F(\cdot, \eta) \, dV, \quad \text{(b)} \quad I_S(\eta) = \int_{S_\eta(\boldsymbol{\theta})} F(\cdot, \eta) \, ds,$$

145 where $\Omega_\eta(\boldsymbol{\theta}) = (\mathbf{I} + \eta\boldsymbol{\theta})(\Omega)$ is a variable domain and $S_\eta(\boldsymbol{\theta}) := (\mathbf{I} + \eta\boldsymbol{\theta})(S)$ a (possibly open) variable curve.
 146 The derivatives of $I_V(\eta)$ and $I_S(\eta)$ are given by the material differentiation identities

$$147 \quad (3.5) \quad (a) \quad \frac{dI_V}{d\eta} \Big|_{\eta=0} = \int_{\Omega} [\dot{F} + F(\cdot, 0) \operatorname{div} \boldsymbol{\theta}] \, dV, \quad (b) \quad \frac{dI_S}{d\eta} \Big|_{\eta=0} = \int_S [\dot{F} + F(\cdot, 0) \operatorname{div}_S \boldsymbol{\theta}] \, ds,$$

148 which are well-known material differentiation formulas of continuum kinematics. In (3.5b), div_S stands for
 149 the tangential divergence operator, which in the present 2D context is given, with κ denoting the curvature
 150 (see Sec. A.1) by

$$151 \qquad \qquad \qquad \text{div}_S \theta = (I - n \otimes n) : \nabla \theta = \partial_s \theta_s - \kappa \theta_n$$

152 where we have set $\boldsymbol{\theta}$ on Γ , using the notations and conventions introduced in (2.1), in the form

$$153 \quad \boldsymbol{\theta} = \theta_s \boldsymbol{\tau} + \theta_n \mathbf{n}.$$

154 **Shape functionals and structure theorem.** The structure theorem for shape derivatives (see e.g. [6,
155 Chap. 8, Sec. 3.3]) then states that the derivative of any shape functional J is a linear functional in the
156 normal transformation velocity $\theta_n = \mathbf{n} \cdot \boldsymbol{\theta}|_{\partial\Omega}$. For PDE-constrained shape optimization problems involving
157 sufficiently smooth domains and data, the derivative $\langle J'(\Omega), \boldsymbol{\theta} \rangle$ has the general form

$$158 \quad (3.6) \quad \langle J'(\Omega), \boldsymbol{\theta} \rangle = \int_{\partial\Omega} g \theta_n \, ds$$

159 where g is the *shape gradient* of J . The structure theorem intuitively means that (i) the shape of Ω_η is
160 determined by that of $\partial\Omega_\eta$, and (ii) tangential components of $\boldsymbol{\theta}$ leave Ω_η unchanged at leading order $O(\eta)$.

161 **Example: shape derivative of channel volume constraint..** Since $|\Omega|$ is given by (3.4a) with
162 $F = 1$, this purely geometric constraint is readily differentiated using (3.5a) and Green's theorem, to obtain

$$163 \quad (3.7) \quad \langle C'_V(\Omega), \boldsymbol{\theta} \rangle = \int_{\Omega} \operatorname{div} \boldsymbol{\theta} \, dV = \int_{\partial\Omega} \theta_n \, ds = \int_{\Gamma} \theta_n \, ds,$$

164 where the last equality results from provision (ii) in (3.3).

165 **3.2. Shape derivative of forward solution.** The power loss and the mass flow rate constraint are
166 expressed in terms of functionals J_{PL} and C_Q that depend on Ω implicitly through the solution $(\mathbf{u}, \mathbf{f}, p)$
167 of the forward problem. Finding their shape derivatives will then involve the solution derivative $(\mathbf{u}, \mathbf{f}, p)^*$.
168 Setting up the governing problem for $(\mathbf{u}, \mathbf{f}, p)^*$ is then a necessary prerequisite.

169 **PROPOSITION 1.** *The governing weak formulation for the shape derivative $(\dot{\mathbf{u}}, \dot{\mathbf{f}}, \dot{p})$ of the solution
170 $(\mathbf{u}, \mathbf{f}, p)$ of problem (2.4) is*

$$171 \quad (3.8) \quad \begin{aligned} (a) \quad a(\dot{\mathbf{u}}, \mathbf{v}) - b(\mathbf{v}, \dot{p}) - \langle \dot{\mathbf{f}}, \mathbf{v} \rangle_{\Gamma} &= -a^1(\mathbf{u}, \mathbf{v}, \boldsymbol{\theta}) + b^1(\mathbf{v}, p, \boldsymbol{\theta}) - \langle \mathbf{f}, \mathbf{v} \operatorname{div}_{\mathcal{S}} \boldsymbol{\theta} \rangle_{\Gamma} \quad \forall \mathbf{v} \in \mathcal{V} \\ (b) \quad b(\dot{\mathbf{u}}, q) &= -b^1(\mathbf{u}, q, \boldsymbol{\theta}) \quad \forall q \in \mathcal{P} \\ (c) \quad \langle \dot{\mathbf{u}}^D, \mathbf{g} \rangle_{\Gamma} - \langle \dot{\mathbf{u}}, \mathbf{g} \rangle_{\Gamma} &= \langle (\mathbf{u} - \mathbf{u}^D) \operatorname{div}_{\mathcal{S}} \boldsymbol{\theta}, \mathbf{g} \rangle_{\Gamma} \quad \forall \mathbf{g} \in \mathcal{F} \end{aligned}$$

172 with the trilinear forms a^1 and b^1 given by

$$173 \quad (3.9a) \quad a^1(\mathbf{u}, \mathbf{v}, \boldsymbol{\theta}) = \int_{\Omega} 2\mu \left\{ (\mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{v}]) \operatorname{div} \boldsymbol{\theta} - \mathbf{D}[\mathbf{u}] : (\nabla \mathbf{v} \cdot \nabla \boldsymbol{\theta}) - (\nabla \mathbf{u} \cdot \nabla \boldsymbol{\theta}) : \mathbf{D}[\mathbf{v}] \right\} \, dV$$

$$174 \quad b^1(\mathbf{u}, q, \boldsymbol{\theta}) = \int_{\Omega} q [\operatorname{div} \mathbf{u} \operatorname{div} \boldsymbol{\theta} - \nabla \mathbf{u} : \nabla \boldsymbol{\theta}] \, dV$$

176 *Proof.* The proposition is obtained by applying the material differentiation identities (3.5) to the weak
177 formulation (2.4), assuming that the test functions are such that $\dot{\mathbf{v}} = \mathbf{0}$, $\dot{\mathbf{g}} = \mathbf{0}$ and $\dot{q} = 0$, i.e. are convected
178 under the shape perturbation. The latter provision is made possible by the absence of boundary constraints
179 in the adopted definition of $\mathcal{V}, \mathcal{F}, \mathcal{P}$ (Sec. 2.3). \square

180 Moreover, the material derivative $\dot{\mathbf{u}}^D$ of the Dirichlet data \mathbf{u}^D , involved in (3.8c), is given in the following
181 lemma, proved in Sec. A.1:

182 **LEMMA 3.1.** *Let \mathbf{u}^D be the prescribed wall velocity (2.2). On either component of the wall Γ , we have*

$$183 \quad (a) \quad \dot{\mathbf{u}}^D = \frac{c\ell}{L} \dot{\boldsymbol{\tau}} + \frac{c\ell}{L} (\partial_s \theta_n + \kappa \theta_s) \mathbf{n}, \quad \text{with} \quad (b) \quad \dot{\ell} = - \int_0^\ell \kappa \theta_n \, ds$$

184 **REMARK 3.** *The provision $\boldsymbol{\theta} \in W^{1,\infty}(\Omega_{all})$ in (3.3) serves to ensure well-definiteness of the trilinear
185 forms a^1, b^1 introduced in Proposition 1 for any $(\mathbf{u}, p) \in \mathcal{V} \times \mathcal{P}$.*

186 **REMARK 4.** *To maintain the zero-mean constraint on p as Ω is perturbed, the mean of \dot{p} must be fixed
187 through $\langle \dot{p}, 1 \rangle_{\Omega} + \langle p \operatorname{div} \boldsymbol{\theta}, 1 \rangle_{\Omega} = 0$ (this provision plays no actual role in the sequel).*

188 We now state an identity involving the trilinear forms a^1, b^1 that will play a crucial role in the derivation
 189 of convenient shape derivative formulas for the functionals involved in this work. The proof of this result is
 190 given in Sec. A.2

191 **LEMMA 3.2.** *Let (\mathbf{u}, p) and $(\hat{\mathbf{u}}, \hat{p})$ respectively satisfy $\operatorname{div} \mathbf{u} = 0$, $\operatorname{div}(\boldsymbol{\sigma}[\mathbf{u}, p]) = \mathbf{0}$ and $\operatorname{div} \hat{\mathbf{u}} = 0$,
 192 $\operatorname{div}(\boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}]) = \mathbf{0}$ in Ω , with $\boldsymbol{\sigma}[\mathbf{u}, p], \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}]$ given for both states by the constitutive relation (2.3b). Moreover,
 193 assume that $\mathbf{u}, \hat{\mathbf{u}}$ and p are periodic, and set $\mathbf{f} := \boldsymbol{\sigma}[\mathbf{u}, p] \cdot \mathbf{n}$, $\hat{\mathbf{f}} := \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] \cdot \mathbf{n}$ and $\Delta \hat{p}(x_2) := \hat{p}(L, x_2) - \hat{p}(0, x_2)$
 194 (i.e. periodicity is not assumed for \hat{p}). Then, the following identity holds:*

195

$$196 (3.10) \quad a^1(\mathbf{u}, \hat{\mathbf{u}}, \boldsymbol{\theta}) - b^1(\mathbf{u}, \hat{p}, \boldsymbol{\theta}) - b^1(\hat{\mathbf{u}}, p, \boldsymbol{\theta}) \\ 197 = \int_{\Gamma} \left\{ (\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}]) \theta_n - \mathbf{f} \cdot \nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta} - \hat{\mathbf{f}} \cdot \nabla \mathbf{u} \cdot \boldsymbol{\theta} \right\} ds + \int_{\Gamma_L} \Delta \hat{p} (\partial_2 u_1) \theta_2 ds.$$

198

199 *Proof.* See Sec. A.2 □

200 **3.3. Shape derivative of power loss functional.** The derivative of the cost functional (2.5) is
 201 given, using the material differentiation identity (3.5b), by

202 (3.11)
$$\langle J'_{\text{PL}}(\Omega), \boldsymbol{\theta} \rangle = \int_{\Gamma} [\mathbf{f} \cdot \dot{\mathbf{u}}^D + (\mathbf{u}^D + \mathbf{e}_1) \cdot (\dot{\mathbf{f}} + \mathbf{f} \operatorname{div}_S \boldsymbol{\theta})] ds$$

203 in terms of the derivatives $\dot{\mathbf{u}}^D$ of the Dirichlet data and $\dot{\mathbf{f}}$ of the stress vector. The former is given by
 204 Lemma 3.1. The latter is part of the solution of the derivative problem (3.8), whose solution therefore
 205 seems necessary for evaluating $\langle J'_{\text{PL}}(\Omega), \boldsymbol{\theta} \rangle$ in a given shape perturbation $\boldsymbol{\theta}$. However, a more effective
 206 approach allows to bypass the actual evaluation of $\dot{\mathbf{f}}$ by combining the forward and derivative problems
 207 with appropriate choices of test functions:

208 **LEMMA 3.3.** *The following identity holds:*

209
$$\int_{\Gamma} (\mathbf{u}^D + \mathbf{e}_1) \cdot (\dot{\mathbf{f}} + \mathbf{f} \operatorname{div}_S \boldsymbol{\theta}) ds = -a^1(\mathbf{u}, \mathbf{u}, \boldsymbol{\theta}) + 2b^1(\mathbf{u}, p, \boldsymbol{\theta}) + \int_{\Gamma} \mathbf{f} \cdot \dot{\mathbf{u}}^D ds$$

210 *Proof.* Consider the forward problem (2.4) with $(\mathbf{v}, \mathbf{g}, q) = (\dot{\mathbf{u}}, \dot{\mathbf{f}}, \dot{p})$ and the derivative problem (3.8)
 211 with $(\mathbf{v}, \mathbf{g}, q) = (\mathbf{u} + \mathbf{e}_1, \mathbf{f}, p)$. Making these substitutions and forming the combination (3.8a) – (3.8b) –
 212 (3.8c) – (2.4a) + (2.4b) + (2.4c), one obtains

213
$$\int_{\Gamma} \dot{\mathbf{u}}^D \cdot \mathbf{f} ds - \int_{\Gamma} (\mathbf{u}^D + \mathbf{e}_1) \cdot \dot{\mathbf{f}} ds = -a^1(\mathbf{u}, \mathbf{u}, \boldsymbol{\theta}) + 2b^1(\mathbf{u}, p, \boldsymbol{\theta}) + \int_{\Gamma} \mathbf{f} \cdot (2\mathbf{u} + \mathbf{e}_1 - \mathbf{u}^D) \operatorname{div}_S \boldsymbol{\theta} ds$$

214 The Lemma follows from using $\mathbf{u} = \mathbf{u}^D$ on Γ and rearranging the above equality. □

215 Then, using Lemma 3.3 in (3.11) and evaluating $a^1(\mathbf{u}, \mathbf{u}, \boldsymbol{\theta}) - 2b^1(\mathbf{u}, p, \boldsymbol{\theta})$ by means of Lemma 3.2 with
 216 $(\hat{\mathbf{u}}, \hat{\mathbf{f}}, \hat{p}) = (\mathbf{u} + \mathbf{e}_1, \mathbf{f}, p)$ (implying that $\Delta p = 0$), the derivative of J_{PL} is recast in the following form, which
 217 no longer involves the solution of the derivative problem:

218 (3.12)
$$\langle J'_{\text{PL}}(\Omega), \boldsymbol{\theta} \rangle = \int_{\Gamma} \left\{ (2\mu \mathbf{D}[\mathbf{u}] : \mathbf{D}[\mathbf{u}]) \theta_n + 2\mathbf{f} \cdot (\dot{\mathbf{u}}^D - \nabla \mathbf{u} \cdot \boldsymbol{\theta}) \right\} ds$$

219 This expression is still somewhat inconvenient as it involves (through $\mathbf{D}[\mathbf{u}]$) the complete velocity gradient
 220 on Γ . This can be alleviated by using the decomposition

221
$$\nabla \mathbf{u} = \nabla_S \mathbf{u} + \partial_n \mathbf{u} \otimes \mathbf{n}$$

222 of the velocity gradient (where $\nabla_S \mathbf{u}$ and $\partial_n \mathbf{u}$ respectively denote the tangential gradient and the normal
 223 derivative of \mathbf{u}) and expressing $\partial_n \mathbf{u}$ in terms of \mathbf{f} by means of the constitutive relation (2.3b). In view of
 224 the specific form (2.2) of the Dirichlet data, the latter step is here conveniently carried out explicitly (in
 225 Sec. A.3), using curvilinear coordinates, and yields:

LEMMA 3.4. Let $(\mathbf{u}, \mathbf{f}, p)$ solve the forward problem (2.4). On the channel wall Γ , we have

$$(a) \quad \nabla \mathbf{u} = \frac{\kappa c \ell}{L} \mathbf{n} \otimes \boldsymbol{\tau} + \left(\frac{f_s}{\mu} - \frac{\kappa c \ell}{L} \right) \boldsymbol{\tau} \otimes \mathbf{n}, \quad (b) \quad 2\mathbf{D}[\mathbf{u}] = \frac{f_s}{\mu} (\mathbf{n} \otimes \boldsymbol{\tau} + \boldsymbol{\tau} \otimes \mathbf{n}), \quad (c) \quad \mathbf{f} = -p \mathbf{n} + f_s \boldsymbol{\tau}$$

where $f_s := \mathbf{f} \cdot \boldsymbol{\tau}$ (hence the viscous part of \mathbf{f} is tangential to Γ).

Finally, we evaluate the density of the integral in (3.12) using the formulas of Lemmas 3.1 and 3.4. On performing straightforward algebra and rearranging terms, we obtain the following final result for $\langle J'_{PL}(\Omega), \boldsymbol{\theta} \rangle$, which is suitable for a direct implementation using the output of a boundary integral solver:

PROPOSITION 2. The shape derivative of the power loss cost functional J_{PL} in a shape perturbation whose transformation velocity field $\boldsymbol{\theta}$ satisfies assumptions (3.3) is given (with $f_s := \mathbf{f} \cdot \boldsymbol{\tau}$) by

$$\langle J'_{PL}(\Omega), \boldsymbol{\theta} \rangle = \sum_{\epsilon=+,-} \int_{\Gamma^\epsilon} \left\{ \left[2 \frac{c \ell^\epsilon \kappa}{L} f_s - \frac{1}{\mu} f_s^2 \right] \theta_n + \frac{2c}{L} \left(\ell^\epsilon f_s - \ell^\epsilon (\partial_s \theta_n) p \right) \right\} ds.$$

where $\epsilon \in \{+, -\}$ refers to the upper wall Γ^+ or the lower wall Γ^- .

REMARK 5. The shape derivative $\langle J'_{PL}(\Omega), \boldsymbol{\theta} \rangle$ as given by Proposition 2 is a linear functional on $\theta_n|_\Gamma$

(since ℓ is one, see Lemma 3.1), as predicted by the structure theorem. Moreover, it is insensitive to the pressure being possibly defined up to an additive constant: indeed, replacing p with $p + \Delta p$ adds

$$- \frac{2c\ell^+}{L} \int_{\Gamma^+} \partial_s \theta_n ds - \frac{2c\ell^-}{L} \int_{\Gamma^-} \partial_s \theta_n ds$$

to $\langle J'_{PL}(\Omega), \boldsymbol{\theta} \rangle$ as given by Proposition 2, and this quantity vanishes due to the assumed periodicity of θ_n .

3.4. Shape derivative of mass flow rate functional. The derivative of the mass flow rate functional

C_Q , defined by (2.7), is given (recalling (3.7) for the shape derivative of $|\Omega|$) by

$$(3.13) \quad \langle C'_Q(\Omega), \boldsymbol{\theta} \rangle = \langle I'(\Omega), \boldsymbol{\theta} \rangle + \frac{c}{L} \int_{\Gamma} \theta_n ds, \quad \text{with } I(\Omega) := \frac{1}{L} \int_{\Omega} \mathbf{u}_\Omega \cdot \mathbf{e}_1 dV.$$

To evaluate $\langle I'(\Omega), \boldsymbol{\theta} \rangle$, with \mathbf{u} solving the forward problem (2.3), we recast $I(\Omega)$ as an integral over the end section Γ_0 by means of the divergence theorem, recalling that \mathbf{u}_Ω is divergence-free, tangential on Γ and periodic:

$$I(\Omega) = \frac{1}{L} \int_{\Omega} [\operatorname{div}(x_1 \mathbf{u}_\Omega) - x_1 \operatorname{div} \mathbf{u}_\Omega] dV = \frac{1}{L} \left\{ \int_{\Gamma_L} x_1 (\mathbf{u}_\Omega \cdot \mathbf{e}_1) ds - \int_{\Gamma_0} x_1 (\mathbf{u}_\Omega \cdot \mathbf{e}_1) ds \right\} = \int_{\Gamma_L} \mathbf{u}_\Omega \cdot \mathbf{e}_1 ds.$$

Consequently, using identity (3.5b) with provision (ii) of (3.3), we find:

$$(3.14) \quad \langle I'(\Omega), \boldsymbol{\theta} \rangle = \int_{\Gamma_L} (\dot{\mathbf{u}} + \mathbf{u} \operatorname{div}_S \boldsymbol{\theta}) \cdot \mathbf{e}_1 ds = \int_{\Gamma_L} (\dot{u}_1 + u_1 \partial_2 \theta_2) dx_2$$

The forward solution derivative $\dot{\mathbf{u}}$ in the above expression will now be eliminated with the help of an adjoint problem. Let the adjoint state $(\hat{\mathbf{u}}, \hat{\mathbf{f}}, \hat{p})$ be defined as the solution of the mixed weak formulation

$$(3.15) \quad \begin{aligned} (a) \quad a(\hat{\mathbf{u}}, \mathbf{v}) - b(\mathbf{v}, \hat{p}) - \langle \hat{\mathbf{f}}, \mathbf{v} \rangle_{\Gamma} &= -\langle 1, \mathbf{v} \cdot \mathbf{e}_1 \rangle_{\Gamma_0} \quad \forall \mathbf{v} \in \mathcal{V}, \\ (b) \quad b(\hat{\mathbf{u}}, q) &= 0 \quad \forall q \in \mathcal{P}, \\ (c) \quad -\langle \hat{\mathbf{u}}, \mathbf{g} \rangle_{\Gamma} &= 0 \quad \forall \mathbf{g} \in \mathcal{F}. \end{aligned}$$

The adjoint state $(\hat{\mathbf{u}}, \hat{\mathbf{f}}, \hat{p})$ thus results from applying a unit pressure difference $\Delta \hat{p} = 1$ between the channel end sections while prescribing a no-slip condition on the channel walls, i.e. Problem (2.14–2.18) of [18] with homogeneous Dirichlet data on the walls (see Remark 6).

257 Then, combining the adjoint problem (3.15) with $(\mathbf{v}, \mathbf{g}, q) = (\dot{\mathbf{u}}, \dot{\mathbf{f}}, \dot{p})$ and the derivative problem (3.8)
258 with $(\mathbf{v}, \mathbf{g}, q) = (\hat{\mathbf{u}}, \hat{\mathbf{f}}, \hat{p})$ and recalling the no-slip condition $\hat{\mathbf{u}} = \mathbf{0}$ on Γ yields the identity

259
$$\int_{\Gamma_L} \dot{u}_1 \, dx_2 = a^1(\mathbf{u}, \hat{\mathbf{u}}, \boldsymbol{\theta}) - b^1(\hat{\mathbf{u}}, p, \boldsymbol{\theta}) - b^1(\mathbf{u}, \hat{p}, \boldsymbol{\theta}) + \int_{\Gamma} \dot{\mathbf{u}}^D \cdot \hat{\mathbf{f}} \, ds.$$

260 We next use this identity in (3.14) and substitute the resulting expression of $\langle I'(\Omega), \boldsymbol{\theta} \rangle$ into (3.13), to obtain

261
$$\langle C'_Q(\Omega), \boldsymbol{\theta} \rangle = a^1(\mathbf{u}, \hat{\mathbf{u}}, \boldsymbol{\theta}) - b^1(\hat{\mathbf{u}}, p, \boldsymbol{\theta}) - b^1(\mathbf{u}, \hat{p}, \boldsymbol{\theta}) + \int_{\Gamma} \left(\frac{c}{L} \theta_n + \hat{\mathbf{f}} \cdot \dot{\mathbf{u}}^D \right) \, ds + \int_{\Gamma_L} u_1 \partial_2 \theta_2 \, dx_2$$

262 We first apply Lemma 3.2 with $\Delta \hat{p} = 1$ to the above expression, to obtain

263 (3.16)
$$\langle C'_Q(\Omega), \boldsymbol{\theta} \rangle = \int_{\Gamma} \left(-(2\mu \mathbf{D}[\mathbf{u}] : \mathbf{D}[\hat{\mathbf{u}}]) \theta_n + \frac{c}{L} \theta_n - \mathbf{f} \cdot \nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta} - \hat{\mathbf{f}} \cdot (\nabla \mathbf{u} \cdot \boldsymbol{\theta} - \dot{\mathbf{u}}^D) \right) \, ds + \int_{\Gamma_L} \partial_2(u_1 \theta_2) \, dx_2,$$

264 whose form is similar to (3.12). The first integral in (3.16) can be reformulated with the help of Lemma 3.1,
265 Lemma 3.4 and its following counterpart for the adjoint solution (whose proof is given in Sec. A.3):

266 LEMMA 3.5. *Let $(\hat{\mathbf{u}}, \hat{\mathbf{f}}, \hat{p})$ solve the adjoint problem (3.15). On the channel wall Γ , we have*

267
$$(a) \quad \nabla \hat{\mathbf{u}} = \frac{\hat{f}_s}{\mu} \boldsymbol{\tau} \otimes \mathbf{n}, \quad (b) \quad 2\mathbf{D}[\hat{\mathbf{u}}] = \frac{\hat{f}_s}{\mu} (\mathbf{n} \otimes \boldsymbol{\tau} + \boldsymbol{\tau} \otimes \mathbf{n}), \quad (c) \quad \hat{\mathbf{f}} = -\hat{p} \mathbf{n} + \hat{f}_s \boldsymbol{\tau}$$

268 where $\hat{f}_s := \hat{\mathbf{f}} \cdot \boldsymbol{\tau}$ (hence the viscous part of $\hat{\mathbf{f}}$ is tangential to Γ).

269 Carrying out these derivations, and evaluating the second integral of (3.16), establishes the following final,
270 implementation-ready, formula for $\langle C'_Q(\Omega), \boldsymbol{\theta} \rangle$:

271 PROPOSITION 3. *The shape derivative of the mass flow rate functional C_Q in a domain shape perturbation such that the transformation velocity field $\boldsymbol{\theta}$ satisfies assumptions (3.3) is given by*

273
$$\langle C'_Q(\Omega), \boldsymbol{\theta} \rangle = \sum_{\epsilon=+,-} \int_{\Gamma^{\epsilon}} \left\{ \left(\frac{c \ell^{\epsilon} \kappa}{L} - \frac{1}{\mu} f_s \hat{f}_s + \frac{c}{L} \right) \theta_n + \frac{c}{L} (\ell^{\epsilon} \hat{f}_s - \ell^{\epsilon} (\partial_s \theta_n) \hat{p}) \right\} \, ds$$

274
$$+ [\theta_2 u_1](\mathbf{z}^+) - [\theta_2 u_1](\mathbf{z}^-)$$

276 where f_s and (\hat{p}, \hat{f}_s) are components of the solutions of the forward problem (2.4) and the adjoint problem (3.15), respectively, and $\epsilon \in \{+, -\}$ refers to the upper wall Γ^+ or the lower wall Γ^- .

278 REMARK 6. *Let the Stokes solution $(\hat{\mathbf{u}}, \hat{p})$, periodic up to a constant (unit) pressure drop, be defined by*

279
$$- \operatorname{div}(2\mu \mathbf{D}[\hat{\mathbf{u}}] - \hat{p} \mathbf{I}) = \mathbf{0} \quad \text{in } \Omega, \quad \operatorname{div} \hat{\mathbf{u}} = 0, \quad \hat{\mathbf{u}} = \mathbf{0} \quad \text{on } \Gamma, \quad \hat{p}(\cdot) - \hat{p}(\cdot - L \mathbf{e}_1) = 1 \quad \text{on } \Gamma_p^+$$

280 (i.e. Problem (2.14–2.18) of [18] with homogeneous Dirichlet data on the walls). Taking the dot product
281 of the first equation by $\mathbf{v} \in \mathbf{V}$, integrating by parts and using the periodicity of \mathbf{v} and $2\mu \mathbf{D}[\hat{\mathbf{u}}]$, we obtain
282 equation (3.15a), while equations (3.15b,c) express the incompressibility and no-slip conditions.

283 4. Numerical algorithm. We now formally define the shape optimization problem and describe a
284 numerical algorithm to solve it based on the shape sensitivity formulas derived in the previous section.

285 4.1. Optimization method. Our goal is to find the shape of the peristaltic pump in the wave frame
286 that minimizes the power loss functional subject to constant volume and flow rate constraints, that is,

287 (4.1)
$$\Omega^* = \arg \min_{\Omega \in \mathcal{O}} J_{PL}(\Omega) \quad \text{subject to } C_Q(\Omega) = 0, C_V(\Omega) = 0,$$

288 with \mathcal{O} defined as in (3.2). While there are numerous approaches for solving constrained optimization
289 problems [20], we use an Augmented Lagrangian (AL) approach and avoid second-order derivatives of the

Algorithm 4.1 Augmented Lagrangian method for problem (4.1)

```

1: Choose initial design shape parameters  $\xi^0$ , which determines initial domain  $\Omega_0$ 
  Set convergence tolerance  $\zeta^* = 10^{-3}$ 
  Set  $\lambda^0 = (0, 0)$ 
  Set  $\sigma_1^0 = 10, \sigma_2^0 = 10$  or  $\sigma_2^0 = 100$  (depending on  $\Omega_0$ )
  Set  $\zeta^1 = (\sigma^0)^{-0.1}$ 
2: for  $m = 1, 2, \dots$  do
3:   # Solve unconstrained minimization subproblem (4.2) for  $\Omega_m$ 
4:   From  $\xi^{m-1} = \xi^{m-1,0}$  and an approximate (positive definite) Hessian matrix  $B_0$ , repeat the
  following steps until  $\xi^{m-1,j}$  converges to the solution  $\xi^m$ :
5:   1) Obtain a perturbation direction  $\mathbf{p}_j$  by solving  $B_j \mathbf{p}_j = -\nabla_{\xi} \mathcal{L}_A(\xi^{m-1,j}, \lambda^{m-1}; \sigma^{m-1})$ 
6:   2) find an acceptable stepsize  $\eta_j$ 
7:   3)  $\xi^{m-1,j+1} = \xi^{m-1,j} + \eta_j \mathbf{p}_j$ 
8:   4) Update the approximate Hessian matrix  $B_{j+1}$  (by BFGS formula)
9:   The solution  $\xi^m$  uniquely determines  $\Omega_m$ .
10:  # Check for convergence and/or update Lagrange multipliers and penalty parameters
11:  if  $|C_V(\Omega_m)| < \zeta_1^m$  and  $|C_Q(\Omega_m)| < \zeta_2^m$  then
12:    if  $|C_V(\Omega_m)| < \zeta^*$  and  $|C_Q(\Omega_m)| < \zeta^*$  then
13:      Set  $\xi^* := \xi^m$ , i.e.,  $\Omega^* := \Omega_m$  STOP
14:    end if
15:     $\lambda_1^m = \lambda_1^{m-1} - \sigma_1^{m-1} C_V(\Omega_m)$ 
16:     $\lambda_2^m = \lambda_2^{m-1} - \sigma_2^{m-1} C_Q(\Omega_m)$ 
17:     $\sigma^m = \sigma^{m-1}$ 
18:     $\zeta^{m+1} = (\sigma^0)^{-0.9} \zeta^m$ 
19:  else
20:     $\lambda^m = \lambda^{m-1}$ 
21:     $\sigma^m = 10\sigma^{m-1}$ 
22:     $\zeta^{m+1} = (\sigma^0)^{-0.1}$ 
23:  end if
24: end for

```

290 cost functional, whose evaluation is somewhat challenging in the case of our shape optimization problem.
 291 It proceeds by forming an augmented Lagrangian, defined by

$$292 \quad \mathcal{L}_A(\Omega, \lambda; \sigma) = J_{PL}(\Omega) - \lambda_1 C_Q(\Omega) - \lambda_2 C_V(\Omega) + \frac{\sigma_1}{2} C_Q^2(\Omega) + \frac{\sigma_2}{2} C_V^2(\Omega),$$

293 where $\sigma = (\sigma_1, \sigma_2)$ are penalty coefficients that are positive and $\lambda = (\lambda_1, \lambda_2)$ are Lagrange multipliers.
 294 Setting the initial values σ^0 and λ^0 using heuristics, the augmented Lagrangian method introduces a sequence
 295 ($m = 1, 2, \dots$) of unconstrained minimization problems:

$$296 \quad (4.2) \quad \Omega_m = \arg \min_{\Omega \in \mathcal{O}} \mathcal{L}_A(\Omega, \lambda^m; \sigma^m),$$

297 with explicit Lagrange multiplier estimates λ^m and increasing penalties σ^m . We use the Broyden-Fletcher-
 298 Goldfarb-Shanno (BFGS) algorithm [20], a quasi-Newton method, for solving (4.2). Equation (3.7), Propo-
 299 sitions 2 and 3 are used in this context for all gradient evaluations.

300 The overall optimization procedure is summarized in Algorithm 4.1.

301 **4.2. Finite-dimensional parametrization of shapes.** In view of both the structure theorem,
 302 see (3.6), and the fact that we rely for the present study on a boundary integral method, we only need
 303 to model shape perturbations of the channel walls. Here we consider, for each wall Γ^{\pm} , parametrizations of

304 the form $\mathbf{x}^\pm = \mathbf{x}^\pm(t, \boldsymbol{\xi})$ with

305 (4.3)
$$\Gamma \ni x_1^\pm(t) := \frac{L}{2\pi}t - \sum_{k=1}^N \xi_{1,k}^\pm + \sum_{k=1}^{2N} \xi_{1,k}^\pm \phi_k(t) \quad t \in [0, 2\pi],$$

306 (4.4)
$$\Gamma \ni x_2^\pm(t) := \xi_{2,0}^\pm - \sum_{k=1}^N \xi_{2,k}^\pm + \sum_{k=1}^{2N} \xi_{2,k}^\pm \phi_k(t) \quad t \in [0, 2\pi],$$

307

308 where $\phi_k(t)$ are the trigonometric polynomials $\{\cos(t), \cos(2t), \dots, \cos(Nt), \sin(t), \sin(2t), \dots, \sin(Nt)\}$. The
309 set of admissible shapes as in (3.2) indicates $x_1^\pm(0) = 0$ and $x_1^\pm(2\pi) = L$, which are enforced in (4.3). The
310 constraint (iii) of (3.3) is fulfilled by a fixed value $\xi_{2,0}^- = x_2^-(0)$ in (4.4), which will be pre-assigned and
311 excluded from the shape parameters.

312 Therefore, we take as design shape parameters the set $\boldsymbol{\xi} = \{\xi_{1,1}^\pm, \dots, \xi_{1,2N}^\pm, \xi_{2,0}^+, \xi_{2,1}^\pm, \dots, \xi_{2,2N}^\pm\}$ of
313 dimension $8N+1$. Since the parametrization (4.3), (4.4) is linear in $\boldsymbol{\xi}$, transformation velocities $\boldsymbol{\theta}$ associated
314 to perturbed parameters $\boldsymbol{\xi}(\eta) = \boldsymbol{\xi} + \eta \mathbf{p}$, i.e., to the η -dependent parametrization have the form

315
$$\boldsymbol{\theta}(\mathbf{x}(t)) = \frac{1}{\eta} (\mathbf{x}(t; \boldsymbol{\xi} + \eta \mathbf{p}) - \mathbf{x}(t; \boldsymbol{\xi})) \quad t \in [0, 2\pi].$$

316 **4.3. Boundary integral solver.** Solving the unconstrained optimization problem (4.2) requires eval-
317 uating the shape sensitivities (Propositions 2 and 3), which in turn require solving the forward and adjoint
318 problems to obtain the corresponding traction and pressure on the channel walls. In both problems, the
319 fluid velocity and pressure satisfy the Stokes equations:

320
$$-\nabla p + \mu \Delta \mathbf{u} = 0 \quad \text{and} \quad \nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega.$$

321 While the forward problem requires applying prescribed slip on the walls and periodic boundary conditions,
322 the adjoint problem requires a no-slip on the walls and unit pressure drop across the channel. The boundary
323 conditions can be summarized in a slightly modified form as follows.

324 (4.5) *Forward problem:* $\mathbf{u} = \mathbf{u}^D$ on Γ , $\mathbf{u}|_{\Gamma_L} - \mathbf{u}|_{\Gamma_0} = \mathbf{0}$ and $T|_{\Gamma_L} - T|_{\Gamma_0} = \mathbf{0}$.

325 (4.6) *Adjoint problem:* $\mathbf{u} = \mathbf{0}$ on Γ , $\mathbf{u}|_{\Gamma_L} - \mathbf{u}|_{\Gamma_0} = \mathbf{0}$ and $T|_{\Gamma_L} - T|_{\Gamma_0} = \mathbf{e}_1$.

326 Here, T is the *traction* vector, whose components are given by $T_i(\mathbf{u}, p) = \sigma_{ij}(\mathbf{u}, p) \mathbf{n}_j$ and it represents the
327 hydrodynamic force experienced by any interface in the fluid with normal \mathbf{n} . These systems of equations
328 correspond to (2.3) and (3.15) respectively by unique continuation of Cauchy data [18]. The standard
329 boundary integral approach for periodic flows is to use periodic Greens functions obtained by summing over
330 all the periodic copies of the sources [21]. The disadvantage of this approach is the slow convergence rate,
331 specially, for high-aspect ratio domains; moreover, the pressure-drop condition cannot be applied directly.
332 Instead, we use the periodization scheme developed recently in [18] that uses the free-space kernels only
333 and enforces the inlet and outlet flow conditions in (4.5, 4.6) algebraically at a set of collocation nodes.

334 The free-space Stokes single-layer kernel and the associated pressure kernel, given a source point \mathbf{y} and
335 a target point \mathbf{x} , are given by

336 (4.7)
$$S(\mathbf{x}, \mathbf{y}) = \frac{1}{4\pi\mu} \left(-\log |\mathbf{x} - \mathbf{y}| \mathbf{I} + \frac{(\mathbf{x} - \mathbf{y}) \otimes (\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^2} \right) \quad \text{and} \quad Q(\mathbf{x}, \mathbf{y}) = \frac{1}{2\pi} \frac{\mathbf{x} - \mathbf{y}}{|\mathbf{x} - \mathbf{y}|^2}.$$

337 The approach of [18] represents the velocity field as a sum of free-space potentials defined on the unit cell
338 Ω , its nearest periodic copies and at a small number, K , of auxiliary sources located exterior to Ω that act
339 as proxies for the infinite number of far-field periodic copies:

340 (4.8)
$$\mathbf{u} = \mathcal{S}_\Gamma^{\text{near}} \boldsymbol{\tau} + \sum_{m=1}^K \mathbf{c}_m \phi_m,$$

341 where

342 (4.9)
$$(\mathcal{S}_\Gamma^{\text{near}} \boldsymbol{\tau})(\mathbf{x}) := \sum_{|n| \leq 1} \int_\Gamma S(\mathbf{x}, \mathbf{y} + n\mathbf{d}) \boldsymbol{\tau}(\mathbf{y}) d\mathbf{s}_\mathbf{y} \quad \text{and} \quad \phi_m(\mathbf{x}) = S(\mathbf{x}, \mathbf{y}_m).$$

343 Here, \mathbf{d} is the lattice vector i.e. $\mathbf{d} = L\mathbf{e}_1$ and the source locations $\{\mathbf{y}_m\}_{m=1}^K$ are chosen to be equispaced on
 344 a circle enclosing Ω . The associated representation for pressure is given by

345 (4.10)
$$p = \mathcal{P}_\Gamma^{\text{near}} \boldsymbol{\tau} + \sum_{m=1}^K \mathbf{c}_m \cdot \boldsymbol{\varphi}_m,$$

346 where

347
$$(\mathcal{P}_\Gamma^{\text{near}} \boldsymbol{\tau})(\mathbf{x}) := \sum_{|n| \leq 1} \int_{\Gamma} Q(\mathbf{x}, \mathbf{y} + n\mathbf{d}) \cdot \boldsymbol{\tau}(\mathbf{y}) ds_{\mathbf{y}} \quad \text{and} \quad \boldsymbol{\varphi}_m(\mathbf{x}) = Q(\mathbf{x}, \mathbf{y}_m).$$

348 The pair (\mathbf{u}, p) as defined by this representation satisfy the Stokes equations since S and Q , defined in (4.7),
 349 are the Green's functions. The unknown density function $\boldsymbol{\tau}$ and the coefficients $\{\mathbf{c}_m\}$ are then determined
 350 by enforcing the boundary conditions. For the forward problem, applying the conditions in (4.5) produces
 351 a system of equations in the following form [18]:

352 (4.11)
$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \boldsymbol{\tau} \\ \mathbf{c} \end{bmatrix} = \begin{bmatrix} \mathbf{u}^D \\ \mathbf{0} \end{bmatrix}.$$

353 The first row applies the slip condition on Γ by taking the limiting value of $\mathbf{u}(\mathbf{x})$, defined in (4.8), as
 354 \mathbf{x} approaches Γ from the interior. The second row applies the periodic boundary conditions on velocity
 355 and traction as defined in (4.5). The operators A, B, C and D are correspondingly defined based on the
 356 representation formulas (4.8) and (4.10). In the case of the adjoint problem, the operators remain the same
 357 but the right hand side of (4.11) is modified according to the boundary conditions (4.6).

358 *REMARK 7.* Note that the representation (4.8) implies that A is a first-kind boundary integral operator
 359 and in general is not advisable for large-scale problems due to ill-conditioning of resulting discrete linear
 360 systems. However, for the problems we consider here, the dimension of linear system is usually small ~ 100 -
 361 200 and we always solve it using direct solvers. For large-scale problems requiring iterative solution (e.g., in
 362 peristaltic pumps transporting rigid or deformable particles), well-conditioned systems can be produced from
 363 second-kind operators, which can readily be constructed using double-layer potentials as was done in [18].

364 Finally, we use M quadrature nodes each on Γ^+ and Γ^- to evaluate smooth integrals using the standard
 365 periodic trapezoidal rule and weakly singular integrals, such as (4.9) evaluated on Γ , using a spectrally-
 366 accurate Nyström method (with periodic Kress corrections for the log singularity, see Sec. 12.3 of [16]).
 367 Thereby, a discrete linear system equivalent to (4.11) is obtained, which is solved using a direct solver for
 368 the unknowns $\boldsymbol{\tau}$ and $\{\mathbf{c}_m\}$. The traction vector for a given pipe shape, required for evaluating the shape
 369 derivatives (Props. 2 and 3), can then be obtained by a similar representation as (4.8) but with the kernel
 370 replaced by the traction kernel, given by,

371
$$T(S, Q)(\mathbf{x}, \mathbf{y}) = -\frac{1}{\pi} \frac{(\mathbf{x} - \mathbf{y}) \otimes (\mathbf{x} - \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^2} \frac{(\mathbf{x} - \mathbf{y}) \cdot \mathbf{n}^{\mathbf{x}}}{|\mathbf{x} - \mathbf{y}|^2}.$$

372 **5. Results.** In this section, we present validation results for our numerical PDE solver and test the
 373 performance of our shape optimization algorithm. First, we demonstrate the performance of our forward
 374 problem (2.3) solver on an arbitrary pump shape as shown in Figure 5.1(a). To illustrate the convergence of
 375 the numerical scheme, we consider two scalar quantities: the objective function J_{PL} and the mass flow rate
 376 Q , both of which depend on the traction vector obtained by solving the forward problem. In 5.1(b), we show
 377 the accuracy of the solver in computing these quantities as well as the CPU time it takes to solve as the
 378 number of quadrature points on each of the walls, M , is increased. Since we are using a spectrally-accurate
 379 quadrature rule, notice that the error decays rapidly and a small number of points are sufficient to achieve
 380 six-digit accuracy, which is more than enough for our application. The number of proxy points and the
 381 number of collocation points on the side walls are chosen following the analysis of [18]—both typically are
 382 small again owing to the spectral convergence of the method w.r.t these parameters. Consequently, each
 383 forward solve takes less than a second to obtain the solution to six-digit accuracy as can be observed from
 384 Figure 5.1(b).

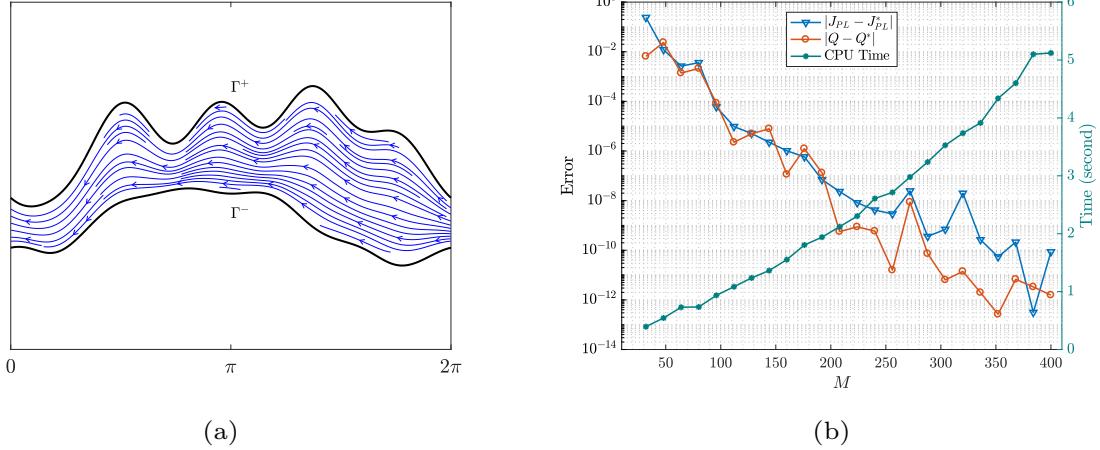


FIG. 5.1. (a) An arbitrarily shaped channel and the streamlines of flow induced by a prescribed slip on the walls, as defined in (2.3), obtained using our boundary integral solver. (b) Plot of convergence and CPU times as a function of the spatial resolution M used in the forward problem solver. The reference solution (denoted by superscript $*$) is obtained using $M = 1024$. Notice that we get single-precision accuracy ($1e-6$) even with a small number of points (~ 100) and corresponding cost of forward solve is less than a second.

385 Next we consider two different initial pump shapes and perform the shape optimization by imposing
386 the same constraints on the flow rate Q^* and the volume V^* . The initial and the intermediary shapes
387 produced by our numerical optimization procedure are shown in Figure 5.2. Based on our earlier analysis of
388 the forward solver, we set $M = 64$ and the number of modes N (e.g., in (4.3) and (4.4)) is set to 5, thereby,
389 the number of the shape design parameters is 41. We use the Augmented Lagrangian approach described
390 in Algorithm 4.1 with the values of the penalty parameters as listed. Each AL iteration requires solving an
391 unconstrained optimization problem, which entails taking several BFGS iterations (steps 5-9 of Algo 4.1).
392 Both the number of AL iterations and the number of BFGS iterations are shown for each shape update
393 in Figure 5.2. In total, it costs 143 solves of the forward and adjoint problems (4.5)–(4.6) for the case in
394 Fig. 5.2(a) and 197 for the case in Fig. 5.2(b).

395 We show the evolution of the objective function and the constraints with the iteration index, corre-
396 sponding to these two test cases, in Fig. 5.3. Due to the fact that we are using an AL approach, the
397 constraints are enforced progressively by increasing the penalty coefficients σ and as a result, the objective
398 function approaches a local minimum in a non-monotonic fashion. In the second test case (Fig. 5.2b), for
399 instance, J_{PL} increases significantly since the initial shape doesn't satisfy the constraints. On the other
400 hand, in the first test case, the initial values for the Q and V , obtained by a forward solve, match the
401 target values Q^* and V^* , thereby J_{PL} is reduced as the optimization proceeds, to nearly half of its initial
402 value. While not guaranteed in general (due to the possibility of getting stuck in a local minimum), the
403 final shapes in both cases coincide, which is another validation of our analytic shape sensitivity calculations.

404 The equilibrium shapes and their interior fluid flow shown in Figure 5.2 reaffirm the classical observation
405 [12] of *trapping* i.e., an enclosed bolus of fluid particles near the center line indicated by the closed streamlines
406 in the waveframe. As is also well-known, trapping occurs beyond a certain pumping range only; in Fig. 5.4,
407 we show the optimal shapes obtained by our algorithm at different flow rates but containing the same
408 volume of fluid. Here, we fixed the bottom wall to be flat. Notice that the bolus appears to form for shapes
409 beyond $Q = 0.9$. Moreover, as expected, the optimal value of power loss is higher for higher flow rates with
410 the extreme case of a flat pipe transporting zero net flow with no power loss.

411 **6. Conclusions.** We derived new analytic formulas for evaluating the shape derivatives of the power
412 loss and the mass flow rate functionals that arise in the shape optimization of Stokesian peristaltic pumps.
413 While we restricted our attention to two-dimensional shapes, extension of these formulas to rotationally-
414 symmetric shapes is rather straightforward. We applied the recently developed periodic boundary integral
415 solver of [18] to solve the forward/adjoint PDE problems efficiently.

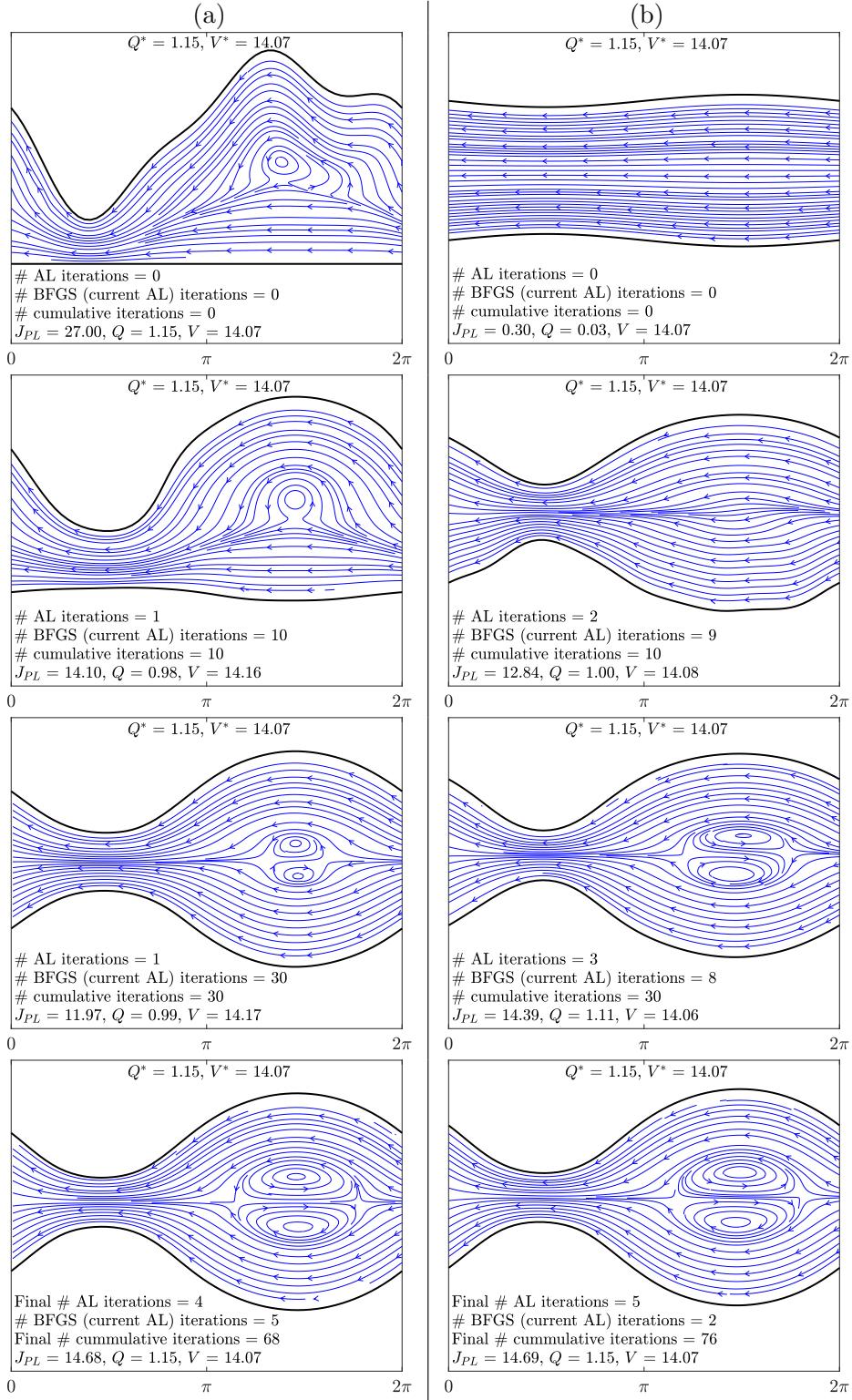


FIG. 5.2. Optimizing power loss with mass flow rate and volume constraints, starting with two different initial shapes, (a) a random top wall with a flat bottom wall, and (b) a symmetric slight bump shape. In both cases, the constraints on Q^* and V^* are the same. We observe that both arrive at the same equilibrium shape.

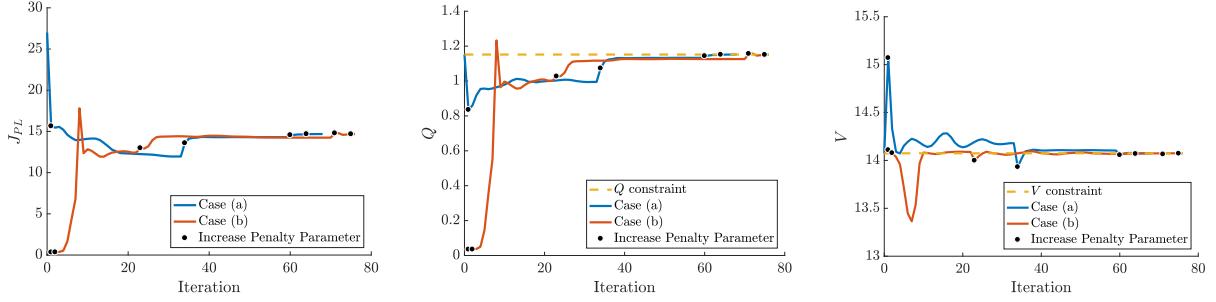


FIG. 5.3. Evolution of the power loss, mass flow rate, and volume as a function of the optimization iteration index corresponding to the two test cases shown in Fig. 5.2. Since we are using an Augmented Lagrangian approach, as expected, we can observe that the constraints—of prescribed mass flow rate and volume indicated by dashed lines—are satisfied progressively as the penalty parameters are increased.

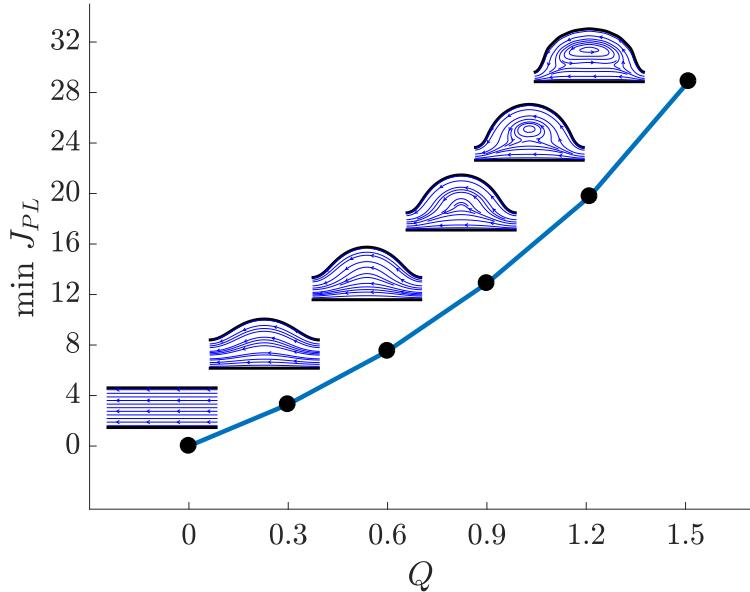


FIG. 5.4. Optimal shapes and minimized power losses for varying mass flow rates. The bottom wall is fixed as flat. The constraint of volume is identical for all shapes.

416 One of the main directions of our future investigation is to consider optimal shapes for transporting
 417 passive (e.g., colloids, bubbles or vesicles) and/or active (e.g., spermatozoa, bacteria) particles in Stokes
 418 flow. This is of current interest in both science and technological applications. Clearly, they are more
 419 computationally intensive since transient PDEs need to be solved as opposed to the quasi-static ones considered
 420 here. However, particulate flow solvers based on BIEs are proven to be efficient and scalable to simulating
 421 millions of deformable particles [22]; our work lays the foundation for applying these methods to shape
 422 optimization of peristaltic pumps transporting such complex fluids.

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 425 Foundation, and by the *Fondation Mathématique Jacques Hadamard* (France).

426 **Appendix A. Proofs.**

427 **A.1. Proof of Lemma 3.1.** We use the Frenet formulas (2.1) and associated conventions. To evaluate
428 $\dot{\mathbf{u}}^D$, we let Γ depend on the fictitious time η , setting

429
$$\Gamma_\eta \ni \mathbf{x}_\eta(s) = \mathbf{x}(s) + \eta \boldsymbol{\theta}(s) \quad (0 \leq s \leq \ell),$$

430 (where Γ stands for Γ^+ or Γ^- , and likewise for ℓ) and seek the relevant derivatives w.r.t. η evaluated at
431 $\eta = 0$. Note that for $\eta \neq 0$, s is no longer the arclength coordinate along Γ_η , and $\partial_s \mathbf{x}_\eta$ is no longer of unit
432 norm; moreover, the length of Γ_η depends on η . The wall velocity $\mathbf{U} = (c\ell/L)\boldsymbol{\tau}$ for varying η is then given
433 by

434 (A.1)
$$\mathbf{U}_\eta(s) = \frac{c\ell_\eta}{Lg_\eta} \partial_s \mathbf{x}_\eta \quad (0 \leq s \leq \ell),$$

435 having set $g_\eta = |\partial_s \mathbf{x}_\eta|$ (note that $g_0 = 1$). Our task is to evaluate $d/d\eta \mathbf{U}_\eta(s)$ at $\eta = 0$. We begin by
436 observing that the derivative of g is (since $\partial_s \mathbf{x}_\eta = \boldsymbol{\tau}$ and $g = 1$ for $\eta = 0$)

437
$$\partial_\eta g = (\partial_s \mathbf{x}_\eta \cdot \partial_{\eta s} \mathbf{x}_\eta)/g = \boldsymbol{\tau} \cdot \partial_s \boldsymbol{\theta} = \partial_s \theta_s - \kappa \theta_n$$

438 and the length ℓ_η of Γ_η and its derivative $\dot{\ell}$ are given (noting that s spans the fixed interval $[0, \ell]$ for all
439 curves Γ_η) by

440
$$(i) \quad \ell_\eta = \int_0^\ell g_\eta \, ds, \quad (ii) \quad \dot{\ell} = \int_0^\ell (\partial_s \theta_s - \kappa \theta_n) \, ds = - \int_0^\ell \kappa \theta_n \, ds.$$

441 The last equality in (ii), which results from the assumed periodicity of $\boldsymbol{\theta}$, proves item (b) of the lemma.

442 Using these identities in (A.1), the sought derivative $\dot{\mathbf{u}}^D$ of the wall velocity is found as

443
$$\dot{\mathbf{u}}^D = \partial_\eta \mathbf{U}_\eta(s) \Big|_{\eta=0} = \frac{c}{L} (\dot{\ell} - \ell (\partial_s \theta_s - \kappa \theta_n)) \boldsymbol{\tau} + \frac{c}{L} \ell \partial_s \boldsymbol{\theta} = \frac{c\ell}{L} \boldsymbol{\tau} + \frac{c\ell}{L} (\partial_s \theta_n + \kappa \theta_s) \mathbf{n},$$

444 thus establishing item (a) of the lemma. The proof of Lemma 3.1 is complete.

445 **A.2. Proof of Lemma 3.2.** The proof proceeds by verification, and rests on evaluating $\operatorname{div} \mathbf{A}$, with
446 the vector function \mathbf{A} defined by

447
$$\mathbf{A} := (\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}]) \boldsymbol{\theta} - \boldsymbol{\sigma}[\mathbf{u}, p] \cdot \nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta} - \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] \cdot \nabla \mathbf{u} \cdot \boldsymbol{\theta}$$

448 First, it is easy to check, e.g. using component notation relative to a Cartesian frame, that

449 (A.2a)
$$\operatorname{div} [(\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}]) \boldsymbol{\theta}] = (\nabla \boldsymbol{\sigma}[\mathbf{u}, p] \cdot \boldsymbol{\theta}) : \mathbf{D}[\hat{\mathbf{u}}] + \boldsymbol{\sigma}[\mathbf{u}, p] : (\nabla \mathbf{D}[\hat{\mathbf{u}}] \cdot \boldsymbol{\theta}) + (\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}]) \operatorname{div} \boldsymbol{\theta}$$

450 (A.2b)
$$\operatorname{div} [\boldsymbol{\sigma}[\mathbf{u}, p] \cdot \nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta}] = (\operatorname{div} \boldsymbol{\sigma}[\mathbf{u}, p]) \cdot (\nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta}) + \boldsymbol{\sigma}[\mathbf{u}, p] : (\nabla \hat{\mathbf{u}} \cdot \nabla \boldsymbol{\theta}) + \boldsymbol{\sigma}[\mathbf{u}, p] : (\nabla \mathbf{D}[\hat{\mathbf{u}}] \cdot \boldsymbol{\theta})$$

452 Next, invoking the constitutive relation (2.2b) for both states, one has

453
$$\boldsymbol{\sigma}[\mathbf{u}, p] : (\nabla \mathbf{D}[\hat{\mathbf{u}}] \cdot \boldsymbol{\theta}) = -p \nabla(\operatorname{div} \hat{\mathbf{u}}) \cdot \boldsymbol{\theta} + 2\mu \mathbf{D}[\mathbf{u}] : (\nabla \mathbf{D}[\hat{\mathbf{u}}] \cdot \boldsymbol{\theta})$$

454
$$(\nabla \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] \cdot \boldsymbol{\theta}) : \mathbf{D}[\mathbf{u}] = -(\nabla \hat{p} \cdot \boldsymbol{\theta}) \operatorname{div} \mathbf{u} + 2\mu (\nabla \mathbf{D}[\hat{\mathbf{u}}] \cdot \boldsymbol{\theta}) : \mathbf{D}[\mathbf{u}].$$

456 i.e. (using incompressibility)

457 (A.3)
$$\boldsymbol{\sigma}[\mathbf{u}, p] : (\nabla \mathbf{D}[\hat{\mathbf{u}}] \cdot \boldsymbol{\theta}) = (\nabla \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] \cdot \boldsymbol{\theta}) : \mathbf{D}[\mathbf{u}].$$

458 Finally, using (A.3) in (A.2a) and the balance equation in (A.2b), together with the corresponding identities
459 obtained by switching (\mathbf{u}, p) and $(\hat{\mathbf{u}}, \hat{p})$, one obtains

460
$$\operatorname{div} \mathbf{A} = \operatorname{div} [(\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}]) \boldsymbol{\theta} - \boldsymbol{\sigma}[\mathbf{u}, p] \cdot \nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta} - \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] \cdot \nabla \mathbf{u} \cdot \boldsymbol{\theta}]$$

461
$$= \operatorname{div} [\frac{1}{2}(\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}]) \boldsymbol{\theta} + \frac{1}{2}(\boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] : \mathbf{D}[\mathbf{u}]) \boldsymbol{\theta} - \boldsymbol{\sigma}[\mathbf{u}, p] \cdot \nabla \hat{\mathbf{u}} \cdot \boldsymbol{\theta} - \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] \cdot \nabla \mathbf{u} \cdot \boldsymbol{\theta}]$$

462
$$= \frac{1}{2} [\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}] + \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] : \mathbf{D}[\mathbf{u}]] \operatorname{div} \boldsymbol{\theta} - \boldsymbol{\sigma}[\mathbf{u}, p] : (\nabla \hat{\mathbf{u}} \cdot \nabla \boldsymbol{\theta}) - \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] : (\nabla \mathbf{u} \cdot \nabla \boldsymbol{\theta})$$

463
$$= 2\mu (\mathbf{D}[\mathbf{u}] : \mathbf{D}[\hat{\mathbf{u}}]) \operatorname{div} \boldsymbol{\theta} - 2\mu \mathbf{D}[\mathbf{u}] : (\nabla \hat{\mathbf{u}} \cdot \nabla \boldsymbol{\theta}) - 2\mu \mathbf{D}[\hat{\mathbf{u}}] : (\nabla \mathbf{u} \cdot \nabla \boldsymbol{\theta}) + (p \nabla \hat{p} + \hat{p} \nabla p) : \nabla \boldsymbol{\theta}$$

465 (with the second equality stemming from $\boldsymbol{\sigma}[\mathbf{u}, p] : \mathbf{D}[\hat{\mathbf{u}}] = 2\mu\mathbf{D}[\mathbf{u}] : \mathbf{D}[\hat{\mathbf{u}}] = 2\mu\mathbf{D}[\hat{\mathbf{u}}] : \mathbf{D}[\mathbf{u}] = \boldsymbol{\sigma}[\hat{\mathbf{u}}, \hat{p}] : \mathbf{D}[\mathbf{u}]$).
466 Using definitions (3.9a,b) of a^1 and b^1 , we therefore observe that

467
$$a^1(\mathbf{u}, \hat{\mathbf{u}}, \boldsymbol{\theta}) - b^1(\mathbf{u}, \hat{p}, \boldsymbol{\theta}) - b^1(\hat{\mathbf{u}}, p, \boldsymbol{\theta}) = \int_{\Omega} \operatorname{div} \mathbf{A} \, dV.$$

468 The last step consists of applying the first Green identity (divergence theorem) to the above integral. The
469 Lemma follows, with the contribution of the end section Γ_L therein stemming from condition (ii) in (3.3)
470 and the periodicity conditions at the end sections. The latter hold by assumption for both \mathbf{u} and $\hat{\mathbf{u}}$, and
471 the interior regularity of solutions in the whole channel then implies the same periodicity for $\nabla \mathbf{u}$ and $\nabla \hat{\mathbf{u}}$;
472 moreover, periodicity is also assumed for p (but not necessarily for \hat{p}) as well as for $\boldsymbol{\theta}$.

473 **A.3. Proof of Lemmas 3.4 and 3.5.** Let points \mathbf{x} in a tubular neighborhood V of Γ be given in
474 terms of curvilinear coordinates (s, z) , so that

475
$$\mathbf{x} = \mathbf{x}(s) + z\mathbf{n}(s),$$

476 and let $\mathbf{v}(\mathbf{x}) = v_s(s, z)\boldsymbol{\tau}(s) + v_n(s, z)\mathbf{n}(s)$ denote a generic vector field in V . Then, at any point $\mathbf{x} = \mathbf{x}(s)$
477 of Γ , we have

478
$$\nabla \mathbf{v} = (\partial_s v_s - \kappa v_n) \boldsymbol{\tau} \otimes \boldsymbol{\tau} + (\partial_s v_n + \kappa v_s) \mathbf{n} \otimes \boldsymbol{\tau} + \partial_n v_s \boldsymbol{\tau} \otimes \mathbf{n} + \partial_n v_n \mathbf{n} \otimes \mathbf{n},$$

479
$$\operatorname{div} \mathbf{v} = \partial_s v_s - \kappa v_n + \partial_n v_n.$$

481 Assuming incompressibility, the condition $\operatorname{div} \mathbf{v} = 0$ can be used for eliminating $\partial_n v_n$ and we obtain

482
$$\nabla \mathbf{v} = (\partial_s v_s - \kappa v_n) (\boldsymbol{\tau} \otimes \boldsymbol{\tau} - \mathbf{n} \otimes \mathbf{n}) + (\partial_s v_n + \kappa v_s) \mathbf{n} \otimes \boldsymbol{\tau} + \partial_n v_s \boldsymbol{\tau} \otimes \mathbf{n},$$

483 Recalling now that the forward and adjoint solutions respectively satisfy $\mathbf{u} = (c\ell/L)\boldsymbol{\tau}$ and $\hat{\mathbf{u}} = \mathbf{0}$ on Γ , and
484 that $2\mathbf{D}[\mathbf{v}] = \nabla \mathbf{v} + \nabla \mathbf{v}^T$, we have

485 (A.4)
$$\begin{aligned} \nabla \mathbf{u} &= \frac{\kappa c\ell}{L} \mathbf{n} \otimes \boldsymbol{\tau} + \partial_n u_s \boldsymbol{\tau} \otimes \mathbf{n} & 2\mathbf{D}[\mathbf{u}] &= \left(\frac{\kappa c\ell}{L} + \partial_n u_s \right) (\mathbf{n} \otimes \boldsymbol{\tau} + \boldsymbol{\tau} \otimes \mathbf{n}) \\ \nabla \hat{\mathbf{u}} &= \partial_n \hat{u}_s \boldsymbol{\tau} \otimes \mathbf{n} & 2\mathbf{D}[\hat{\mathbf{u}}] &= \partial_n \hat{u}_s (\mathbf{n} \otimes \boldsymbol{\tau} + \boldsymbol{\tau} \otimes \mathbf{n}) \end{aligned} \quad \left. \right\} \quad \text{on } \Gamma.$$

486 The corresponding stress vectors $\mathbf{f} = -p\mathbf{n} + 2\mu\mathbf{D}[\mathbf{u}] \cdot \mathbf{n}$ and $\hat{\mathbf{f}} = -\hat{p}\mathbf{n} + 2\mu\mathbf{D}[\hat{\mathbf{u}}] \cdot \mathbf{n}$ on Γ are found as

487
$$\mathbf{f} = -p\mathbf{n} + f_s \boldsymbol{\tau}, \quad \hat{\mathbf{f}} = -\hat{p}\mathbf{n} + \hat{f}_s \boldsymbol{\tau} \quad \text{with} \quad f_s = \mu \left(\frac{\kappa c\ell}{L} + \partial_n u_s \right), \quad \hat{f}_s = \mu \partial_n \hat{u}_s,$$

488 which in particular prove items (c) of Lemmas 3.4 and 3.5. Finally, using the above in (A.4) establishes the
489 remaining items (a), (b) of both lemmas.

490

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