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Shape optimization for the generalized Graetz problem

Frédéric de Gournay · Jérôme Fehrenbach · Franck Plouraboué

Abstract We apply shape optimization tools to the generalized Graetz problem which is a convection-diffusion equation. The problem boils down to the optimization of generalized eigenvalues on a two phases domain. Shape sensitivity analysis is performed with respect to the evolution of the interface between the fluid and solid phase. In particular physical settings, counterexamples where there is no optimal domains are exhibited. Numerical examples of optimal domains with different physical parameters and constraints are presented. Two different numerical methods (level-set and mesh-morphing) are show-cased and compared.

Keywords Graetz problem · Shape sensitivity · Generalized eigenvalues · Shape optimization

1 Introduction

Convective heat or mass transfer occur in many industrial processes, with application to cooling or heating systems, pasteurisation, crystallization, distillation, or different purifications processes. We are interested in exchange of heat or mass without contact between a fluid phase, and a solid phase in parallel flow designs, as illustrated in Fig. 1.

The simplest parallel convection-dominated stationary transport problem in a single tube associated with a parabolic axi-symmetrical Poiseuille velocity profile is named after its first contributor the Graetz problem (Graetz 1885). The associated eigenmodes provide a set of longitudinally exponentially decaying solutions, and the decomposition of the entrance boundary condition in the orthogonal basis formed by these eigenmodes provides the solution in the entire domain. This allows to reduce three-dimensional computations to two-dimensional eigenvalue problems. This framework is adapted when longitudinal diffusion is negligible compared with longitudinal convection. The role of longitudinal diffusion, especially in the solid compartments in micro-exchangers, is more and more stringent from advances in miniaturization (Fedorov and Viskanta 2000; Foli et al. 2006). But the extension of a generalized Graetz orthogonal eigenmode decomposition to treat non convection-dominated convective transport is not a simple task. To make a long story short, it was shown in Papoutsakis et al. (1980) that a linear operator acting on a two-component temperature/longitudinal gradient vector can provide a symmetric operator and the eigenmode decomposition in a single tube configuration.

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The purpose of the present contribution is to propose shape optimization tools associated to the generalized Graetz problem. The optimization of the section of a pipe in order to maximize or minimize the characteristic length of heat transport amounts to find the optimal insulating pipe (large characteristic length), or the optimal heat exchanger (small characteristic length). This problem finds applications in various contexts (Fabri 1998; Bau 1998; Foli et al. 2006; Bruns 2007; Iga et al. 2009; Canhoto and Reis 2011). The characteristic lengths are the inverses of the Graetz operator eigenvalues, and more precisely the dominant downstream (resp. upstream) characteristic length is the inverse of the smallest negative (resp. positive) eigenvalue $\lambda_{-1}$ (resp. $\lambda_1$). In the context of exchangers, the first Graetz eigenvalue controls the thermal entrance length associated with longitudinal relaxation of the temperature, which subsequently controls the most active transfer region, as discussed, for example in Canhoto and Reis (2011). Hence, for exchanger compactness, it is useful to find the shape which can maximize the first Graetz eigenvalue in order to obtain the more compact device. The shape optimization problem we address is thus naturally an eigenvalue optimization problem for the Graetz operator. Eigenvalue optimization is a very natural problem in structural design, and it was addressed in many works, see e.g., Osher and Santosa (2001), Conca et al. (2009) or de Gournay (2006) for the case of multiple eigenvalues. Topology optimization tools have also been applied to transfer problems over the last few years (Bruns 2007; Iga et al. 2009; Canhoto and Reis 2011).

The point of view adopted here is to assume that the boundary of the outer domain is fixed, this amounts to say that the outer shape of the pipe is fixed, and we compute the shape sensitivity with respect to the variation of the inner domain (the shape of the fluid domain). The fluid flow is described as a Poiseuille flow, which means that the longitudinal velocity $u$ of the fluid is the solution of Poisson’s equation with a constant source term in the fluid domain and Dirichlet boundary conditions. The shape optimization problem that we consider takes into account two nested partial differential equations: Poisson’s equation which provides the velocity of the fluid in the fluid domain, and Graetz operator whose eigenvalues are to be optimized, and where the velocity of the fluid appears as a coefficient. Therefore the sensitivity analysis is performed in two successive steps: variation of the fluid velocity (which is a standard result), and then the variation of the bilinear forms associated to the eigenvalue problem for the Graetz operator.

It is clear that without any normalization constraint, the best insulating pipe is empty, and the best conducting pipe is full. Therefore it appears necessary for the problem to be tractable and physically meaningful to add some constraints. We considered three natural normalizations for this problem: the first one is to set the total flow in the pipe, the second one is to set the viscous dissipation in the flow, and the last one is to set the total work of the pump. The shape sensitivity analysis leads to a shape optimization algorithm, by gradient descent. This algorithm was implemented using the level-set method (Allaire et al. 2004) and the mesh-morphing method (Pironneau 1982) and we discuss the advantages and drawbacks of each different method. We present numerical results in different configurations and parameters, for each of the constraint listed above.

The paper is organized as follows: The first section is dedicated to setting the direct problem. In Section 3, we recall basic facts about shape sensitivity analysis and provide the shape sensitivity of the flow. In Section 4, the shape sensitivity analysis of the eigenvalues is performed and our main result is stated in Proposition 4. The proof of this result is new in nature, although the formula for the gradient is the expected one. In Section 5, we exhibit a counterexample to the existence of an optimal shape. Finally, numerical results obtained by a steepest descent algorithm are presented and discussed in Section 6.

2 Setting
In this Section, we present the direct problem to be optimized also known as the generalized Graetz problem. This problem is a generalized eigenvalue problem on a system of PDE. We state the mathematical results of existence of the first eigenvalue.
2.1 The generalized Graetz problem

A fluid constrained in a cylindrical pipe \( \omega \times I \), where \( \omega \subset \Omega \), advects the temperature that diffuses outside the pipe. The fluid velocity inside the pipe is denoted by \( u(\xi , z) \), whereas the temperature is denoted by \( T(\xi , z) \) for \( \xi = (x, y) \in \Omega \) and \( z \in I \). The temperature \( T \) in the stationary regime satisfies the following convection-diffusion equation:

\[
\text{div}(\kappa \nabla T) = u \cdot \nabla T,
\]

where \( \kappa = \kappa(\xi , z) \) is the conductivity tensor that describes the conductivity of the fluid in \( \omega \) and the conductivity of the solid in \( \Omega \setminus \omega \). We assume that the outer boundary of the pipe is at a constant temperature, and (1) is completed by the following Dirichlet boundary condition:

\[
T = 0 \quad \text{on } \partial \Omega \times I. 
\]

The velocity flow \( u \) is assumed to be a laminar Poiseuille pressure-driven flow directed along the \( z \) direction and constant in the \( z \) variable, that is \( u(\xi , z) = u(\xi) e_z \), where \( e_z \) is the unit vector in the \( z \) direction. The velocity amplitude \( u \) is given as \( u(\xi) = \alpha v(\xi) \), \( \alpha \in \mathbb{R} \), where the velocity profile \( v \) solves Poisson’s equation

\[
-\Delta v = 1 \quad \text{in } \omega, \quad v = 0 \quad \text{on } \partial \omega, 
\]

and where \( \alpha \) is a normalization factor that corresponds to one of the following normalization processes:

Definition 1 We define three different normalization processes:

- The “prescribed total flow”: in this case, \( \int_{\omega} u \) is set to be equal to a constant \( F \) and we have \( \alpha = F(\int_{\omega} v)^{-1} \).
- The “prescribed dissipation”. In this case, we set \( \int_{\omega} |\nabla u|^2 = D \) and hence \( \alpha = D^{-1/2}(\int_{\omega} |\nabla v|^2)^{-1/2} \).
- The “prescribed work of the pump”, where we set \( \int_{\omega} \Delta u = P \) and then \( \alpha = P/|\omega|^{-1} \).

Note that (3) provides the solution of Stokes and Navier–Stokes equations for an unidirectional incompressible flow (Leal 1992).

Let us now describe the conduction problem. The conductivity matrix is supposed to be symmetric bounded, coercive and anisotropic in the \( \xi \) direction only, i.e., it is of the form

\[
\kappa(\xi , z) = \begin{pmatrix} \sigma(\xi) & 0 \\ 0 & c(\xi) \end{pmatrix},
\]

and there exists a constant \( C > 1 \) such that \( \forall \xi \in \Omega, \eta \in \mathbb{R}^2, C|\eta|^2 \geq \sigma(\xi)\eta \geq C^{-1}|\eta|^2 \) and \( C \geq c(\xi) \geq C^{-1} \).

It is required that \( c \) and \( \sigma \) are regular on both \( \omega \) and \( \Omega \setminus \omega \) but may admit a jump between the fluid phase and the solid phase. Hence, for \( i = 1, 2 \) there exist \( c_i \in C^\infty(\Omega) \) and \( \sigma_i \) a \( C^\infty(\Omega) \) matrix field such that

\[
c = \chi_\omega c_1 + (1 - \chi_\omega)c_2, \quad \sigma = \chi_\omega \sigma_1 + (1 - \chi_\omega)\sigma_2, 
\]

where \( \chi_\omega \) is the characteristic function of \( \omega \) and where \( c_i \) and \( \sigma_i \) are uniformly bounded from above and below such that (4) holds. We recall that, on any point of \( \partial \omega \), the operator \([c]_{\partial \omega} \) refers to the jump discontinuity across \( \omega \), for instance we have \([c]_{\partial \omega}(\xi) = c_1(\xi) - c_2(\xi) \).

In this setting (see Figs. 1 and 2), (1–2) reduce to the following (2+1)-dimensional convection-diffusion equation, referred to as the generalized Graetz problem:

\[
\left\{ \begin{array}{ll}
c(\xi) \partial_t T + \text{div} \left( \sigma(\xi) \nabla T \right) - u(\xi) \partial_z T = 0 & \text{in } \Omega \times I, \\
T = 0 & \text{on } \partial \Omega \times I, \\
T \text{ given} & \text{on } \Omega \times \partial I.
\end{array} \right.
\]

In the sequel, the subscript \( \xi \) will be omitted and we will simply write: \( \Delta = \Delta_\xi, \nabla = \nabla_\xi, \text{div} = \text{div}_\xi \) for the Laplacian, gradient and divergence operators in the section \( \Omega \).

Treating \( z \) as a time variable, the study of the evolution equation (6) reduces (see (Fehrenbach et al. 2012)) to the study of the associated eigenproblem

\[
\left\{ \begin{array}{ll}
c \lambda_\xi^2 T_k + \text{div}(\sigma \nabla T_k) - \lambda_k u T_k = 0 & \text{in } \Omega, \\
T_k = 0 & \text{on } \partial \Omega, \\
T_k \text{ given} & \text{on } \partial I.
\end{array} \right.
\]

and the aim of the present work is to study the shape optimization of the eigenvalues associated to (7), that is to maximize or minimize the value of the smallest positive or biggest negative eigenvalue by changing the domain \( \omega \).

We can already point out the influence of the domain \( \omega \) on the different terms in (7). First \( v \) depends on \( \omega \) in (3), and \( \sigma \) depends on \( \omega \) via Definition 1 and finally \( u = \alpha v \) depends on \( \omega \). Moreover, throughout their definition (5), \( c \) and \( \sigma \) both depend on \( \omega \). The fact that the sensitivity with respect to the shape of \( \omega \) is computed implies that an interface between two materials with different conductivities evolves.
This requires a more subtle treatment than the cases where the outer boundary of the domain is varying. Shape sensitivity in the case of an interface between two materials was already studied, see Hettlich and Rundell (1998), Bernardi and Pironneau (2003), Pantz (2005), Conca et al. (2009), Allaire et al. (2009) and Neittaanmäki and Tiba (2012) for a recent review article. To our knowledge the eigenvalue problem for the Graetz operator, where some coefficient of the operator depends on an auxiliary partial differential equation, was not addressed previously.

2.2 Solving the direct problem

In this paragraph, we discuss the resolution of the eigenvalue problem (7) when ω is fixed and the regularity results that can be deduced. We shall suppose that ω is a smooth set with $C^\infty$ boundary.

Assuming that ω and Ω are regular domains, by elliptic regularity, $v$ which solves (3) is a regular function on ω that can be extended by zero outside ω such that the resulting function is $C^0(\Omega) \cap H^1(\Omega)$, of course this regularity result implies the same regularity for the function $u = av$.

In order to solve the eigenproblem, we introduce the operators

$A : (T, s) \mapsto (-\div(\sigma \nabla T), cs)$

and

$B : (T, s) \mapsto (cs - uT, cT)$.

The operators $A$ and $B$ are unbounded operators from $L^2(\Omega)^2$ to $L^2(\Omega)^2$. The domain of $B$ is $L^2(\Omega)^2$ whereas the domain of $A$ is

$D(A) = \left\{(T, s) \in \left(L^2(\Omega)\right)^2 : \text{s.t. } \div(\sigma \nabla T) \in L^2(\Omega)\right\}$.

By duality $A$ may be extended to an operator from $L^2(\Omega)^2$ to the dual space of $D(A)$. This extension may still be denoted as $A$ and is a symmetric operator on the space $\mathcal{G} = H^1_0(\Omega) \times L^2(\Omega)$. It follows from an integration by part and Poincaré’s identity that $A$ is coercive in the sense that there exists a constant $C$ such that

$\langle A\phi, \phi \rangle_{L^2} \geq C\|\phi\|_{\mathcal{G}}^2 \quad \forall \phi \in \mathcal{G}$.

It follows from these definitions that $T_k \in H^1_0(\Omega)$ is a solution of (7), if and only if $\phi_k = (T_k, \lambda_k) \in \mathcal{G}$ solves

$A\phi_k = \lambda_k B\phi_k$.

It has been shown in Pierre and Plouraboué (2009) that this problem has a compactness property and that it’s spectrum is a double sequence going to infinity on both sides, i.e., it consists of $\lambda_k$ such that:

$-\infty \leftarrow \lambda_{-k} < \cdots < \lambda_{-1} < 0 < \lambda_1 < \lambda_2 < \ldots \lambda_k \rightarrow +\infty$.

Moreover, for each $k \in \mathbb{Z}^*$, the eigenspace $E_k$ associated to $\lambda_k$ is of finite dimension. The compactness of this eigenproblem relies on the fact that $A$ is an operator involving second spatial derivatives of $T$ (operator of order 2) while $B$ is an operator of order 0 in $T$. Note that $A$ and $B$ are both operators of order 0 in the variable $s$, so that there is no stricto sensu jump of orders between $A$ and $B$ in the $s$ variable, but the coupling of the equations allows to retrieve compactness in the variable $s$ from compactness in the variable $T$. Moreover, the Rayleigh’s quotient giving the smallest positive eigenvalue (resp. largest negative) denoted as $\lambda_1$ (resp. $\lambda_{-1}$) is:

$\lambda_{-1} = \max_{\phi \in \mathcal{G}} \frac{(B\phi, \phi)}{(A\phi, \phi)}, \quad \text{resp. } (\lambda_{-1})^{-1} = \min_{\phi \in \mathcal{G}} \frac{(B\phi, \phi)}{(A\phi, \phi)}$.

(8)

For fixed $k \in \mathbb{Z}^*$, we have the following regularity properties on $T_k$:

Proposition 1 For every $(T_k, \lambda_k T_k)$ in $E_k$, then $T_k$ is $H^1_{\text{div}}(\Omega)$ and

$[T_k]_{\partial \omega} = 0$ and $[\sigma \nabla T_k \cdot n]_{\partial \omega} = 0$.

If $\omega$ is smooth, $T_k$ is smooth in both $\omega$ or $\Omega \setminus \omega$ and for any $\tau$, tangent vector to $\partial \omega$, we have $[\nabla T_k \cdot \tau]_{\partial \omega} = 0$.

Proof Since $T_k$ is $H^1_{\text{div}}(\Omega)$, then $[T_k]_{\partial \omega}$ exists and is equal to 0 (in the sense of the difference of the trace of $T_k$ on both sides of $\omega$), the equation $[\sigma \nabla T_k \cdot n]_{\partial \omega} = 0$ pops up when writing the variational equation of (7). Since the domain $\omega$ is regular, the regularity of $T_k$ follows from bootstrap arguments on equation (7):

$-\div(\sigma \nabla T_k) = c\lambda_k^2 T_k - \lambda_k u T_k$.

and considering this equation on $\omega$ or $\Omega \setminus \omega$ which are regular sets where the coefficients $c$ and $u$ are regular. Finally the equation $[\nabla T_k \cdot \tau]_{\partial \omega} = 0$ comes from differentiating with respect to $\tau$ the equation $[T_k]_{\partial \omega} = 0$ and supposing that $\omega$ is regular enough for that purpose. □

3 Shape sensitivity of the flow

In this Section, we present the framework of shape sensitivity and state classical results for the sensitivity of the flow profile $v$ and the scaling constant $\alpha$. The reader can refer to one of the following reference books (Allaire 2007; Henrot and Pierre 2005) or the numerous references therein. We also refer to the review article (Neittaanmäki and Tiba 2012) and its references for shape sensitivity of domains with varying coefficients (the so-called transmission problems).
3.1 Notation and general framework

Shape sensitivity analysis amounts to advect the domain with a diffeomorphism and to differentiate in the tangent space around identity which is the space of vector fields, see Murat and Simon (1976). Contrariwise to standard shape sensitivity analysis, we do not want to change the domain \( \Omega \) but only to study how the changes in \( \omega \) affect the eigenvalue. This leads to the following definition:

**Definition 2** Define
\[
\Theta = \left\{ \theta \in W^{1,\infty}(\mathbb{R}^2, \mathbb{R}^2), \text{ such that } \theta = 0 \text{ in } \mathbb{R}^2 \setminus \Omega \right\},
\]
then for any \( \theta \in \Theta \) such that \( \|	heta\|_{W^{1,\infty}} < 1 \), the vector field \( F_\theta = Id + \theta \) defines a diffeomorphism such that \( F_\theta(\Omega) = \Omega \). For each such \( \theta \), we define
\[
\omega(\theta) = F_\theta(\omega) = [x + \theta(x)] | x \in \omega] .
\]

We use the notation of Section 2, and choose to write the dependence on \( \theta \) explicitly. Hence \( \nu(\theta) \), \( T_\theta(\theta) \) will denote functions that solve (3) and (7) with \( \omega \) replaced by \( \omega(\theta) \). Similarly \( \alpha(\theta) \), \( \lambda_\pm(\theta) \) are real numbers that satisfy Definition 1 and (7) with \( \omega \) replaced by \( \omega(\theta) \). Note that normalization factors, \( F, D \) or \( P \) involved in Definition 1 are supposed to be independent of \( \theta \). Our aim is to study the derivative of the mapping \( \theta \mapsto \lambda_1(\theta) \) and \( \theta \mapsto \lambda_{-1}(\theta) \). The eigenvalues \( \lambda_{\pm}(\theta) \) are defined via the following Rayleigh’s quotient:
\[
\lambda_{\pm}(\theta) = \min_{\phi \in G} \frac{(B(\theta)\phi, \phi)}{\langle A(\theta)\phi, \phi \rangle}, \quad \lambda_{-1}(\theta) = \min_{\phi \in G} \frac{(B(\theta)\phi, \phi)}{\langle A(\theta)\phi, \phi \rangle}, \quad \lambda_1(\theta) = \max_{\phi \in G} \frac{(B(\theta)\phi, \phi)}{\langle A(\theta)\phi, \phi \rangle}, \quad (9)
\]
where, if \( \phi = (T, s) \in G \).

\[
(B(\theta)\phi, \phi) = \int_\Omega 2c(\theta)TS - u(\theta)T^2,
\]
\[
(A(\theta)\phi, \phi) = \int_\Omega \sigma(\theta) \nabla T \cdot \nabla T + c(\theta)s^2,
\]
\[
c(\theta) = \chi_{\omega(\theta)}c_1 + (1 - \chi_{\omega(\theta)})c_2 \quad \text{ and } \quad \sigma(\theta) = \chi_{\omega(\theta)}\sigma_1 + (1 - \chi_{\omega(\theta)})\sigma_2 .
\]

There are two ways to obtain the differentiability result, the first one is the Lagrangian method of Céa, see Céa (1986), that we shall not follow here since it does not rigorously prove the existence of the derivative but rather computes it when it exists. Since we deal with eigenvalues which are known not to be differentiable but rather directionally derivable, we use the second method which is more challenging but mathematically correct. This method reads as follows:

- Perform a change of variable to obtain a variational formulation on a fixed domain with coefficients depending on \( \theta \).
- Differentiate the coefficients with respect to \( \theta \).
- At some point, use an integration by part on \( \theta \), in our case, we will use the following Lemma:

**Lemma 1** (Technical result) Let \( \mathcal{O} \subset \Omega \) be an open set with \( C^1 \) boundary. Suppose that \( \theta \in \Theta \) and \( \sigma \in C^1(\mathcal{O}) \), then for every \( a, b \in H^2(\mathcal{O}) \) we have:

\[
\int_\Omega \text{div}\theta(\sigma \nabla a \cdot \nabla b) - (\nabla \theta^T \sigma \nabla a \cdot \nabla b - (\sigma \nabla \theta \nabla a) \cdot \nabla b = \int_\Omega -\nabla \sigma \cdot (\nabla a \cdot \nabla b) + \text{div}(\sigma \nabla a)(\nabla b \cdot \theta) + \text{div}(\sigma \nabla b) (\nabla a \cdot \theta) + \int_{\partial \mathcal{O}} (\theta \cdot n)(\sigma \nabla a \cdot \nabla b - (\nabla b \cdot \theta)(\sigma \nabla a \cdot n) - (\nabla a \cdot \theta)(\sigma \nabla b \cdot n)
\]

*If \( \sigma \) is a symmetric matrix with \( C^1(\mathcal{O}) \) coefficients, the same formula holds true except that the term \( (\nabla \sigma \cdot \theta)(\nabla a \cdot \nabla b) \) has to be replaced by the term*
\[
\sum_{i,j,k} \frac{\partial \sigma_{ij}}{\partial x^k} \frac{\partial a}{\partial x^i} \frac{\partial b}{\partial x^j} .
\]

*Proof* The formula follows from an integration by part. \( \square \)

3.2 Derivative of the flow profile

Let \( \nu(\theta) \) be the material derivative which is the pullback of the flow profile \( \nu(\theta) \) by the transformation \( F_\theta \), in other words \( \nu = \nu(\theta) \circ F_\theta \in H^1_0(\omega) \). Since \( \nu \) belongs to a space that does not vary with \( \theta \), it makes sense to study the derivatives of \( \nu \) with respect to \( \theta \).

**Proposition 2** (Derivative of \( \nu(\theta) \)) The application \( \theta \mapsto \nu(\theta) \) is \( C^\infty \) at \( \theta = 0 \) for the natural norms. The derivative of this application at the point \( \theta \) in the direction \( \theta \), denoted hereafter \( Y \in H^1_0(\omega) \) is implicitly given by: \( \forall \psi \in H^2(\omega) \cap H^1_0(\omega) \),

\[
\int_\omega \nabla Y \cdot \nabla \psi = - \int_\omega (\Delta \psi)(\nabla v \cdot \theta) + \int_{\partial \theta}(\theta \cdot n)(\nabla v \cdot \nabla \psi) .
\]

*Proof* see Henrot and Pierre (2005), Allaire (2007). \( \square \)

3.3 Derivative of the scaling constant \( \alpha \)

**Proposition 3** (Derivatives of the scaling factors) The mapping \( \theta \in \Theta \mapsto \alpha(\theta) \in \mathbb{R} \) as defined in Definition 1
is differentiable at the point $\theta = 0$ and the value of its differential at the point 0 in direction $\theta$ is given by:

$$d\alpha(\theta) = \begin{cases} -F \left( \int_\omega v \right)^{-2} \int_\omega (\theta \cdot n)(\partial_n v)^2 & \text{in the “prescribed flow” case,} \\ -\frac{\sqrt{D}}{2} \left( \int_\omega v \right)^{-\frac{1}{2}} \int_\omega (\theta \cdot n)(\partial_n v)^2 & \text{in the “prescribed dissipation” case,} \\ -P|\alpha|^{-2} \int_{\partial\omega} \theta \cdot n & \text{in the “prescribed work” case.} \end{cases}$$

(11)

**Proof** The derivative of $\alpha$ in the “prescribed work of the pump” case is straightforward, since it relies on the derivative with respect to $\theta$ of the volume of $\omega$ (Allaire 2007):

$$|\omega(\theta)| = |\omega| + \int_{\partial\omega} \theta \cdot n + o(||\theta||_{1,\infty}).$$

We now turn our attention to the “prescribed dissipation” case and to the “prescribed flow” case. Since

$$\int_{\omega(\theta)} v(\theta) = \int_{\omega(\theta)} |\nabla v(\theta)|^2,$$

it is sufficient to compute the derivative of this expression (the compliance) which is a standard result. 

\[\square\]

4 Domain sensitivity of the eigenvalue

The objective of this Section is to establish the main result of this paper, which is the directional derivability of the eigenvalue. This section presents the main novelty of this article since our problem has the following features:

- It is a linear generalized eigenvalue system of PDE with transmission coefficient (jumps in the coefficients).
- One of the coefficient depends on the domain via a PDE.
- There is no gap of derivative on the second equation of the eigenproblem, hence no compactness. Compactness is gained via the coupling of the first equation and the second.

4.1 Statement of the main result

Our main claim is:

**Proposition 4** Suppose that $\omega$ is smooth. For $\phi = (T, \lambda_1 T)$ any eigenvector relative to $\lambda_1$ associated to the eigenproblem (7), let the adjoint $p \in H^2(\omega)$ be the unique solution in $H^1_0(\omega)$ of

$$\int_\omega \nabla p \cdot \nabla \psi = \int_\omega T^2 \psi \quad \forall \psi \in H^1_0(\omega).$$

(12)

Then the mapping $\theta \mapsto \lambda_1(\theta)$ is directionally derivable at the point 0 and its derivative in the direction $\theta$ is given by

$$d\lambda_1(\theta) = \min_{\phi \in E_1} \int_{\partial\omega} (\theta \cdot n) e(\phi),$$

(13)

where $e(\phi)$ depends quadratically on $\phi$ and is given by

$$e(\phi) = \alpha \lambda_1 \nabla v \cdot \nabla p - \left[\sigma^{-1}\right]|_{\partial\omega} (\sigma \nabla T \cdot n)^2 + [\sigma]|_{\partial\omega}(\nabla T \cdot \tau)^2 - [c]|_{\partial\omega} \lambda_1^2 T^2 + C,$$

(14)

where the term $C$ depends on the normalization case and is equal to

$$C = \begin{cases} -\lambda_1 F \left( \int_\omega T^2 v \right)^{-2} (\partial_n v)^2 & \text{in the “prescribed flow” case,} \\ -\frac{\lambda_1 D^{1/2}}{2} \left( \int_\omega T^2 v \right)^{-3/2} (\partial_n v)^2 & \text{in the “prescribed dissipation” case,} \\ -\lambda_1 P|\alpha|^{-2} \left( \int_\omega T^2 v \right)^2 & \text{in the “prescribed work of the pump” case,} \end{cases}$$

(15)

and where $(\nabla T \cdot \tau)^2$ is the tangential part of the gradient of $T$ that may be also defined as:

$$(\nabla T \cdot \tau)^2 = \nabla \cdot T \nabla T - (\nabla T \cdot n)^2$$

The shape derivative of $\lambda_{-1}$ is obtained via formulae similar to (13), (14) and (15) if $\lambda_1$ is replaced by $\lambda_{-1}$, $E_1$ by $E_{-1}$ and the min is replaced by a max.

Note that (13) is similar to the standard results of eigenvalue optimization (Haug and Rousselet 1980; Seyranian et al. 1994; de Gournay 2006), and that (14) incorporates jump terms that are typical of shape sensitivity with discontinuous coefficients (Bernardi and Pironneau 2003; Pantz 2005). Note also that (13) holds for any eigenvalue (and not only the first one) and in the case of a simple eigenvalue $d\lambda$ is linear w.r.to $\theta$, hence Fréchet differentiability holds.

The proof of Proposition 4 is decomposed into three parts, the first one (Proposition 6 in paragraph 3.2) shows that the operators $\mathcal{A}(\theta)$ and $\mathcal{B}(\theta)$ are differentiable as operators. The second part (Proposition 7 in paragraph 3.3) is an abstract result showing that the eigenvalue admits directional derivatives when the operators are differentiable. The third part is presented in paragraph 3.4, it is the application of Proposition 7 that leads to (13). The end of the present paragraph is devoted to introducing some notation.
Write $\mathfrak{F}(\theta) = u_\theta \circ F_\theta$. It follows from Propositions 2, 3 and the chain rule that the mapping $\theta \in \Theta \mapsto \bar{u} \in H^1_0(\omega)$ is differentiable with respect to $\theta$ at the point $\theta = 0$ and that its derivative at 0 in the direction $\theta$ hereafter denoted $\bar{Y}$ is given by:

$$\bar{Y} = \alpha Y + d\alpha(\theta) u + o(\|\theta\|_{W^{1,\infty}}).$$

(16)

In order to compute the shape derivative of $\lambda_{\pm 1}$, we perform a change of variable by $F_0$ in the Rayleigh quotient (9) defining the eigenvalue, this leads to:

**Proposition 5** Define the operators $\mathcal{B}(\theta)$ and $\mathcal{A}(\theta)$ by

$$(\mathcal{B}(\theta) \phi, \phi) = \int_\Omega 2\delta(\theta) T s - \gamma(\theta) T^2$$

and

$$(\mathcal{A}(\theta) \phi, \phi) = \int_\Omega \beta(\theta) \nabla T \cdot \nabla T + \delta(\theta) s^2,$$

where $\delta, \beta$ and $\gamma$ are defined as

$$\delta(\theta) = |\det \nabla F_\theta| (\chi_{\omega} c_1 \circ F_\theta + (1 - \chi_{\omega}) c_2 \circ F_\theta),$$

$$\beta(\theta) = |\det \nabla F_\theta| (\nabla F_\theta)^{-T} (\chi_{\omega} c_1 \circ F_\theta + (1 - \chi_{\omega}) c_2 \circ F_\theta)(\nabla F_\theta)^{-1},$$

$$\gamma(\theta) = |\det \nabla F_\theta| \overline{u}(\theta).$$

Then

$$\left(\lambda_{1}(\theta)\right)^{-1} = \max_{\phi \in \mathcal{G}} \frac{(\mathcal{B}(\theta) \phi, \phi)}{(\mathcal{A}(\theta) \phi, \phi),}$$

and $\left(\lambda_{-1}(\theta)\right)^{-1}$ is given as the minimum of the same ratio.

**Proof** We perform a change of variable in (9) together with the property that when $\phi$ describes $\mathcal{G}$ then $\bar{\phi} = \phi \circ F_0$ describes $\mathcal{G}$. We shall only prove that $(\mathcal{B}(\theta) \bar{\phi}, \bar{\phi}) = (\mathcal{B}(\theta) \phi, \phi)$. Denote $\Omega_1 = \omega$ and $\Omega_2 = \Omega \setminus \omega$. We have, if $\phi = (T, s)$ and $\bar{\phi} = (\bar{T}, \bar{s}) = (T \circ F_0, s \circ F_0)$,

$$(\mathcal{B}(\theta) \phi, \phi) = \left(\sum_{i=1}^2 \int_{\Omega_2} 2c_i T s \right) - \int_{\omega(\theta)} u(\theta) T s$$

$$= \left(\sum_{i=1}^2 \int_{\Omega_2} 2 |\det \nabla F_\theta|(c_i \circ F_\theta) \bar{T} \bar{s} \right) - \int_{\omega(\theta)} |\det \nabla F_\theta| \overline{u}(\theta) \bar{T} \bar{s} = (\mathcal{B}(\theta) \bar{\phi}, \bar{\phi}).$$

The development for $\mathcal{A}(\theta)$ is done exactly the same way.

\[ \square \]

4.2 Derivative of the bilinear forms

In this paragraph, the shape derivative of the operators $\mathcal{A}$ and $\mathcal{B}$ (as bilinear forms) is calculated.

**Proposition 6** There exists a neighborhood $\mathcal{V}$ of 0 in $W^{1,\infty}(\mathbb{R}^2, \mathbb{R}^2)$ and operators $d\mathcal{B}$ and $d\mathcal{A} : W^{1,\infty}(\mathbb{R}^2, \mathbb{R}^2) \times \mathcal{G} \to \mathbb{R}$, linear in the first variable and quadratic in the second such that for any $\phi \in \mathcal{G}$ and $\Theta \in \mathcal{V}$,

$$(\mathcal{B}(\theta) \phi, \phi) = (\mathcal{B}(\theta_0) \phi, \phi) + d\mathcal{B}(\theta, \phi) + o\left(\|\theta\|_{W^{1,\infty}} \|\phi\|_{\mathcal{G}}^2\right),$$

$$(\mathcal{A}(\theta) \phi, \phi) = (\mathcal{A}(\theta_0) \phi, \phi) + d\mathcal{A}(\theta, \phi) + o\left(\|\theta\|_{W^{1,\infty}} \|\phi\|_{\mathcal{G}}^2\right).$$

(17)

Moreover, denoting $\mathcal{O}_1 = \omega$ and $\mathcal{O}_2 = \Omega \setminus \omega$, we have:

$$d\mathcal{B}(\theta, \phi) = \left(\sum_{i=1}^2 \int_{\mathcal{O}_1} 2 |\det \nabla F_\theta|(c_i \circ F_\theta) \bar{T} \bar{s} \right) - \int_{\omega(\theta)} (\gamma(\theta) u + \bar{Y}) T^2,$$

$$d\mathcal{A}(\theta, \phi) = \sum_{i=1}^2 \int_{\mathcal{O}_1} (\sigma_i \gamma(\theta) - \nabla \theta^T \bar{c}_i + \nabla \sigma_i \cdot \bar{T} + \nabla(\theta) c_1 \circ F_\theta) T^2.$$

(18)

**Proof** We prove that the quadratic forms associated to $\mathcal{A}(\theta)$ and $\mathcal{B}(\theta)$ as defined in Proposition 5 are differentiable, this implies -by polarization- that the operators themselves are differentiable. We partition the domain $\Omega$ into $\mathcal{O}_1 = \omega$ and $\mathcal{O}_2 = \Omega \setminus \omega$, we obtain for $\bar{A}$:

$$(\mathcal{A}(\theta) \phi, \phi) = \sum_{i=1}^2 \int_{\mathcal{O}_1} |\det \nabla F_\theta|(c_i \circ F_\theta) \bar{T} \bar{s} +$$

$$|\det \nabla F_\theta| (\sigma_i \circ F_\theta)(\nabla F_\theta)^{-1} \bar{T} \cdot \nabla T.$$

$$= \beta(\theta)$$

For all $i = 1, 2$, the mappings $\theta \in \Theta \mapsto \beta(\theta) \in L^\infty(\mathcal{O}_i)$ and $\theta \in \Theta \mapsto \delta(\theta) \in L^\infty(\mathcal{O}_i)$ are differentiable, this ensures the existence of $d\mathcal{A}$. Computing the differential of the mappings $\beta$ and $\delta$, we obtain the required formula for $d\mathcal{A}$. The differentiation of $\mathcal{B}(\theta)$ is a little bit more involved, indeed we have:

$$d\mathcal{B}(\theta, \phi) = \left(\sum_{i=1}^2 \int_{\mathcal{O}_1} 2 |\det \nabla F_\theta|(c_i \circ F_\theta) T s \right)$$

$$- \int_{\omega(\theta)} |\det \nabla F_\theta| \overline{u}(\theta) T^2$$

The term $\delta(\theta)$ poses no problem but the term $\gamma(\theta)$ does not belong to $L^\infty$. Since $\theta \in \Theta \mapsto \bar{u} \in H^1_0(\omega)$ is differentiable, Sobolev embedding theorems in dimension 2 ensure that this mapping is also differentiable as a mapping $\theta \in \Theta \mapsto \bar{u} \in L^q(\Omega)$ for each $q \in \mathbb{N}^*$. Then the mapping $\theta \in \Theta \mapsto \gamma(\theta) \in L^q(\Omega)$ is also differentiable. It is then sufficient to bound $T^2$ in $L^q(\Omega)$ by $\|\theta\|_{H^1_0(\omega)}^2$ to obtain the desired development. \[ \square \]
4.3 Derivability of the eigenvalue

In this paragraph, the shape derivative of the eigenvalues is calculated, based on the results of Section 4.2.

**Proposition 7** (Existence of the derivative of the eigenvalue)

Using the notation of Proposition 6, the mapping \( \theta \mapsto \lambda_1(\theta) \in \mathbb{R} \) is directionally derivable at the point 0, and the value of the derivative in direction \( \dot{\theta} \) is given by

\[
d\lambda_1(\theta) = \min_{\phi \in E_1} dA(\theta, \phi) - \lambda_1 dB(\theta, \phi),
\]

where \( E_1 \) is the eigenspace associated to the eigenvalue \( \lambda_1 \) and where \( dA \) and \( dB \) are defined in Proposition 6. The same result holds true for \( \lambda_{-1} \) upon replacing \( \lambda_1 \) by \( \lambda_{-1} \), \( E_1 \) by \( E_{-1} \) and the minimum by a maximum.

**Proof** Before digging into the proof, let us give some insight about the formula. A formal way to derive Proposition 7 would be to set the direction and to write the equation \( A(\theta)\phi(\theta) = \lambda(\theta)B(\theta)\phi(\theta) \) and to suppose that \( \lambda(\theta) \) and \( \phi(\theta) \) are derivable in this direction (note that \( \phi \) may not even be continuous), deriving the above equation yields

\[
A'\phi + A\phi' = \lambda'B\phi + \lambda'B\phi + \lambda'B\phi'.
\]

Using the scalar product with \( \phi \) and using that \( \phi \) is an eigenvector, hence that \( (A\phi', \phi) = \lambda(B\phi', \phi) \), we have

\[
\lambda'(B\phi, \phi) = (A'\phi, \phi) - \lambda'(B'\phi, \phi).
\]

By homogeneity with respect to \( \phi \), we restrict ourselves to the \( \phi \) such that \( (A\phi, \phi) = 1 \). Finally, if the eigenspace is of dimension greater than 1, each eigenvector of the ball \( (B\phi, \phi) \) would give rise to a \( \lambda' \), they all compete to yield the smallest positive eigenvalue, the winning eigenvector is the one with the smallest derivative, and hence we have

\[
\lambda' = \min_{\phi \in E_1} (A'\phi, \phi) - \lambda(B'\phi, \phi),
\]

which is exactly the result of Proposition 7.

Our approach follows the ideas of Clarke (1990), which is similar to the one developed in de Gournay (2006). Since there is no -strictly speaking- gap of derivative between the operators \( A \) and \( B \) (and hence no straightforward compactness), we prove the result by hand. We recall that \( \lambda_1(\theta)^{-1} \) is given as the maximum over \( \mathcal{G} \) of the ratio:

\[
K(\theta, \phi) = \frac{(B(\theta)\phi, \phi)}{(A(\theta)\phi, \phi)}.
\]

We choose a direction \( \dot{\theta} \), an \( \epsilon \) small enough (that only depends on \( \theta \)) and a sequence \( t_n \to 0 \). We denote the directional derivative of \( K \) with respect to \( \theta \) at the point \( \theta = 0 \) as:

\[
dK(\phi) = \frac{dK(\theta, \phi)}{d\theta} = \frac{dA(\theta, \phi)(B(\theta, \phi), \phi)}{(A(\theta, \phi))^2}.
\]

where we recall that \( dB \) and \( dA \) are defined in Proposition 6, that \( \bar{B}(0) = B \) and that \( \bar{A}(0) = A \). Proving Proposition 7 amounts to proving that if \( a_n = \frac{1}{\epsilon} (\lambda_1^{-1}(t_n\theta) - \lambda_1^{-1}(0)) \) then

\[
\lim_{n \to +\infty} a_n = \max_{\phi \in E_1} dK(\phi).
\]

In order to prove this assertion, take \( \phi^* \in E_1 \) such that \( (A\phi^*, \phi^*) = 1 \), then \( \phi^* \) is a maximizer of the functional \( \phi \mapsto K(0, \phi) \). Since \( (A\phi^*, \phi^*) = 1 \), then \( \|\phi^*\| \leq 1 \) is bounded (uniformly in the choice of \( \phi^* \)). By the differentiability of \( \theta \mapsto (\bar{A}(\theta)\phi^*, \phi^*) \) and \( \theta \mapsto (\bar{B}(\theta)\phi^*, \phi^*) \) and the chain rule theorem it follows that

\[
K(t_n\theta, \phi^*) = K(0, \phi^*) + t_n dK(\phi^*) + O\left(\frac{t_n^2}{n}\right),
\]

where the term \( O\left(\frac{t_n^2}{n}\right) \) does not depend on the choice of \( \phi^* \), since \( \|\phi^*\| \) is uniformly bounded. We then have

\[
a_n = \max_{\phi \in \mathcal{G}} \frac{1}{t_n}(K(t_n\theta, \phi) - K(0, \phi^*))
\geq \frac{1}{t_n}(K(t_n\theta, \phi^*) - K(0, \phi^*)) = dK(\phi^*) + O(t_n).
\]

Maximizing on every \( \phi^* \in E_1 \), such that \( (A\phi^*, \phi^*) = 1 \), and taking the limit inf, we then have

\[
\liminf_{n \to +\infty} a_n \geq \max_{\phi^* \in E_1} dK(\phi^*),
\]

By homogeneity of \( dK(\phi^*) \), the latest maximum can be taken on the whole set \( E_1 \). In order to prove equality (20), it is then sufficient to prove that \( \limsup a_n \leq \max_{\phi \in \mathcal{G}} dK(\phi^*) \).

For that purpose, for each \( n \), consider \( \psi_n = (t_n, s_n) \) a maximizer of \( \psi \mapsto K(t_n\theta, \psi) \) such that \( \bar{A}(t_n\theta)\phi_n, \bar{\psi}_n = 1 \). Upon restricting \( \epsilon \), the coefficients \( \beta(t_n\theta) \) and \( \gamma(t_n\theta) \) can be supposed uniformly (with respect to \( n \)) bounded from above and below. This restriction in \( \epsilon \) depends on the choice of \( \theta \) only. Then the operator \( \bar{A}(t_n\theta) \) is uniformly coercive and continuous in the \( \mathcal{G} \) norm in the sense that:

\[
m\|\psi\|_{\mathcal{G}}^2 \leq (\bar{A}(t_n\theta)\phi_n, \phi_n) \leq M\|\phi\|_{\mathcal{G}}^2,
\]

for some constants \( m \) and \( M \) independent of \( n \).

Thanks to (22), the sequence \( t_n \) is uniformly bounded in \( H_0^1(\Omega) \) whereas the sequence \( s_n \) is uniformly bounded in \( L^2(\Omega) \), so that, up to a subsequence, they converge weakly in those respective spaces to some \( T^* \) and \( s^* \). Denoting \( \phi^* = (T^*, s^*) \), we first aim at proving that \( \phi^* \in E_1 \). By weak semi-continuity then \( (A\phi^*, \phi^*) \leq 1 \). Moreover

\[
\lim_{n \to +\infty} (\bar{B}(t_n\theta)\phi_n, \phi_n) = \lim_{n \to +\infty} \int_{\Omega} 2\delta(t_n\theta)\phi_n T_n + \gamma(t_n\theta) T_n^2 = (B\phi^*, \phi^*),
\]

by strong convergence of \( T_n \) towards \( T^* \) in \( L^p(\Omega) \) for any \( p \in \mathbb{N}^* \), weak convergence of \( s_n \) towards \( s^* \) in \( L^2(\Omega) \), strong convergence of \( \delta(t_n\theta) \) towards \( \delta(0) \) in \( L^\infty(\Omega) \) and
strong convergence of $\gamma(t_\alpha \theta)$ towards $\gamma(0)$ in any $L^q(\Omega)$ for $q \in \mathbb{N}^*$. As a consequence

$$\lim_{n \to +\infty} \lambda_{1}^{-1}(t_n \theta, \phi_n) = \lim_{n \to +\infty} K(t_n \theta, \phi_n) \leq K(0, \phi^*)$$

By (21), we already know that

$$\liminf_{n \to +\infty} \lambda_{1}^{-1}(t_n \theta, \phi) \geq \lambda_{1}^{-1}(0) = \max K(0, \phi) \geq K(0, \phi^*).$$

Hence, we have equality in this inequality and $\phi^*$ is a maximizer of $\phi \mapsto K(0, \phi)$ and hence is an eigenvector and $(A \phi^*, \phi^*) = 1$. Since the $G$-norm of $\phi_n$ converges strongly to the $G$-norm of $\phi^*$, then $\phi_n$ converges strongly towards $\phi^*$ in the $G$-norm. Since the sequence $\phi_n$ is uniformly bounded in the $G$-norm, we have:

$$K(t_n \theta, \phi_n) = K(0, \phi_n) + t_n dK(\phi_n) + O\left(t_n^2\right).$$

Using that $K(0, \phi_n) \leq \lambda_{1}^{-1}$, then

$$a_n = \frac{1}{t_n} \left(K(t_n \theta, \phi_n) - \lambda_{1}^{-1}\right) \leq dK(\phi_n) + O(t_n).$$

Since $\phi_n$ converges strongly towards $\phi^*$ in the $G$-norm, by continuity of $\phi \mapsto dK(\phi)$ for this norm and taking the limit sup, we have

$$\limsup_{n \to +\infty} a_n = dK(\phi^*) \leq \max_{\phi \in E_1} dK(\phi).$$


4.4 Proof of the main result

We are now in position to prove Proposition 4. By Proposition 7, the eigenvalue is directionally derivable and its derivative in the direction $\theta$ is given by (19). For any $\phi = (T, s) \in E_1$, using (17, 18) and $s = \lambda_{1}T$, we have

$$dA(\theta, \phi) - \lambda_{1} dB(\theta, \phi)$$

$$= \frac{1}{2} \left(\sigma \Delta \theta + (\nabla \theta) \cdot \nabla \theta + \nabla \sigma \cdot \theta - \sigma \nabla \theta\right) \nabla T \cdot \nabla T$$

$$- \frac{1}{2} \left(\Delta \theta + \sigma(T) \nabla \theta^2 + \lambda_{1} \int_{\omega} \left(\nabla \theta u + \tilde{Y}\right)^2 T^2\right)$$

Since, for $i = 1, 2, T$ is in $H^2(C_1)$ whereas $\sigma$ is in $C^1(C_1)$ we apply twice Lemma 1 with $a = b = T$, and we obtain

$$dA(\theta, \phi) - \lambda_{1} dB(\theta, \phi)$$

$$= \frac{1}{2} \left(\sigma \Delta \theta + (\nabla \theta) \cdot \nabla \theta + \nabla \sigma \cdot \theta - \sigma \nabla \theta\right) \nabla T \cdot \nabla T$$

$$- \frac{1}{2} \left(\Delta \theta + \lambda_{1} \int_{\omega} \left(\nabla \theta u + \tilde{Y}\right)^2 T^2\right)$$

$$+ \int_{\omega} \left(\theta \cdot n\right) [\sigma \nabla T \cdot \nabla T]_{\omega} - 2[(\nabla T \cdot \theta)(\sigma \nabla T \cdot n)]_{\omega}.$$ 

where we used $\theta = 0$ and $T = 0$ on $\partial \Omega$ and where $[\bullet]_{\omega}$ represents the jump discontinuity across $\omega$. Since $\phi \in E_1$, then $\lambda_{1}T + \sigma(T) - \lambda_{1}T = 0$ in $L^2(\Omega)$ and we also have $\nabla T \cdot \theta \in L^2(\Omega)$. We then replace the term denoted (1) by $-\lambda_{1}^2 T + \lambda_{1}uT$ and we obtain:

$$dA(\theta, \phi) - \lambda_{1} dB(\theta, \phi)$$

$$= \frac{1}{2} \left(\sigma \Delta \theta + (\nabla \theta) \cdot \nabla \theta + \nabla \sigma \cdot \theta - \sigma \nabla \theta\right) \nabla T \cdot \nabla T$$

$$- \frac{1}{2} \left(\Delta \theta + \lambda_{1} \int_{\omega} \left(\nabla \theta u + \tilde{Y}\right)^2 T^2\right)$$

$$+ \int_{\omega} \left(\theta \cdot n\right) [\sigma \nabla T \cdot \nabla T]_{\omega} - 2[(\nabla T \cdot \theta)(\sigma \nabla T \cdot n)]_{\omega}.$$
Plugging the expression of \( d\sigma(\theta) \) obtained in Proposition 3, we obtain the required expression as soon as we show that

\[
(\theta \cdot n)[\sigma \nabla T \cdot \nabla T]_{\partial \omega} = (\theta \cdot n)[\sigma \nabla T \cdot \nabla T]_{\partial \omega} - 2[\nabla \cdot \theta + \varphi \sigma \nabla T \cdot n]_{\partial \omega}.
\]

In order to obtain the above equation, recall that \( [\sigma \nabla T \cdot \nabla T]_{\partial \omega} = 0 = [\nabla \cdot \theta + \varphi \sigma \nabla T \cdot n]_{\partial \omega} \). Hence, we have

\[
[\sigma \nabla T \cdot \nabla T]_{\partial \omega} = \left[ \sigma^{-1}(\sigma \nabla T \cdot n)^2 \right]_{\partial \omega} + \left[ \sigma(\nabla T \cdot \nabla T) \right]_{\partial \omega}.
\]

And similarly

\[
[(\nabla \cdot \theta)(\sigma \nabla T \cdot n)]_{\partial \omega} = [\nabla \cdot \theta(\sigma \nabla T \cdot n)]_{\partial \omega} + [\sigma(\nabla T \cdot \nabla T)]_{\partial \omega}.
\]

which proves (23) which in turn proves the formulas (13) and (14).

5 A counterexample

In this Section, we prove that some shape optimization problems in the class that we consider do not admit a solution.

This is the case when one tries to minimize \( \lambda_1 \) or \( \lambda_{-1} \) under the “prescribed work of the pump” constraint. Non-existence of solutions for shape optimization problems is standard and is linked to the homogenization theory of microstructures and/or to failure of compactness for a certain topology. For instance, amongst the different additional hypotheses that one may require to ensure compactness in the Hausdorff topology, let us quote the perimeter constraint (Bucur and Zolesio 1994), the uniform cone condition (Chenais 1975), the uniform segment property (Neittaanmäki et al. 2006, A.3.9) and Sverak’s topological constraint (Sverak 1993) on the number of connected component of the complementary. Our counterexample verifies Sverak’s hypothesis but none of the other.

Our counterexample is stated in Proposition 8, it relies on the following lemma.

Lemma 2 Let \( \omega \) be a \( C^2 \) domain. There exists a sequence of regular domains \( \omega_n \) included in \( \omega \) such that

i) Every point in \( \partial \omega_n \) is at a distance at most \( 1/n \) along the vertical direction from a point of the boundary \( \partial \omega_n \).

ii) The characteristic function of \( \omega_n \) tends to the characteristic function of \( \omega \) strongly in \( L^1(\Omega) \).

As a consequence of i), the Poincaré inequality applied to the domain \( \omega_n \) reads

\[
\forall f \in H^1_0(\omega_n), \quad \int_{\omega_n} f^2 \leq \frac{1}{2n^2} \int_{\omega_n} |\nabla f|^2.
\]

Proof The domain \( \omega_n \) is obtained by removing \( O(n) \) thin stripes of width \( 1/n^2 \) and length \( O(1) \) from the domain \( \omega \). This construction is illustrated in Fig. 3 where the corners are rounded in order to make \( \omega_n \) as regular as wanted. The stripes are thin enough so that their union forms a set whose measure tends to zero, which proves ii). The proof of Poincaré’s inequality is standard from i) using Fubini’s theorem, see e.g., Dautray and Lions (1988).

Proof Let \( \omega \) be a fixed domain with a \( C^2 \) boundary. We consider the sequence of sets \( \{\omega_n\} \) given by Lemma 2, and denote \( u_n = u(\omega_n) \) the flow velocity in the domain \( \omega_n \). Let us prove that there exists a constant \( K \) such that for \( T \in H^1_0(\Omega) \),

\[
\int_\Omega u_n T^2 \leq \frac{K}{n^2} ||T||_{H^1(\Omega)}^2.
\]

From Cauchy-Schwarz inequality it follows that:

\[
\int_\Omega u_n T^2 \leq ||v_n||_{L^2(\Omega)} ||T||_{L^2(\Omega)} = ||v_n||_{L^2(\Omega)} ||T||_{L^2(\Omega)}^2.
\]

It follows successively from Sobolev’s embedding theorem and the fact that \( \Omega \) is bounded that

\[
||T||_{L^4(\Omega)} \leq ||T||_{W^{1,4}(\Omega)} \leq C ||T||_{H^1(\Omega)}.
\]

On the other hand, Poincaré’s inequality on the domain \( \omega_n \), an integration by parts and the use of (3) implies that

\[
||v_n||_{L^2(\Omega)}^2 = \int_{\omega_n} v_n^2 \leq \frac{1}{2n^2} \int_{\omega_n} |\nabla v_n|^2 = \frac{1}{2n^2} \int_{\omega_n} v_n^2.
\]

Caucahy-Schwarz inequality implies that

\[
\int_{\omega_n} v_n^2 \leq \frac{1}{2n^2} \int_{\omega_n} v_n \leq \frac{1}{2n^2} \left( \int_{\omega_n} v_n^2 \right)^{1/2} ||\omega_n||.
\]
hence
\[|v_n| |\lambda_1^{(\omega)}| \leq \frac{1}{2n^2} |\omega_n| \leq \frac{1}{2n^2} |\omega|,\]
which proves (24).

Let \(\phi^* \in \mathcal{G}\) be an eigenvector relative to the first eigenvalue \(\lambda_1^{\text{steady}}\) for the steady problem defined by
\[
(\lambda_1^{\text{steady}})^{-1} = \max_{\phi \in \mathcal{G}} \frac{(\mathbf{B}^{\text{steady}} \phi, \phi)}{(A^{\text{steady}} \phi, \phi)},
\]
where \(\mathbf{B}^{\text{steady}}\) corresponds to setting \(u = 0\) and hence is given by
\[
(\mathbf{B}^{\text{steady}} \phi, \phi) = \int_\Omega 2c(\omega) T s.
\]
It follows from inequality (24) that \((\mathcal{B}(\omega_n) \phi^*, \phi^*) \rightarrow (\mathbf{B}^{\text{steady}} \phi^*, \phi^*)\). It is also clear from point ii) in Lemma 2 and (4) that \((A^{\text{steady}})(\omega_n) \phi^*, \phi^*) \rightarrow (A(\phi^*, \phi^*)\). Therefore, when \(n\) tends to \(+\infty\), we have
\[
(\mathcal{B}(\omega_n) \phi^*, \phi^*) \rightarrow (\mathbf{B}^{\text{steady}} \phi^*, \phi^*) = (\lambda_1^{\text{steady}})^{-1}.
\]
Therefore, \(\limsup \lambda_1(\omega_n) \leq \lambda_1^{\text{steady}}\). Since the eigenvalues for the steady problem are strictly smaller than the eigenvalues of the original problem in \(\omega\), this proves that \(\omega\) is not optimal for the minimization of \(\lambda_1\).

Let us treat the case of \(\lambda_{-1}\). Denote \(\phi_n = (T_n, \gamma_n T_n)\) a sequence of eigenvectors associated to the eigenvalue \(\gamma_n = \lambda_{-1}(\omega_n)\) such that \((A(\omega_n) \phi_n, \phi_n) = 1\). The sequence \(\gamma_n\) is bounded in \(\mathbb{R}\) and so converges up to a subsequence to a certain \(\gamma^*\) and the sequence \(T_n\) is a bounded sequence in \(H^1_0(\Omega)\) that weakly-\(H^1\) converges to a certain \(T^*\). Moreover \(T_n\) verifies:
\[-\text{div}(c(\omega_n) \nabla T_n) = f_n \text{ with } f_n = \gamma_n u_n T_n - c(\omega_n) y_n^2 T_n.\]

The strong convergence of \(T_n\) towards \(T^*\) in \(L^2\) norm and \(u_n\) towards 0 in \(L^2\) norm ensures that \(f_n\) strongly converges to
\[-c(\omega)(\gamma^*)^2 T^*\]
in \(L^1(\Omega)\) and subsequently in \(H^{-1}(\Omega)\). Homogenization theory (Murat and Tartar 1978; Čerkaev and Kohn 1997) ensures that \(T^*\) verifies the equation
\[-\text{div}(\sigma^* \nabla T^*) = -c(\omega)(\gamma^*)^2 T^*,\]
where \(\sigma^*\) is the homogenized matrix associated to the sequence \(\chi_{\omega_1} \sigma_1 + (1 - \chi_{\omega_1}) \sigma_2\). Since the strong \(L^1\)-convergence of \(\chi_{\omega_n}\) towards \(\chi_{\omega}\) holds, then homogenization theory ensures that \(\sigma^* = \chi_{\omega} \sigma_1 + (1 - \chi_{\omega}) \sigma_2 = \sigma(\omega)\), see Allaire (2002). Hence, \(T^*\) is an eigenvector of the steady problem and
\[
(\gamma^*)^{-1} \geq (\lambda_1^{\text{steady}})^{-1} > (\lambda_{-1})^{-1}
\]
this proves that for \(n\) sufficiently large, \(\lambda_{-1}(\omega_n) = \gamma_n < \lambda_{-1}(\omega)\).

\[\square\]

6 Numerical results

We perform several tests while changing the type of normalization (either “prescribed flow”, “dissipation” or “work” see Definition 1), changing the factor of normalization (the quantity \(F\), \(D\) or \(P\) introduced in Definition 1), varying the conductivities in the solid phase (\(c_2\) and \(\sigma_2\)). The outer domain \(\Omega\) is the square \([-1, 1] \times [-1, 1]\). The conductivity in the fluid phase (\(c_1\) and \(\sigma_1\)) are set to be equal to one, after a normalization of (7). We study test-cases concerning the maximization of the smallest positive eigenvalue in Section 6.2. In view of the non-existence results of Section 5, when dealing with the minimization of the smallest positive eigenvalue, an additional geometric constraint is added, see Section 6.3.

6.1 Presentation of the numerical algorithm

The numerical implementation is performed with the finite element method and \(P^2\) finite elements for computing both the velocity and the eigenvectors. The optimization uses a steepest descent method based on the computation of the gradient with respect to the shape of the domain presented in Proposition 4.

There exist two major ways to represent the domain. The first method consists in parameterizing the nodes of the boundary of the domain and to advect those nodes according to the direction of descent given by the gradient, this
method is called thereafter “mesh-morphing”. To be more precise, the initial data is a non self-intersecting curve discretized by $N$ points inside the prescribed domain $\Omega$. Mesh its interior $\omega$ and its exterior $\Omega \setminus \omega$, compute $v$, compute the eigenvalue and the value of $e(\phi)$ as in (13), since the corresponding eigenspace is supposed to be of dimension 1, $e(\phi)$ can only take one value. If every point defining the boundary is advected by the velocity $e(\phi)n$ where $n$ is the outward normal to $\omega$, then the eigenvalue rises. Drop the mesh and advect only the $N$ points of the boundary by this velocity in order to obtain new coordinates for the points. If necessary, modify the points so that they define a non self-intersecting curve and are uniformly spaced on the curve. Re-mesh and repeat to reach convergence.

The second method consists in working on a fixed Cartesian mesh and to parameterize the boundary of $\omega$ as the zero level-set of a given function $\psi$. Given a level set $\psi$ defined on the nodes of the mesh, cut the cells along the lines $\psi = 0$. Define $\omega = \{ \psi < 0 \}$ and $\Omega \setminus \omega = \{ \psi > 0 \}$. Compute $v$, the eigenvalue and the value of $e(\phi)$ as in (13), since the corresponding eigenspace is supposed to be of dimension 1, $e(\phi)$ can only take one value. If $\psi$ is advected with the Hamilton-Jacobi equation

$$\partial_t \psi + V|\nabla \psi| = 0$$

with $V = e(\phi)$ on $\partial \Omega$, then the derivative of the eigenvalue w.r.t. time is positive (see Osher and Santosa (2001)). We define $V$ as $V = e(\phi)$ on $\partial \omega$, $V = 0$ on $\partial \Omega$ and $\Delta V = 0$ in $\omega$ and $\Omega \setminus \omega$. The final time $t_f$ of the Hamilton-Jacobi equation plays the role of the step of the gradient method. Repeat the process with domains defined as the level-sets of $\psi(t_f)$ until convergence is reached. This second method is known as the “level-set” method, for further details on the implementation see Allaire et al. (2004).

In both cases, we adapt the gradient step such that, if the eigenvalue decreases after one iteration, we come back to the previous iteration and reduce the step. This ensures that the eigenvalue always increases during the optimization procedure.

Those methods have the following advantages and drawbacks

- The mesh-morphing method allows for fine control of the final shape, but cannot change the topology of $\omega$, in our case, the main problem is when the boundary of $\omega$ reaches $\partial \Omega$. This method also requires to remesh at each iteration, thankfully, the remeshing operation is not very time-consuming in 2D, indeed it is of the same order as the cost of the eigenvalue problem. In order to speed up the algorithm, the boundary is first meshed with a few number of points which is increased along the iterations. Moreover, if two points of the boundary are too far apart, a new point of the boundary is added in between them in order to keep the mesh structured.

- The level-set method does not preserve the topology of $\omega$ and since the computations are performed on a fixed mesh, is more stable and less prone to errors due to re-meshing operations. The main drawback is that the precision of the result is linked to the original Cartesian grid.

We performed the tests with the two methods separately, in order to document the advantages of each. Of course, an algorithm for industrial production would mix the two methods, starting with a level-set method and then a mesh-morphing one.

6.2 Discussion of the numerical results

In all the tests shown, the number of triangles of the mesh is approximatively $10^4$. We used Python programming language and Getfem++ (Pommier and Renard) finite element library, the re-mesh operations are performed by the BAMG (Hecht) software.

In Figs. 4 and 5, we show optimal forms for the fixed dissipation case for the same parameters. It is interesting to note that some of the resulting optimal shape share similar features with those obtained in figure 17 of Iga et al. (2009). Figure 4 are the optimal shapes obtained by the mesh-morphing method whereas Fig. 5 shows the optimal shapes for the level-set method.

![Fig. 4 The optimal shapes for the mesh-morphing method and fixed dissipation. The conductivity of the solid phase $c_2 = \sigma_2$ are equal to (from left to right) : 1, 5, 10 and the total dissipation is set equal to (from top to bottom) : $D = 0.1, 1, 10$](image)
In Fig. 6, we show optimal forms for the prescribed flow case and the mesh morphing method, the optimal shapes for the level set method being show-cased in Fig. 7. Finally, Fig. 8 displays optimal forms for the fixed work of the pump case and the mesh morphing method whereas Fig. 9 presents optimal shapes obtained by the level-set method.

We observe that the mesh-morphing and level-set method optimal shapes are comparable, that the mesh-morphing optimal shapes are more accurate than the ones obtained by the level-set method but that they do not always converge, see for instance the last line of Fig. 4 which corresponds to a fixed viscosity of 100 and an optimal domain $\omega$ that touches the boundary of $\Omega$ which prevented the mesh-morphing algorithm to converge. We verify here the rule of thumb that the level-set method is more stable but less accurate than the mesh-morphing one. An other interesting case were the mesh-morphing method fails to converge is the very first case of Fig. 6 that corresponds to $\sigma_2 = 1$ and to a prescribed total flow of 0.1. Indeed in this case, the optimal domain seems to be a disk of small radius but the mesh-morphing method is stuck in a local minimizer composed of four small disks linked together by rods. For this special case, the mesh morphing methods is trying to remove the rods which is impossible because it may not change the topology of the optimal domain, this case is an example of the limitations of the mesh morphing methods when topology changes are involved. Of course the optimal shape given by the mesh morphing method in this case is not to be trusted, one should prefer the one yielded by the level-set method.

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**Fig. 5** The optimal shapes for the level-set method and fixed dissipation. The conductivity of the solid phase $c_2 = \sigma_2$ are equal to (from left to right): 1, 5, 10 and the total dissipation is set equal to (from top to bottom): $D = 0.1, 1, 10, 100$

**Fig. 6** The optimal shapes for the mesh-morphing method and fixed flow. The conductivity of the solid phase $c_2 = \sigma_2$ are equal to (from top to bottom): 1, 5, 10 and the total flow is set equal to (from left to right): $F = 0.1, 1, 10$

**Fig. 7** The optimal shapes for the level-set method and fixed flow. The conductivity of the solid phase $c_2 = \sigma_2$ are equal to (from top to bottom): 1, 5, 10 and the total flow is set equal to (from left to right): $F = 0.1, 1, 10$
There is a third instance where the mesh-morphing method presents a drawback and is illustrated in Fig. 8, the first (and second) optimal shape of the last column, that correspond to exterior conductivities of 10 and to a prescribed total flow of 0.1 (resp. of 1). Observe that the optimal shape in this case roughly resembles a rounded square with four “cuts”, two in the horizontal and in the vertical direction. In this case, the mesh-morphing method is striving to improve the cups-like cuts, reducing the step of the method due to a strict condition of non-overlapping of the boundary along this cups and fails to improve the rest of the shape. Moreover, even if those kind of cups might improve the objective function in the continuous setting, they yield a smaller improvement in the numerical sense, since they require a (prohibitive) denser mesh around the cups for the computations to be accurately rendered. Hence the mesh-morphing method performs slightly worse than the level-set method in those cases (an eigenvalue of 3.53 in the level-set method against an eigenvalue of 3.4 for the mesh-morphing method).

6.3 Geometric constraints

It is a well known fact that shape sensitivity analysis is only valid in a regularity regime of the domain under consideration that is violated during the optimization procedure, see Henrot and Pierre (2005). We implemented the standard trick that consists of adding geometric constraints to the

Fig. 9 The optimal shapes for the level-set method and prescribed work of the pump. The conductivity of the solid phase $c_2 = \sigma_2$ are equal to (from left to right) : 1, 5, 10 and the total work is prescribed to be equal (from top to bottom) : $P = 0.1, 1, 10, 100$

Fig. 10 Two final shapes for the minimization of the first negative eigenvalue in the “prescribed work of the pump” constraint. On the left, without a perimeter constraint, the algorithm fails to converge and tries to build a shape similar to the counterexample of Section 5. On the right, the final shape of the algorithm with a perimeter constraint implemented.
objective function in order to ensure that the resulting optimal shapes are more regular. These geometric constraints may be driven by:

- Practical considerations concerning the manufacturing of the shape.
- Numerical considerations related to the meshing and the advection of domains with irregular boundary.
- Mathematical considerations concerning the non-existence of optimal shapes, as in the case discussed in Section 5.

We chose to impose a perimeter constraint by adding the perimeter to the objective function. Namely (e.g. in the case of the first positive eigenvalue) the objective function becomes

\[ J(\Omega) = \lambda_1 + v|\partial \Omega|, \]

where \( v \) is a given number, positive in the case of the minimization of \( J \) and negative in the case of the maximization of \( J \). This term contributes to the gradient by adding a multiple of the mean curvature \( H = \text{div}(n) \) (see Allaire et al. (2004)), i.e., (13) is replaced by

\[
dJ(\theta) = \min_{\phi \in E_1, (\Delta \phi) = 0} \int_{\partial \omega} (\theta \cdot n)[e(\phi) + vH]. \tag{26}
\]

We re-tested every case of Section 6.1, the optimal shapes that were obtained after adding the perimeter constraint were similar to the one described above. In our experiments (moderate value for \( v \)) the perimeter constraint removed the jagged character of the boundary of the optimal shape only by a marginal factor.

We implemented the perimeter constraint in the case of Section 5, when dealing with minimization of the eigenvalues under the “prescribed work of the pump” constraint. In this case, the perimeter constraint allows to circumvent the counter-example and the perimeter constraint stabilizes the algorithm. An example of this phenomenon is illustrated in Fig. 10.

**Conclusion**

In this paper, we presented a novel application of shape optimization tools. We gave a rigorous proof of eigenvalue sensitivity analysis in the case of biphasic domains with coefficient depending themselves on an auxiliary PDE. Numerous optimal shapes are provided using two different numerical methods, proving the capacity of shape sensitivity analysis to provide original shapes. The framework presented here is merely a proof of concept, the constraints and the objective functions are to be adapted to specific applications.

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