

Adjoint-aided homogenisation for flows through heterogeneous membranes

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Porous membranes, like nets or filters, are thin structures that allow fluid to flow through their pores. Homogenisation can be used to rigorously link the flow velocity with the stresses on the membrane via several coefficients (e.g. permeability and slip) stemming from the solution of Stokes problems at the pore level. For a periodic microstructure, the geometry of a single pore determines these coefficients for the whole membrane. However, many biological membranes are not periodic, and the porous microstructure of industrial membranes can be modified to address specific needs, resulting in non-periodic patterns of solid inclusions and pores. In this case, multiple microscopic calculations are needed to retrieve the local non-periodic membrane properties, negatively affecting the efficiency of the homogenised model. In this paper, we introduce an adjoint-based procedure that drastically reduces the computational cost of these operations by computing the pore-scale solution's first- and second-order sensitivities to geometric modifications. This adjoint-based technique only requires the solution of a few problems on a reference geometry and allows us to find the homogenised solution on any number of modified geometries. This new adjoint-based homogenisation procedure predicts the macroscopic flow around a thin aperiodic porous membrane at a fraction of the computational cost of classical approaches while maintaining comparable accuracy.

Key words: porous media, membranes

1. Introduction

Fluid flows permeating a porous, thin membrane, have attracted a wide interest in engineering and natural sciences. Biological cells exchange water and nutrients with the environment using protein-based channels on their membranes (Verkman & Mitra 2000; Jensen *et al.* 2016). Glass sponges like the *Euplectella aspergillum* show interesting thin porous skeletons, which ensure their structural stability and allow the feeding of the organisms living inside them. Filtration and separation systems are widely used in the chemical and biomedical industry (Catarino *et al.* 2019), water purification technologies (Mohanty & Purkait 2011) and batteries (Lu *et al.* 2017; Dai *et al.* 2022). Periodic porous media are adopted in some applications such as regenerators (i.e. porous matrices working as heat exchangers) for refrigerators used in cryogenic applications (Roberts & Desai 2003) and offer obvious modelling advantages, such as the possibility of retrieving the whole medium properties from the geometric unit cell repeating along the membrane. On the other hand, biological porous membranes can be very irregular (Verkman & Mitra 2000) and periodic membranes can become aperiodic due to the loads applied by a fluid flowing across it (Fagbemi *et al.* 2018), erosion or fouling or by the presence of defects in the fabrication process. Non-periodicity is also leveraged to improve the efficiency of filtration devices (Dalwadi *et al.* 2015).

The precise and efficient description of flows through porous media plays a key role in many engineering fields. We can classify the modelling of flows across porous media into two families: direct solutions and averaged models. In the first case, we consider the actual geometry of the porous medium and solve the governing equations at all scales of interest. Periodic and aperiodic structures in various flow conditions (Icardi *et al.* 2014; Falcucci *et al.* 2021) can be studied using this technique with very high accuracy, since the fluid flow solution is accessible up to the smallest scale of interest in time and space. However, these simulations easily become prohibitively computationally expensive, they are rarely scalable and do not adapt well to large parametric studies or optimisation routines. The second family relies on a simplified physical description. We substitute a fictitious homogeneous domain to the actual geometry of the medium characterised by coefficients representing the average properties of the porous structure (Darcy 1856; Dagan 1987). Some authors (Hasimoto 1958; Conca 1987; Wang 1994; Bourgeat *et al.* 2001) analytically computed these coefficients in simple, periodic geometries and flow configurations. However, in most cases, they have been empirically found. Non-periodicity of the medium's microstructure is often introduced in these models using additional correction coefficients (Jensen *et al.* 2014). Such techniques are computationally very cheap compared with direct solutions, but their empiricism limits their predictive power. Averaged models with predictive capabilities are thus an active field of research since they represent a good trade-off between accuracy and computational cost. Multiscale methods such as the volume averaging method (Whitaker 1999) and homogenisation (Hornung 1997; Mei & Vernescu 2010) are at the core of these techniques.

In most homogenisation and volume averaging works, the porous microstructure must show periodicity or exhibit a representative elementary volume (REV), i.e. the minimal geometrical portion of the medium where some properties like permeability are univocally determined in a statistical sense. We refer to the book by Bear & Bachmat (1990) for a formal definition of the REV. In the periodic case, there exists a unit cell containing one (Lăcis & Bagheri 2017; Luckins *et al.* 2023) or more pores (Shipley & Chapman 2010), repeating along the medium geometry. In the REV case, there is no such geometrical repetition along the membrane, but if the microstructure is sufficiently regular, an enclosing volume with the same full membrane statistical

properties can be found (Whitaker 1999). This, however, requires several iterations. For example, Rolland du Roscoat *et al.* (2007) experimentally determined the extension of such entity in some industrial paper materials using microtomography. Auriault *et al.* (2009) also pointed out that typically 10 heterogeneities along a direction in the REV are sufficient in several real situations and that the REV reduces to the unit cell for periodic media. Using the REV assumption, Valdés-Parada & Alvarez-Ramírez (2011) studied asymmetric diffusion in stratified and fractured porous media and Chernyavsky *et al.* (2011) studied haemodynamic transport across the villous branches of the human placenta. However, microstructures with slow geometry modifications have also been considered, effectively bridging the gap between the periodic and non-periodic cases. For example, van Noorden (2009) studied precipitation and dissolution in a pore of varying volume and Van Noorden & Muntean (2011) studied the transport across porous structures with varying diffusivities, while Auton *et al.* (2022) studied the transport and sorption in a longitudinally heterogeneous and transversely periodic medium and Alavi *et al.* (2024) introduced a conformal transformation to analyse quasiperiodic porous structures. In many cases, considering spatially varying geometry or flow conditions requires the construction of surrogate models to contain the computational cost. For example, in a previous work (Wittkowski *et al.* 2024), we adopted a clustering technique (i.e. algorithms used to divide a given dataset into clusters based on a notion of similarity between the elements) to reduce the computational cost of a coupling procedure for inertial flows across thin porous membranes. The problem of coupling the pore-scale and the far-field scale dynamics for reacting flows in bulk porous media has also been investigated by Karimi & Bhattacharya (2024a,b) using recurrent neural networks.

The works mentioned above were mainly related to bulk porous media, while homogenisation has been proposed as a methodology for the analysis of fluid flows (Zampogna & Gallaire 2020) and transport of diluted species (Zampogna *et al.* 2022, 2023) across thin porous membranes with periodic microstructure. In this framework, the membrane average properties (i.e. the so-called Navier tensors) are the spatially averaged solutions of solvability conditions derived from the equations valid at the pore scale. The Navier tensors encrypt the ability of the fluid to pass across and along the membrane and they are useful in the design of efficient filtration devices (Park *et al.* 2013). These tensors correspond to and extend the concept of permeability and slip in the case of bulk porous media and impervious rough surfaces, respectively. Ledda *et al.* (2021) embedded homogenisation into an adjoint-based loop for the design of thin, porous membranes, finding optimal aperiodic microstructures maximizing drag for a given macroscopic flow configuration. In their work, the link between the shape of a single solid inclusion and the Navier tensors was mapped for different geometrical parameters using direct solutions of the equations valid at the pore scale. The cost of this mapping scales with the number of pores/inclusions. The interest in a theoretical tool able to efficiently predict how geometrical modifications in the microstructure of a porous thin membrane affect the local average microscopic properties is thus clear. In other words, we search for a mathematical tool able to handle many shape modifications of the microstructure while keeping the computational cost lower than a series of direct evaluations. This is a common situation in many engineering fields, such as in the automotive and aerospace industries, where the shape of vehicles can be optimised to reach a desired objective such as minimizing drag. In many cases, the resulting gradient-based optimisation routines are solved using adjoint equations, see Skinner & Zare-Behtash (2018) for a review.

Adjoint-based approaches have proven an efficient physics-based technique to forecast how shape changes affect given integral quantities of a flow field in external aerodynamics (Jameson 1988; Jameson *et al.* 1998; Mohammadi & Pironneau 2001). In other techniques,

such as finite differentiation (Reneaux & Thibert 1985), a set of control points are used to control the shape of objects immersed in a flow. These control points are displaced one by one, and the flow is recomputed for each modified geometry. An approximation of the shape sensitivity is then constructed component by component using finite differences. This simple approach does not require solving additional flow equations, but its cost increases with the number of evaluation points and its precision depends on the discretisation. On the other hand, adjoint methods to compute shape sensitivity are more precise and their cost does not depend on the number of evaluation points on the geometry. However, these techniques require the solution of additional flow equations, the adjoint equations, which allow us to evaluate the gradient mentioned above directly.

In the present paper, we focus on the efficient evaluation of the properties of non-periodic membranes via adjoint-based techniques. To develop our methodology, we consider the model developed in Zampogna & Gallaire (2020) for flows past membranes with perfectly periodic pore structure and introduce a technique based on adjoint equations to estimate the gradient of the Navier tensors with respect to an infinitesimal modification of the shape of the solid inclusion, i.e. the shape sensitivity. In § 2 we summarise the model by Zampogna & Gallaire (2020) and derive the adjoint problems from the equations governing the system at the pore scale; in § 3 we compare the direct solution of the pore-scale problems with the adjoint-based prediction for a series of shape changes; in § 4 we use the so-developed tools to analyse the fluid flow across non-periodic thin membranes. In § 5, we summarise the main results and discuss future perspectives.

2. Modelling shape changes in porous membranes using first- and second-order adjoint methods

We consider the incompressible flow of a Newtonian fluid of density ρ and viscosity μ across a thin permeable membrane, depicted in figure 1(a). We denote with $\hat{x}_i = (\hat{x}_1, \hat{x}_2, \hat{x}_3)$ the (dimensional) global coordinate system, with $\hat{u}_i$ and $\hat{p}$ the dimensional fluid flow velocity and pressure and with $\hat{t}$ the dimensional time. We also introduce the outward-pointing normal and two tangent vectors to any boundary $(\hat{n}, \hat{t}, \hat{s})$, specified case by case. Locally, on the surface, we can isolate a control volume containing few pores/solid inclusions and identify a dimensional local reference frame $(\hat{x}_n, \hat{x}_t, \hat{x}_s)$. Assuming that the membrane curvature is negligible at the pore scale, the local frame of reference $(\hat{x}_n, \hat{x}_t, \hat{x}_s)$ is aligned with the normal and tangent vectors $(\hat{n}, \hat{t}, \hat{s})$ to the membrane centreline $\mathbb{C}$ at that location. In the following, the absence of the $\hat{\cdot}$ symbol indicates the non-dimensional quantities and when an index is not repeated, it runs implicitly for 1, 2, 3 for the quantities written on the $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ coordinate system and for n, t, s for the quantities written in the $(\hat{x}_n, \hat{x}_t, \hat{x}_s)$ coordinate system.

In the case of an aperiodic porous medium satisfying a precise set of hypotheses based on statistics, such as ergodicity, it is possible to apply homogenisation within a REV. The REV can be regarded as the minimal subset of the medium at which some properties, such as its porosity or the permeability, are statistically constant if the subset size is enlarged (Bear & Bachmat 1990). We denote with l' (cf. figure 1c) the REV size, with l the distance between two subsequent pore centres and L the membrane characteristic length. We can estimate that $l' \sim ml$, where m is the number of pores we count crossing the REV along some direction. Bear & Bachmat (1990) adopted statistical arguments to conclude the need for the scale relation $l \ll l' \ll L$. Based on experimental evidence, Auriault *et al.* (2009) have shown that the relation above is relaxed as $l \leq l' \ll L$, where the equality is attained in the case of periodic microstructure, i.e. $m = 1$, and the REV reduces to the unit cell. A common choice to compute the permeability associated with some REV

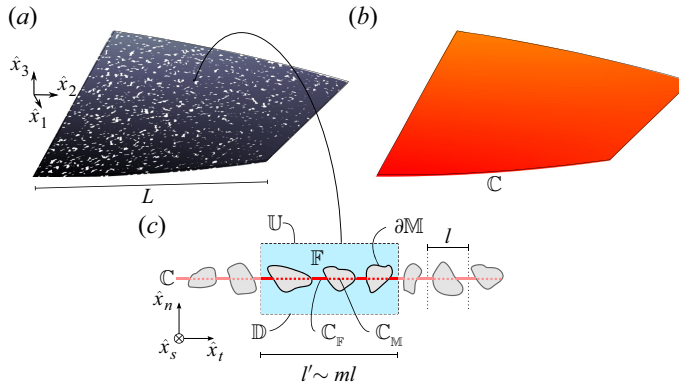


Figure 1. (a) Porous aperiodic thin membrane as it appears in the physical world. We denote with $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ the (dimensional) global coordinate system and with L the characteristic size of the membrane. (b) Membrane centre surface $\mathbb{C}$, which serves as a fictitious interface to divide the original fluid domain into two macroscopic subdomains. (c) Section of the local aperiodic microstructure of the full-scale membrane, neglecting the curvature of $\mathbb{C}$. $(\hat{x}_n, \hat{x}_t, \hat{x}_s)$ is the local coordinate system, aligned with the normal and tangent vectors to the membrane midsurface, $\mathbb{C}$ (red). Along the membrane, we identify a REV (dashed black line in the zoom box) of size l' , which counts m unit cells of typical size l (distance between two subsequent pore centres). We denote with $\mathbb{F}$ the fluid domain inside it and with $\mathbb{U}$, $\mathbb{D}$ and $\partial\mathbb{M}$ its upward and downward sides and its boundary with any solid inclusion, respectively. The portions of the (rectified) membrane centreline $\mathbb{C}$ in the REV crossing the fluid and the solid are denoted with $\mathbb{C}_F$ (red line) and $\mathbb{C}_M$ (red dots), respectively.

geometry is to employ its periodic extension and impose periodic boundary conditions on the fluid flow variables along the membrane tangential directions, compare with, for example, Hendrick *et al.* (2012). From a practical point of view, we need to verify that the ergodicity hypothesis at the basis of the REV concept applies to a given microstructure: a strategy to establish which REV is statistically representative of the whole geometry is to calculate the membrane properties in sets of nested REV and determine when the property of interest converges with the size and location of the REV. Identifying such a REV requires many direct evaluations of the average medium properties. In this paper, we propose an efficient procedure to evaluate the properties of such different REV geometries. To perform this task, we postulate the existence of a REV and we consider simple pore geometries. This procedure can also be applied to explore geometrical modifications of periodic porous media, where the unitary cell replaces the REV.

In our domain, the fluid region in the REV is denoted by $\mathbb{F}$ (figure 1) and all the boundaries of the fluid domain by $\partial\mathbb{F}$. Among the latter, the solid–fluid boundary is called $\partial\mathbb{M}$ and the upward and downward sides of $\mathbb{F}$ are named $\mathbb{U}$ and $\mathbb{D}$, respectively. The Navier–Stokes equations govern the evolution of the dimensional flow velocity $\hat{u}_i$ and pressure $\hat{p}$ in the whole fluid domain,

$$\begin{cases} \rho(\hat{\tau}_\tau \hat{u}_i + \hat{u}_j \hat{\partial}_j \hat{u}_i) = -\hat{\partial}_i \hat{p} + \mu \hat{\partial}_{kk}^2 \hat{u}_i, \\ \hat{\partial}_i \hat{u}_i = 0, \\ \hat{u}_i = 0 \quad \text{on } \partial\mathbb{M}, \end{cases} \quad (2.1)$$

where Einstein's index notation is adopted and $\hat{u}_i = 0$ is intended for each vector component.

Zampogna & Gallaire (2020) proposed a predictive homogeneous model to compute the average flow fields across a periodic thin membrane. In this model, the membrane is treated as a fictitious interface on which equivalent stress-jump conditions are imposed to mimic

the macroscopic effect of the real porous structure on the fluid flow. These conditions, explicitly given in § 2.1.5, contain some coefficients which represent the membrane properties and are the solution of Stokes problems within the REV. We summarise the homogenised model in § 2.1 and introduce in § 2.2 the adjoint-based method used to compute the sensitivity of the above-mentioned coefficients with respect to shape changes.

2.1. From the pore geometry to the macroscopic flow

Starting from the Navier–Stokes equations (2.1), the homogenisation procedure described in Zampogna & Gallaire (2020) relies on the following steps: (i) define and normalise the inner equations, valid at the pore scale, (ii) define and normalize the outer equations, valid far from the membrane, (iii) match the inner and outer equations and solve the inner (microscopic) problem and (iv) average the inner solution and deduce the macroscopic conditions, i.e. the equivalent interface conditions to account for the presence of the membrane in the outer (macroscopic) problem. In the present analysis, we develop a new methodology to efficiently compute the average solution of the microscopic problems for different microstructures. We thus consider a small number of pores per REV, i.e. $m = \mathcal{O}(1)$ (when $m = 1$, we have a fully periodic geometry). We introduce a small scale-separation parameter $\epsilon = l/L$, that is the ratio between the typical interpore distance and the membrane characteristic size. Auriault *et al.* (2009) suggested that real heterogeneous media exhibit a typical m of approximately 10. The relevant separation of scales parameter ϵ is not modified by the introduction of a REV of typical size l' , since $l \sim l'$. The relation $\epsilon = l/L \sim l'/L$ holds, which is consistent with considering a small number of pores per REV.

2.1.1. The inner, pore-scale problem

We first focus on the inner, pore-scale flow description within the REV. We introduce the following non-dimensionalisation for equation (2.1):

$$\hat{x}_i = lx_i \quad \hat{p} = \Delta P p = \frac{\mu U}{l} p \quad \hat{u}_i = U u_i \quad \hat{\tau} = T \tau = \frac{l}{U} \tau, \quad (2.2)$$

where ΔP and U are the (dimensional) microscale characteristic pressure difference and microscale velocity, respectively. The governing equations become

$$\begin{cases} Re_l (\partial_\tau u_i + u_j \partial_j u_i) = -\partial_i p + \partial_{kk}^2 u_i, \\ \partial_i u_i = 0, \\ u_i = 0 \quad \text{on } \partial \mathbb{M}, \end{cases} \quad (2.3)$$

where $Re_l = \rho U l / \mu$ is the Reynolds number based on the microscopic length l and microscale characteristic velocity U . We assume that the flow variables (u_i, p) exhibit periodicity along the tangential-to-the-membrane direction in the REV, but not at the macroscale, i.e. they are locally periodic but macroscopically aperiodic. This approach has already been proposed for homogenizing fluid flows and solute transport across bulk, heterogeneous porous media by, for example, Dalwadi *et al.* (2015) and Auton *et al.* (2022).

2.1.2. The outer, membrane-scale problem

In the macroscopic domain, the following non-dimensionalisation is employed to scale the equations:

$$\hat{x}_i = L X_i \quad \hat{p} = \Delta P^\circ p^\circ = \frac{\mu U^\circ}{L} p^\circ, \quad \hat{u}_i = U^\circ u_i^\circ, \quad \hat{\tau} = T^\circ \tau^\circ = \frac{L}{U^\circ} \tau^\circ, \quad (2.4)$$

where $\Delta P^\ominus$, $U^\ominus$ and $T^\ominus$ are the (dimensional) outer pressure difference, velocity and time scales, respectively. The governing equations of the outer problem become

$$\begin{cases} Re_L \left(\partial_{\tau^\ominus} u_i^\ominus + u_j^\ominus \partial_j u_i^\ominus \right) = -\partial_i p^\ominus + \partial_{kk}^2 u_i^\ominus, \\ \partial_i u_i^\ominus = 0, \end{cases} \quad (2.5)$$

where $Re_L = \rho U^\ominus L / \mu$ is the Reynolds number based on the macroscopic length L and outer velocity $U^\ominus$.

2.1.3. Matching inner and outer normalisations

On the upward $\mathbb{U}$ and downward $\mathbb{D}$ sides of the fluid domain $\mathbb{F}$, the fluid flow is continuous, i.e. the (dimensional) velocity and fluid stresses match

$$u_i U = u_i^{\ominus, \mathbb{U}} U^\ominus, \quad u_i U = u_i^{\ominus, \mathbb{D}} U^\ominus, \quad \Sigma_{ij} n_j = \epsilon \frac{U^\ominus}{U} \Sigma_{ij}^{\ominus, \mathbb{U}} n_j, \quad \Sigma_{ij} n_j = \epsilon \frac{U^\ominus}{U} \Sigma_{ij}^{\ominus, \mathbb{D}} n_j, \quad (2.6)$$

where $\Sigma_{ij} = -p \delta_{ij} + (\partial_i u_j + \partial_j u_i)$ is the stress tensors normalised with the inner scales and $\Sigma_{ij}^{\ominus, \mathbb{U}} = -p^{\ominus, \mathbb{U}} \delta_{ij} + (\partial_i u_j^{\ominus, \mathbb{U}} + \partial_j u_i^{\ominus, \mathbb{U}})$ and $\Sigma_{ij}^{\ominus, \mathbb{D}} = -p^{\ominus, \mathbb{D}} \delta_{ij} + (\partial_i u_j^{\ominus, \mathbb{D}} + \partial_j u_i^{\ominus, \mathbb{D}})$ are the stress tensors normalised with the outer scales and evaluated on $\mathbb{U}$ or $\mathbb{D}$, respectively.

2.1.4. Solving the inner problem

Exploiting the separation between the pore and membrane length scales, we can decompose the inner spatial variable into a fast (x_i) and a slow (X_i) variable and perform an asymptotic expansion of the flow fields,

$$x_i \rightarrow x_i + \epsilon X_i, \quad \partial_i \rightarrow \partial_i + \epsilon \partial_{X_i}, \quad (u_i, p) \rightarrow (u_i^{(0)}, p^{(0)}) + \epsilon (u_i^{(1)}, p^{(1)}) + O(\epsilon^2), \quad (2.7)$$

where the capital subscript denotes the derivation with respect to the macroscopic slow spatial variable X_i . Substituting (2.7) into (2.3), supposing that the flow inertia is negligible at the pore scale (as in Malone *et al.* 1974; Tio & Sadhal 1994; Zampogna & Gallaire 2020; Ledda *et al.* 2021; Zampogna *et al.* 2023), i.e. $Re_l \sim \epsilon$, and collecting each order term in ϵ , we obtain the leading-order problem

$$\begin{cases} -\partial_i p^{(0)} + \partial_{kk}^2 u_i^{(0)} = 0, \\ \partial_i u_i^{(0)} = 0, \\ \Sigma_{ij}^{(0)} n_j = \Sigma_{ij}^{\ominus, \mathbb{U}} n_j \text{ on } \mathbb{U}, \\ \Sigma_{ij}^{(0)} n_j = \Sigma_{ij}^{\ominus, \mathbb{D}} n_j \text{ on } \mathbb{D}, \\ u_i^{(0)} = 0 \text{ on } \partial \mathbb{M}, \\ u_i^{(0)}, p^{(0)} \text{ periodic along } t_i, s_i, \end{cases} \quad (2.8)$$

where t_i, s_i are the tangents to the membrane centreline $\mathbb{C}$ (cf. figure 1*b,c*). In problem (2.8), the quantities $\Sigma_{jk}^{\ominus, \mathbb{U}}$ and $\Sigma_{jk}^{\ominus, \mathbb{D}}$ do not depend on the integration variable x_i and they act as non-homogeneous source terms. As shown by Zampogna & Gallaire (2020), the linearity of the governing equations allows us to formally write the velocity and pressure fields as a linear combination of the source terms, i.e. the outer stresses acting on the upward $\mathbb{U}$ and downward $\mathbb{D}$ sides of the REV. Naming M_{ij} , N_{ij} , Q_j and R_j the

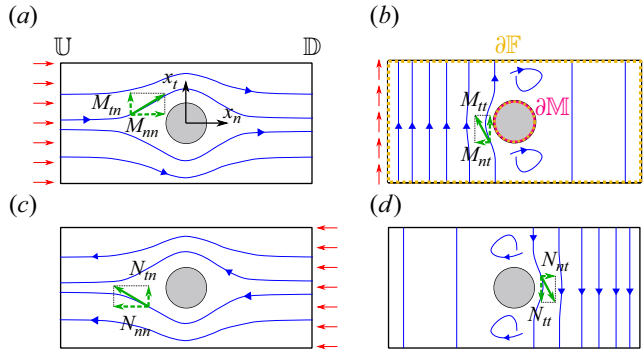


Figure 2. Sketch showing the physical meaning of M_{ij} and N_{ij} . A 2-D configuration is chosen, with a membrane formed by the periodical repetition of circular solid inclusions. In each panel, the left-hand and right-hand sides of the rectangular cell, $\mathbb{U}$, $\mathbb{D}$, are the upward and downward sides of the fluid domain $\mathbb{F}$ as in figure 1(c). The union of all fluid boundaries, $\partial\mathbb{F}$, and the fluid–solid boundary alone, $\partial\mathbb{M}$, are shown in (b) in yellow and magenta, respectively. The red arrows represent the direction of the vector Σ_{ijn_j} , while the blue lines represent the flow streamlines. Solid green arrows represent the local flow direction and the corresponding dashed arrows its components along the principal axes: (a) (M_{nn}, M_{tn}) ; (b) (M_{nt}, M_{tt}) ; (c) (N_{nn}, N_{tn}) ; (d) (N_{nt}, N_{tt}) .

coefficients of the linear combination, the formal solution of problem (2.8) is written as

$$\begin{cases} u_i^{(0)} = M_{ij} \Sigma_{jk}^{\mathbb{O}, \mathbb{U}} n_k + N_{ij} \Sigma_{jk}^{\mathbb{O}, \mathbb{D}} n_k, \\ p^{(0)} = Q_j \Sigma_{jk}^{\mathbb{O}, \mathbb{U}} n_k + R_j \Sigma_{jk}^{\mathbb{O}, \mathbb{D}} n_k. \end{cases} \quad (2.9)$$

Substituting (2.9) into (2.8), we obtain the closure problems (the so-called microscopic problems) for the quantities M_{ij} , N_{ij} , Q_j and R_j within the REV, i.e.

$$\begin{cases} -\partial_i Q_j + \partial_{kk}^2 M_{ij} = 0 & \text{in } \mathbb{F}, \\ \partial_i M_{ij} = 0 & \text{in } \mathbb{F}, \\ \Sigma_{hq}(M_{.j}, Q_j) n_q = \delta_{jh} & \text{on } \mathbb{U}, \\ \Sigma_{hq}(M_{.j}, Q_j) n_q = 0 & \text{on } \mathbb{D}, \\ M_{ij} = 0 & \text{on } \partial\mathbb{M}, \\ M_{ij}, Q_j & \text{periodic along } t_i, s_i, \end{cases} \quad \begin{cases} -\partial_i R_j + \partial_{kk}^2 N_{ij} = 0 & \text{in } \mathbb{F}, \\ \partial_i N_{ij} = 0 & \text{in } \mathbb{F}, \\ \Sigma_{hq}(N_{.j}, R_j) n_q = 0 & \text{on } \mathbb{U}, \\ \Sigma_{hq}(N_{.j}, R_j) n_q = -\delta_{jh} & \text{on } \mathbb{D}, \\ N_{ij} = 0 & \text{on } \partial\mathbb{M}, \\ N_{ij}, R_j & \text{periodic along } t_i, s_i, \end{cases} \quad (2.10)$$

where δ_{jh} is the Kronecker delta and we adopt the notation $\Sigma_{hq}(A_{.j}, B_j) = -B_j \delta_{hq} + (\partial_h A_{qj} + \partial_q A_{hj})$, that is, fixing j , the dimensionless stress tensor built from B_j acting as pressure and $A_{.j}$ as velocity field.

For the sake of clarity, we describe the physical significance of the entries of the quantities M_{ij} , N_{ij} , Q_j and R_j for the two-dimensional (2-D) configuration depicted in figure 2. We thus forget for a moment about the s components and focus on the n, t ones. For a fixed j , the vector field M_{ij} (N_{ij}) and the scalar field Q_j (R_j) play the role of flow velocity and pressure in a problem governed by Stokes's flow with no-slip boundary conditions on the fluid–solid interface $\partial\mathbb{M}$, periodicity along the tangential direction and an external unitary stress applied along the normal – if $j = n$ – or tangential – if $j = t$ – direction on the upward $\mathbb{U}$ (downward $\mathbb{D}$) side of the domain. Thus, $M_{.n}$ and $M_{.t}$ ($N_{.n}$ and $N_{.t}$) represent the flow field caused by normal and tangential unitary stresses applied on $\mathbb{U}$ ($\mathbb{D}$), respectively. Similarly, Q_n and Q_t (R_n and R_t) represent the pressure fields caused by normal and tangential unitary stress on $\mathbb{U}$ ($\mathbb{D}$), respectively.

However, to represent the effect of the membrane microstructure, we are interested in the average values of these tensor quantities. Indeed, the average value of M_{nn} can be interpreted as a permeability coefficient and the average value of M_{tt} as a slip coefficient, for example (Zampogna & Gallaire 2020).

2.1.5. The macroscopic conditions

Model (2.9) together with the microscopic problems (2.10) represent a closed description for the flow in the vicinity of the membrane. However, (2.9) still contains the dependence on the microscopic spatial variable x_i , since M_{ij} , N_{ij} , Q_j and R_j depend on it. Our objective is to find an interface condition which depends only on the macroscopic spatial variable X_i . To obtain the membrane macroscopic model, we introduce the spatial average

$$\bar{\cdot} = \frac{1}{|\mathbb{C}_F \cup \mathbb{C}_M|} \int_{\mathbb{C}_F} \cdot dS = \frac{1}{|\mathbb{C}_F \cup \mathbb{C}_M|} \int_{\mathbb{F}} \cdot \delta(x_n - x_n^{\mathbb{C}}) dV, \quad (2.11)$$

where $\delta(x_n - x_n^{\mathbb{C}})$ is the Dirac delta centred in $x_n^{\mathbb{C}}$, dS and dV are an infinitesimal element of surface and volume, respectively, and $\cdot$ represents any of the entries in M_{ij} , N_{ij} , Q_j or R_j , solution of (2.10) and $\mathbb{C}_F$ and $\mathbb{C}_M$ represent the fluid and solid portion of the membrane centreline $\mathbb{C}$ (cf. figure 1). Applying average (2.11) to (2.9) and renormalizing with the outer scales, we obtain the purely macroscopic conditions

$$u_i^{\mathbb{O}} = \epsilon \left(\bar{M}_{ij} \Sigma_{jk}^{\mathbb{O}, \mathbb{U}} n_k + \bar{N}_{ij} \Sigma_{jk}^{\mathbb{O}, \mathbb{D}} n_k \right) \quad \text{on } \mathbb{C}, \quad (2.12)$$

$$p^{\mathbb{O}} = \bar{Q}_j \Sigma_{jk}^{\mathbb{O}, \mathbb{U}} n_k + \bar{R}_j \Sigma_{jk}^{\mathbb{O}, \mathbb{D}} n_k \quad \text{on } \mathbb{C}. \quad (2.13)$$

These equivalent interface conditions quantify the effects of the porous membrane on the flow from a purely macroscopic perspective, without the need to solve the fluid flow in the geometric details of the membrane for each specific flow configuration. The effect of the microstructure is indeed entirely embedded in the tensors $\bar{M}_{ij}$, $\bar{N}_{ij}$, known as Navier tensors (Zampogna & Gallaire 2020), while the vectors $\bar{Q}_j$ and $\bar{R}_j$ are only useful to estimate the pressure on the membrane centreline *a posteriori*, if needed. If the membrane microstructure is periodic, we need to solve the microscopic problem (2.10) once and for all to find the averaged quantities, whereas when the microstructure is non-periodic, in principle, we should solve system (2.10) within each REV. This negatively affects the computational efficiency of the method. In the following, we develop a sensitivity-based procedure to perform this operation with a computational cost similar to the periodic case, independently of the number of REV's. We focus on the microscopic problem (2.10) that defines the Navier tensors and on the adjoint problems needed to compute the sensitivity of these tensors to changes in the geometry of the solid inclusion's boundary $\partial\mathbb{M}$.

2.1.6. Further considerations on the Navier tensors

A few considerations are propaedeutic for a better comprehension of the adjoint analysis which we will perform in the next section.

- (i) The macroscopic problem (2.5) and the boundary condition (2.12) determine the outer macroscopic solution $(u_i^{\mathbb{O}}, p^{\mathbb{O}})$, including $p^{\mathbb{O}}$ on each side of the membrane; Q_j and R_j are only needed if one wishes to evaluate *a posteriori* $p^{\mathbb{O}}$ at the membrane centreline with (2.13). Therefore, we will use the adjoint-based sensitivity to estimate the effect of inclusion geometry changes on M_{ij} and N_{ij} only, i.e. we will compute the gradient of the quantities $\bar{M}_{ij}$ and $\bar{N}_{ij}$ for a shape modification of the boundary

$\partial\mathbb{M}$ by introducing a Lagrangian optimisation problem and deriving adjoint problems for these quantities. The method can easily be adapted to estimate the effect on Q_j and R_j , but it is not necessary for the determination of the flow across the membrane.

- (ii) In the particular case of solid inclusions that are symmetric about the membrane centreline $\mathbb{C}$, the Navier tensors satisfy

$$\bar{N}_{ij} = -\bar{M}_{ij}. \quad (2.14)$$

In the specific configuration of solid inclusions that are also symmetric about the normal membrane direction, then $\bar{M}_{nt} = \bar{M}_{tn} = 0$.

- (iii) Equations (2.10) are a set of Stokes problems normally ($j = n$) or tangentially ($j = t$ or s) forced on the upward side $\mathbb{U}$ or downward side $\mathbb{D}$ of the fluid domain $\mathbb{F}$ (for M_{ij} or N_{ij} , respectively). Equation (2.10) is essentially a set of three independent problems for $\bar{M}_{ij}$ and three for $\bar{N}_{ij}$ (i.e. one for each value of the j subscript). To ease the notation, we rewrite (2.10) column by column by introducing the quantities (v_i, q) such that

$$\begin{cases} -\partial_i q + \partial_{kk}^2 v_i = 0 & \text{in } \mathbb{F}, \\ \partial_i v_i = 0 & \text{in } \mathbb{F}, \\ \Sigma_{ij}(v, q)n_j = a_i & \text{on } \mathbb{U}, \\ \Sigma_{ij}(v, q)n_j = -b_i & \text{on } \mathbb{D}, \\ v_i = 0 & \text{on } \partial\mathbb{M}, \\ v_i, q & \text{periodic along } t_i, s_i, \end{cases} \quad (2.15)$$

where

$$a_i = (1, 0, 0), \quad b_i = 0 \text{ for } M_n, Q_n, \quad a_i = 0, \quad b_i = (1, 0, 0) \text{ for } N_n, R_n, \quad (2.16)$$

$$a_i = (0, 1, 0), \quad b_i = 0 \text{ for } M_t, Q_t, \quad a_i = 0, \quad b_i = (0, 1, 0) \text{ for } N_t, Q_t, \quad (2.17)$$

$$a_i = (0, 0, 1), \quad b_i = 0 \text{ for } M_s, Q_s, \quad a_i = 0, \quad b_i = (0, 0, 1) \text{ for } N_s, R_s, \quad (2.18)$$

and $\Sigma_{ij}(v, q) = -q\delta_{ij} + (\partial_i v_j + \partial_j v_i)$. This gives a total of six independent Stokes problems, which correspond to (2.10). Explicit correspondence between (2.10) and (2.15) is given in [appendix B](#). In the following section, we use the compact form (2.15) to formally write the sensitivity to solid inclusions shape variations.

2.2. Sensitivity to shape changes in the microscopic geometry

In this section, we derive the first- and second-order shape sensitivities of the Navier tensors. The shape sensitivity is a quantity derived from the original microscopic flow and used to estimate the effect of geometric modifications without recomputing the flow past any modified geometry. In particular, we aim to estimate the change in the Navier tensors induced by a local geometric modification of the porous microstructure in order to understand how this local modification affects the macroscale flow. We follow the formal method of Céa (1986). The reader interested in shape optimisation is referred to Chapter 4 of Allaire *et al.* (2021).

We first recall a general result about shape derivatives. Consider a real-valued functional,

$$\mathcal{L}(\mathbb{F}) = \int_{\mathbb{F}} f(x) dV + \int_{\partial\mathbb{M}} g(x) dS, \quad (2.19)$$

where f and g are sufficiently smooth functions defined on the domain $\mathbb{F}$ and on part of its boundary $\partial\mathbb{M} \subset \partial\mathbb{F}$, respectively. The shape derivative of $\mathcal{L}(\mathbb{F})$ is

$$\frac{\partial \mathcal{L}}{\partial \mathbb{F}} \beta = \int_{\partial\mathbb{F}} \beta f \, dS + \int_{\partial\mathbb{M}} \beta \left(\frac{\partial g}{\partial n} + Hg \right) dS, \quad (2.20)$$

where $\beta(x)$ is the amplitude of the deformation applied to boundary $\partial\mathbb{M}$ perpendicularly to it at any point, n is the normal to $\partial\mathbb{M}$, and $H = \partial_i n_i$ is the mean curvature of $\partial\mathbb{M}$ (see e.g. § 5.9 in Henrot & Pierre 2005 or § 4.2 in Allaire *et al.* 2021).

2.2.1. First-order sensitivity

We wish to evaluate the effect of a small-amplitude modification of the shape of an inclusion on the spatially averaged Navier tensors $\bar{M}_{ij}$ and $\bar{N}_{ij}$, which appear in the effective macroscopic boundary condition (2.12). With the compact form introduced in § 2.1.6, each row of M_{ij} and N_{ij} is a vector v_i solution of the general problem (2.15), made specific to the row of interest with a suitable choice of a_i and b_i (see also appendix B). Therefore, we focus on $\bar{v}_i$, the spatial average of v_i (as defined in (2.11)), and consider the objective function $J^{(1)}$ defined as

$$J^{(1)}(v_i, \mathbb{F}) = \bar{v}_i r_i = \frac{1}{|\mathbb{C}_{\mathbb{F}} \cup \mathbb{C}_{\mathbb{M}}|} \int_{\mathbb{F}} v_i r_i \delta(x_n - x_n^{\mathbb{C}}) dV. \quad (2.21)$$

Here r_i is a unit vector defined in the (x_n, x_t, x_s) microscopic reference frame and used to select a specific component of $\bar{v}_i$, i.e. a specific component of $\bar{M}_{ij}$ or $\bar{N}_{ij}$ (see again appendix B),

$$r_i = (1, 0, 0) \quad \text{to select } \bar{M}_n \text{ or } \bar{N}_n, \quad (2.22)$$

$$r_i = (0, 1, 0) \quad \text{to select } \bar{M}_t \text{ or } \bar{N}_t, \quad (2.23)$$

$$r_i = (0, 0, 1) \quad \text{to select } \bar{M}_s \text{ or } \bar{N}_s. \quad (2.24)$$

The objective function $J^{(1)}$ depends both (i) on the solution v_i of the microscopic problem and (ii) on the microscopic fluid domain $\mathbb{F}$ itself, where v_i is computed. We are looking for the first-order sensitivity $S^{(1)}(x)$ of $\bar{v}_i$ with respect to the geometry, such that the first-order variation in $\bar{v}_i r_i$ induced by any small-amplitude normal deformation $\beta(x)$ of the inclusion geometry $\partial\mathbb{M}$ is

$$\delta \bar{v}_i r_i = \int_{\partial\mathbb{M}} \beta S^{(1)} dS. \quad (2.25)$$

Computing this sensitivity under the constraint that v_i is a solution of (2.15) is a constrained problem, which is notoriously difficult as is. However, it can be conveniently recast into an easier unconstrained problem via a standard Lagrangian approach. We introduce the Lagrangian

$$\mathcal{L}^{(1)}(v_i, q, v_i^\dagger, q^\dagger, \lambda_i^\dagger, \mathbb{F}) = J^{(1)} + \int_{\mathbb{F}} \left[v_i^\dagger (-\partial_i q + \partial_{kk}^2 v_i) + q^\dagger \partial_i v_i \right] dV + \int_{\partial\mathbb{M}} \lambda_i^\dagger v_i dS, \quad (2.26)$$

where $(v_i^\dagger, q^\dagger)$ and $\lambda_i^\dagger$ are yet unknown Lagrange multipliers, whose aim is to enforce the constraints acting on (v_i, q) : governing equations in $\mathbb{F}$, and no-slip condition $v_i = 0$ on $\partial\mathbb{M}$, respectively. All the variables in $\mathcal{L}^{(1)}$ are assumed independent. The derivative of $J^{(1)}$ with respect to $\mathbb{F}$ is obtained via the first-order derivatives of the Lagrangian, as follows.

- (i) By construction, equating to zero the partial derivative of the Lagrangian with respect to the Lagrange multipliers,

$$\frac{\partial \mathcal{L}^{(1)}}{\partial (v_i^\dagger, q^\dagger)} = \frac{\partial \mathcal{L}^{(1)}}{\partial \lambda_i^\dagger} = 0, \quad (2.27)$$

yields the direct equations (2.15) for (v_i, q) and the no-slip condition $v_i = 0$ on $\partial\mathbb{M}$.

- (ii) The partial derivative of the Lagrangian with respect to (v_i, q) in the direction $(\delta v_i, \delta q)$ reads after integration by parts as

$$\begin{aligned} \frac{\partial \mathcal{L}^{(1)}}{\partial (v_i, q)} \delta(v_i, q) &= \frac{1}{|\mathbb{C}_{\mathbb{F}} \cup \mathbb{C}_{\mathbb{M}}|} \int_{\mathbb{F}} \delta v_i r_i \delta(x_n - x_n^{\mathbb{C}}) dV + \int_{\mathbb{F}} \left[\delta v_j \partial_i \Sigma_{ij}^\dagger + \delta q \partial_i v_i^\dagger \right] dV \\ &\quad + \int_{\partial\mathbb{F}} \left[-\delta v_i \Sigma_{ij}^\dagger n_j + v_i^\dagger \delta \Sigma_{ij} n_j \right] dS + \int_{\partial\mathbb{M}} \lambda_i^\dagger \delta v_i dS, \end{aligned} \quad (2.28)$$

where $\Sigma_{ij}^\dagger = -q^\dagger \delta_{ij} + (\partial_i v_j^\dagger + \partial_j v_i^\dagger)$ is the adjoint stress tensor. The two domain integrals over $\mathbb{F}$ are zero for any $(\delta v_i, \delta q)$ if the following adjoint equations for $(v_i^\dagger, q_i^\dagger)$ are satisfied:

$$\begin{cases} -\partial_i q^\dagger + \partial_{kk}^2 v_i^\dagger = -\delta(x_n - x_n^{\mathbb{C}}) r_i, \\ \partial_i v_i^\dagger = 0. \end{cases} \quad (2.29)$$

Next, we equate to zero the two boundary integrals over $\partial\mathbb{F}$ and $\partial\mathbb{M} \subset \partial\mathbb{F}$ for each boundary separately. On the lateral sides, periodicity applies in the direct problem and thus in the adjoint problem too; indeed, δv_i takes the same values on the two sides, as $\delta \Sigma_{ij}$ does, whereas $\mathbf{n}$ has opposite signs, therefore we ask that $v_i^\dagger$ and $\Sigma_{ij}^\dagger$ be periodic. On $\mathbb{U}$ and $\mathbb{D}$, the direct stresses Σ_{ij} satisfy Dirichlet conditions, therefore $\delta \Sigma_{ij} = 0$, so we choose $\Sigma_{ij}^\dagger n_j = 0$. On $\partial\mathbb{M}$, we choose $v_i^\dagger = 0$ and therefore obtain $\lambda_i^\dagger = \Sigma_{ij}^\dagger n_j$. To summarise, the adjoint problem for the adjoint variables $(v_i^\dagger, q_i^\dagger)$ is

$$\begin{cases} -\partial_i q^\dagger + \partial_{kk}^2 v_i^\dagger = -\delta(x_n - x_n^{\mathbb{C}}) r_i & \text{in } \mathbb{F}, \\ \partial_i v_i^\dagger = 0 & \text{in } \mathbb{F}, \\ \Sigma_{pq}^\dagger(v_i^\dagger, q^\dagger) n_q = 0 & \text{on } \mathbb{U}, \mathbb{D}, \\ v_i^\dagger = 0 & \text{on } \partial\mathbb{M}, \\ \lambda_i^\dagger = \Sigma_{ij}^\dagger n_j & \text{on } \partial\mathbb{M}, \\ v_i^\dagger, q^\dagger & \text{periodic along } t_i, s_i. \end{cases} \quad (2.30)$$

Note that the relation $\lambda_i^\dagger = \Sigma_{ij}^\dagger n_j$ on $\partial\mathbb{M}$ is not a boundary condition on $(v_i^\dagger, q_i^\dagger)$ but a defining expression for $\lambda_i^\dagger$. Interestingly, this adjoint problem depends on r_i but neither on v_i nor on a_i and b_i , which implies that it needs to be solved only once for each row of M and N , independently of the selected column

- (iii) Finally, we compute the partial derivative of the Lagrangian with respect to a geometry modification in the direction normal to the solid–fluid boundary $\partial\mathbb{M}$. Noting that $\mathcal{L}^{(1)}$ has the same form as in (2.19), with

$$f = \frac{v_i r_i \delta(x_n - x_n^{\mathbb{C}})}{|\mathbb{C}_{\mathbb{F}} \cup \mathbb{C}_{\mathbb{M}}|} + v_i^\dagger (-\partial_i q + \partial_{kk}^2 v_i) + q^\dagger \partial_i v_i, \quad (2.31)$$

$$g = \lambda_i^\dagger v_i, \quad (2.32)$$

we obtain from (2.20)

$$\begin{aligned} \frac{\partial \mathcal{L}^{(1)}}{\partial \mathbb{F}} \beta &= \int_{\partial \mathbb{F}} \beta f \, dS + \int_{\partial \mathbb{M}} \beta \left(\frac{\partial g}{\partial n} + H g \right) \, dS \\ &= \int_{\partial \mathbb{F}} \beta \left[\frac{v_i r_i \delta(x_n - x_n^{\mathbb{C}})}{|\mathbb{C}_{\mathbb{F}} \cup \mathbb{C}_{\mathbb{M}}|} + v_i^{\dagger} (-\partial_i q + \partial_{kk}^2 v_i) + q^{\dagger} \partial_i v_i \right] \, dS \\ &\quad + \int_{\partial \mathbb{M}} \beta \left(\frac{\partial}{\partial n} + H \right) (\lambda_i^{\dagger} v_i) \, dS. \end{aligned} \quad (2.33)$$

If, specifically, the direct field (v_i, q) is a solution of the direct equations (2.15), and the adjoint field $(v_i^{\dagger}, q^{\dagger})$ and Lagrange multiplier $\lambda_i^{\dagger}$ satisfy the adjoint equations (2.30), we obtain the derivative of the objective function with respect to the geometry $\mathbb{F}$ in the direction β ,

$$\begin{aligned} \frac{\partial J^{(1)}}{\partial \mathbb{F}} \beta &= \int_{\partial \mathbb{M}} \beta \left(\lambda_i^{\dagger} \frac{\partial v_i}{\partial n} + \frac{\partial \lambda_i^{\dagger}}{\partial n} v_i + H \lambda_i^{\dagger} v_i \right) \, dS \\ &= \int_{\partial \mathbb{M}} \beta \lambda_i^{\dagger} \frac{\partial v_i}{\partial n} \, dS \\ &= \int_{\partial \mathbb{M}} \beta \left(-q^{\dagger} n_i + \frac{\partial v_i^{\dagger}}{\partial n} \right) \frac{\partial v_i}{\partial n} \, dS \\ &= \int_{\partial \mathbb{M}} \beta \frac{\partial v_i^{\dagger}}{\partial n} \frac{\partial v_i}{\partial n} \, dS. \end{aligned} \quad (2.34)$$

Here the second equality results from the no-slip condition on v_i , and the last equality from the velocity gradient at the wall being purely tangential and thus orthogonal to $-q^{\dagger} n_i$. Therefore, one can identify from (2.25) the first-order shape sensitivity of $\bar{v}_i r_i$ to a deformation of the solid inclusion,

$$S^{(1)}(x) = \frac{\partial v_i^{\dagger}}{\partial n} \frac{\partial v_i}{\partial n}, \quad (2.35)$$

which can be evaluated on $\partial \mathbb{M}$ once v_i and $v_i^{\dagger}$ have been computed by solving the direct and adjoint problems. Here $S^{(1)}$ allows us to estimate the first-order macroscopic effect of a microscopic change of the geometry. Indeed, on the left-hand side of (2.25), we find the variation $\delta \bar{v}_i$ of the average value of v_i , i.e. the variation of the Navier tensors caused by a geometric deformation of magnitude β .

2.2.2. Second-order sensitivity

We now look for the second-order sensitivity $S^{(2)}(x)$ of $\bar{v}_i r_i$ with respect to the geometry, such that, up to second order, the variation in $\bar{v}_i r_i$ induced by any small-amplitude normal deformation $\beta(x)$ of the inclusion geometry $\partial \mathbb{M}$ is

$$\delta \bar{v}_i r_i = \int_{\partial \mathbb{M}} \left[\beta S^{(1)} + \frac{1}{2} \beta^2 S^{(2)} \right] \, dS. \quad (2.36)$$

To compute this second-order sensitivity of $\bar{v}_i r_i$, we consider the new objective function

$$J^{(2)}(v_i, v_i^{\dagger}, \mathbb{F}) = \int_{\partial \mathbb{M}} S^{(1)} \, dS = \int_{\partial \mathbb{M}} \frac{\partial v_i^{\dagger}}{\partial n} \frac{\partial v_i}{\partial n} \, dS, \quad (2.37)$$

and apply the same method as in § 2.2.1, which is justified for purely normal deformations (Henrot & Pierre 2005). The integral is limited to $\partial\mathbb{M}$, the only deformed boundary. The Lagrangian for this objective function subject to the constraints (2.15) and (2.30) is

$$\begin{aligned} \mathcal{L}^{(2)}(v_i, q, v_i^\dagger, q^\dagger, \tilde{v}_i, \tilde{q}, \tilde{\lambda}_i, \tilde{v}_i^\dagger, \tilde{q}^\dagger, \tilde{\lambda}_i^\dagger, \mathbb{F}) = J^{(2)} \\ + \int_{\mathbb{F}} \left[\tilde{v}_i (-\partial_i q + \partial_{kk}^2 v_i) + \tilde{q} \partial_i v_i \right] dV + \int_{\partial\mathbb{M}} \tilde{\lambda}_i v_i dS \\ + \int_{\mathbb{F}} \left[\tilde{v}_i^\dagger (-\partial_i q^\dagger + \partial_{kk}^2 v_i^\dagger) + \tilde{q}^\dagger \partial_i v_i^\dagger \right] dV + \int_{\partial\mathbb{M}} \tilde{\lambda}_i^\dagger v_i^\dagger dS, \end{aligned} \quad (2.38)$$

where $(\hat{v}_i, \hat{q})$, $\hat{\lambda}_i$, $(\hat{v}_i^\dagger, \hat{q}^\dagger)$ and $\hat{\lambda}_i^\dagger$ are yet unknown Lagrange multipliers whose aim is to enforce the constraints acting on (v_i, q) and $(v_i^\dagger, q^\dagger)$.

- (i) By construction, equating to zero the partial derivatives of the Lagrangian with respect to the Lagrange multipliers $(\tilde{v}_i, \tilde{q})$ and $\hat{\lambda}_i$ yields the direct problem (2.15) for (v_i, q) .
- (ii) By construction, equating to zero the partial derivatives of the Lagrangian with respect to the Lagrange multipliers $(\tilde{v}_i^\dagger, \tilde{q}^\dagger)$ and $\hat{\lambda}_i^\dagger$ yields the first-order adjoint problem (2.30) for $(v_i^\dagger, q^\dagger)$.
- (iii) The partial derivative of the Lagrangian with respect to (v_i, q) in the direction $(\delta v_i, \delta q)$ reads after integration by parts as

$$\begin{aligned} \frac{\partial \mathcal{L}^{(2)}}{\partial (v_i, q)} \delta(v_i, q) = \int_{\partial\mathbb{M}} \frac{\partial v_i^\dagger}{\partial n} \frac{\partial \delta v_i}{\partial n} dS + \int_{\mathbb{F}} \left[\delta v_j \partial_i \tilde{\Sigma}_{ij} + \delta q \partial_i \tilde{v}_i \right] dV \\ + \int_{\partial\mathbb{F}} \left[-\delta v_i \tilde{\Sigma}_{ij} n_j + \tilde{v}_i \delta \Sigma_{ij} n_j \right] dS + \int_{\partial\mathbb{M}} \tilde{\lambda}_i \delta v_i dS, \end{aligned} \quad (2.39)$$

with $\hat{\Sigma}_{ij} = -\hat{q} \delta_{ij} + (\partial_i \hat{v}_j + \partial_j \hat{v}_i)$. Equating to zero the domain and boundary integrals yields adjoint equations and boundary conditions for $(\tilde{v}_i, \tilde{q})$, respectively. Periodicity holds on the lateral sides in the direct problem (2.15), and thus for $(\tilde{v}_i, \tilde{q})$, too. On $\mathbb{U}$ and $\mathbb{D}$, the direct stresses Σ_{ij} satisfy Dirichlet conditions, therefore $\delta \Sigma_{ij} = 0$, so we choose $\tilde{\Sigma}_{ij} n_j = 0$. On $\partial\mathbb{M}$, we choose $\tilde{v}_i = -\partial v_i^\dagger / \partial n$ (which also implies $\tilde{v}_i n_i = 0$ because a velocity gradient at a wall is purely tangential) and we deduce $\tilde{\lambda}_i$. The adjoint problem for $(\tilde{v}_i, \tilde{q})$ is summarised as follows:

$$\begin{cases} -\partial_i \tilde{q} + \partial_{kk}^2 \tilde{v}_i = 0 & \text{in } \mathbb{F}, \\ \partial_i \tilde{v}_i = 0 & \text{in } \mathbb{F}, \\ \tilde{\Sigma}_{pq}(\tilde{v}, \tilde{q}) n_q = 0 & \text{on } \mathbb{U}, \mathbb{D}, \\ \tilde{v}_i = -\frac{\partial v_i^\dagger}{\partial n} & \text{on } \partial\mathbb{M}, \\ \tilde{\lambda}_i = -\tilde{q} n_i + \frac{\partial \tilde{v}_i}{\partial n} & \text{on } \partial\mathbb{M} \\ \tilde{v}_i, \tilde{q} & \text{periodic along } t_i, s_i. \end{cases} \quad (2.40)$$

- (iv) Similarly, the partial derivative of the Lagrangian with respect to $(v_i^\dagger, q^\dagger)$ in the direction $(\delta v_i^\dagger, \delta q^\dagger)$ reads after integration by parts as

$$\begin{aligned} \frac{\partial \mathcal{L}^{(2)}}{\partial(v_i^\dagger, q^\dagger)} \delta(v_i^\dagger, p^\dagger) &= \int_{\partial \mathbb{M}} \frac{\partial \delta v_i^\dagger}{\partial n} \frac{\partial v_i}{\partial n} dS + \int_{\mathbb{F}} \left[\delta v_j^\dagger \partial_i \tilde{\Sigma}_{ij}^\dagger + \delta q^\dagger \partial_i \tilde{v}_i^\dagger \right] dV \\ &+ \int_{\partial \mathbb{F}} \left[-\delta v_i^\dagger \tilde{\Sigma}_{ij}^\dagger n_j + \tilde{v}_i^\dagger \delta \Sigma_{ij}^\dagger n_j \right] dS + \int_{\partial \mathbb{M}} \tilde{\lambda}_i^\dagger \delta v_i^\dagger dS, \end{aligned} \quad (2.41)$$

with $\hat{\Sigma}_{ij}^\dagger = -\hat{q}^\dagger \delta_{ij} + (\partial_i \hat{v}_j^\dagger + \partial_j \hat{v}_i^\dagger)$. Equating to zero the domain and boundary integrals yields adjoint equations and boundary conditions for $(\tilde{v}_i^\dagger, \tilde{q}^\dagger)$, respectively. Periodicity holds on the lateral sides in the adjoint problem (2.30), and thus for $(\tilde{v}_i^\dagger, \tilde{q}^\dagger)$, too. On $\mathbb{U}$ and $\mathbb{D}$, the adjoint stresses $\Sigma_{ij}^\dagger$ satisfy Dirichlet conditions, therefore $\delta \Sigma_{ij}^\dagger = 0$, so we choose $\tilde{\Sigma}_{ij}^\dagger n_j = 0$. On $\partial \mathbb{M}$, we choose $\tilde{v}_i^\dagger = -\partial v_i / \partial n$ (which also implies $\tilde{v}_i^\dagger n_i = 0$ because a velocity gradient at a wall is purely tangential) and we deduce $\tilde{\lambda}_i^\dagger$. The adjoint problem for $(\tilde{v}_i^\dagger, \tilde{q}^\dagger)$ is summarised as follows:

$$\begin{cases} -\partial_i \tilde{q}^\dagger + \partial_{kk}^2 \tilde{v}_i^\dagger = 0 & \text{in } \mathbb{F}, \\ \partial_i \tilde{v}_i^\dagger = 0 & \text{in } \mathbb{F}, \\ \tilde{\Sigma}_{pq}^\dagger(\tilde{v}^\dagger, \tilde{q}^\dagger) n_q = 0 & \text{on } \mathbb{U}, \mathbb{D}, \\ \tilde{v}_i^\dagger = -\frac{\partial v_i}{\partial n} & \text{on } \partial \mathbb{M}, \\ \tilde{\lambda}_i^\dagger = -\tilde{q}^\dagger n_i + \frac{\partial \tilde{v}_i^\dagger}{\partial n} & \text{on } \partial \mathbb{M}, \\ \tilde{v}_i^\dagger, \tilde{q}^\dagger & \text{periodic along } t_i, s_i. \end{cases} \quad (2.42)$$

Although very similar, the two second-order adjoint problems (2.40) and (2.42) differ by the Dirichlet boundary condition on $\partial \mathbb{M}$, where $\tilde{v}_i$ and $\tilde{v}_i^\dagger$ are related to the normal gradient of the first-order adjoint variable $v_i^\dagger$ and the direct solution v_i , respectively. As a consequence, (2.42) depends on v_i but not on r_i and $\hat{v}_i$, so, like the direct problem (2.15), it needs to be solved only once for each column of M_{ij} and N_{ij} , independently of the selected row; by contrast, (2.40) depends on $v_i^\dagger$ but not on v_i , a_i and b_i , so, like the first-order adjoint problem (2.30), it needs to be solved only once for each row of M_{ij} and N_{ij} , independently of the selected column.

- (v) Finally, we compute the partial derivative of the Lagrangian with respect to the geometry $\mathbb{F}$ in the direction β . Noting that $\mathcal{L}^{(2)}$ has the same form as in (2.19), with

$$\begin{aligned} f &= \tilde{v}_i (-\partial_i q + \partial_{kk}^2 v_i) + \tilde{q} \partial_i v_i + \tilde{v}_i^\dagger (-\partial_i q^\dagger + \partial_{kk}^2 v_i^\dagger) + \tilde{q}^\dagger \partial_i v_i^\dagger, \\ g &= \frac{\partial v_i^\dagger}{\partial n} \frac{\partial v_i}{\partial n} + \tilde{\lambda}_i v_i + \tilde{\lambda}_i^\dagger v_i^\dagger, \end{aligned} \quad (2.43)$$

we obtain from (2.20) the following:

$$\begin{aligned} \frac{\partial \mathcal{L}^{(2)}}{\partial \mathbb{F}} \beta &= \int_{\partial \mathbb{F}} \beta f dS + \int_{\partial \mathbb{M}} \beta \left(\frac{\partial g}{\partial n} + H g \right) dS \\ &= \int_{\partial \mathbb{F}} \beta \left[\tilde{v}_i (-\partial_i q + \partial_{kk}^2 v_i) + \tilde{q} \partial_i v_i + \tilde{v}_i^\dagger (-\partial_i q^\dagger + \partial_{kk}^2 v_i^\dagger) + \tilde{q}^\dagger \partial_i v_i^\dagger \right] dS \\ &+ \int_{\partial \mathbb{M}} \beta \left(\frac{\partial}{\partial n} + H \right) \left(\frac{\partial v_i^\dagger}{\partial n} \frac{\partial v_i}{\partial n} + \tilde{\lambda}_i v_i + \tilde{\lambda}_i^\dagger v_i^\dagger \right) dS. \end{aligned} \quad (2.44)$$

If, specifically, the direct field (v_i, q) is a solution of the direct problem (2.15), the first-order adjoint field $(v_i^\dagger, q^\dagger)$ and Lagrange multiplier $\lambda_i^\dagger$ satisfy the first-order adjoint problem (2.30), and their second-order counterparts $(\tilde{v}_i, \tilde{q}, \tilde{\lambda}_i)$ and $(\tilde{v}_i^\dagger, \tilde{q}^\dagger, \tilde{\lambda}_i^\dagger)$ satisfy the second-order adjoint problems (2.40) and (2.42), respectively, we obtain the derivative of the objective function with respect to the geometry $\mathbb{F}$ in the direction β ,

$$\begin{aligned} \frac{\partial J^{(2)}}{\partial \mathbb{F}} \beta &= \int_{\partial \mathbb{M}} \beta \left(\frac{\partial}{\partial n} + H \right) \left(\frac{\partial v_i^\dagger}{\partial n} \frac{\partial v_i}{\partial n} + \frac{\partial \tilde{v}_i}{\partial n} v_i + \frac{\partial \tilde{v}_i^\dagger}{\partial n} v_i^\dagger \right) dS \\ &= \int_{\partial \mathbb{M}} \beta \left[\left(\frac{\partial}{\partial n} + H \right) \left(\frac{\partial v_i^\dagger}{\partial n} \frac{\partial v_i}{\partial n} \right) + \frac{\partial \tilde{v}_i}{\partial n} \frac{\partial v_i}{\partial n} + \frac{\partial \tilde{v}_i^\dagger}{\partial n} \frac{\partial v_i^\dagger}{\partial n} \right] dS. \end{aligned} \quad (2.45)$$

Therefore, one can identify from (2.36) the second-order shape sensitivity of $\tilde{v}_i$ to a modification of the solid inclusion shape,

$$S^{(2)}(x) = \left(\frac{\partial}{\partial n} + H \right) \left(\frac{\partial v_i^\dagger}{\partial n} \frac{\partial v_i}{\partial n} \right) + \frac{\partial \tilde{v}_i}{\partial n} \frac{\partial v_i}{\partial n} + \frac{\partial \tilde{v}_i^\dagger}{\partial n} \frac{\partial v_i^\dagger}{\partial n}, \quad (2.46)$$

which can be evaluated on $\partial \mathbb{M}$ once v_i , $v_i^\dagger$, $\tilde{v}_i$ and $\tilde{v}_i^\dagger$ have been computed by solving the direct and first- and second-order adjoint problems.

3. Microscopic problems: comparison between direct and adjoint approaches

In this section, we compare the average values of the tensors M_{ij} obtained by solving the direct microscopic problem (2.15) and evaluating (2.11) on the actual geometry with the prediction obtained by solving the adjoint microscopic problems (2.30), (2.40) and (2.42) on a reference geometry and evaluating (2.36). To simplify the analysis, we consider geometries for which relation (2.14) holds, i.e. $\tilde{N}_{ij} = -\tilde{M}_{ij}$. Details about the numerical solution are given in appendix C. As a test case, we use a REV containing two circular solid inclusions of different radii R_A and R_B , depicted in figure 3(a).

This means that the considered membrane exhibits a periodicity for every two inclusions. We consider two families of small amplitude geometry modifications: a change in the radius of a solid inclusion (without displacing its centre, cf. figure 3b) and a displacement of the centre of one inclusion (without changing its shape, cf. figure 3c). In the following, we leave the compact notation introduced in (2.15) to analyse the direct and adjoint fields component by component. According to the notation introduced in (2.10) and the relations thoroughly explained in appendix B, $M_{ij}^\dagger$, $\tilde{M}_{ij}$ and $\tilde{M}_{ij}^\dagger$ denote the first, second, and third adjoint variables whose associated problems are (2.30), (2.40) and (2.42), respectively.

Figure 4 shows the contours and streamlines (red) of M_{ij} (a, e), $M_{ij}^\dagger$ (b, f), $\tilde{M}_{ij}$ (c, g) and $\tilde{M}_{ij}^\dagger$ (d, h) in the 2-D domain described in figure 3(a) with $R_A = 0.12$, $R_B = 0.15$, $x_t^A = 0.2$ and $x_t^B = -0.2$. Figure 4(a, e) are obtained by computing (2.15), i.e. the direct problem. Figure 4(b, f) are solutions of (2.30) for $r_i = (1, 0)$ and $(0, 1)$, respectively. These two fields do not depend on the direct solution, but only on r_i . They can be computed once and for all for $\tilde{M}_{ij}$ and the solution for the $\tilde{N}_{ij}$ fields is the same. Figure 4(c, g) are obtained by computing (2.40), which depend only on the solution of (2.30) by means of the inhomogeneous boundary condition on $\partial \mathbb{M}$. Figure 4(d, h) are obtained by computing (2.42), which depend only on the direct solution through the inhomogeneous boundary

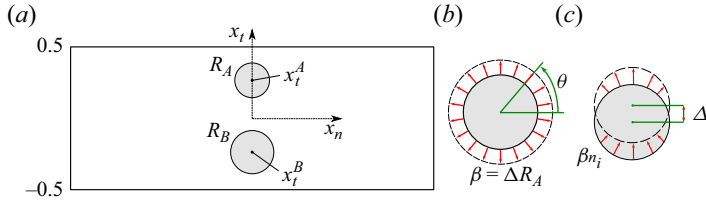


Figure 3. (a) Sketch of a REV containing two circular inclusions with centres in $(x_n^A, x_t^A) = (0, 0.2)$, $(x_n^B, x_t^B) = (0, -0.2)$ and radii $R_A = 0.12$ and $R_B = 0.15$. We consider two cases for the deformation of the boundary of the inclusions $\partial\mathbb{M}$: (b) a purely normal deformation, consisting of a modification of the radius of the upper circular solid inclusion of a quantity $\beta = \Delta R_A$ and (c) an alteration Δ of the position $(x_n^A, 0)$ of its centre. In both cases, the red arrows showing the deformation are directed along the normal to the original boundary (black solid line) and their length is proportional to β . The black dashes in (b) and (c) represent the deformed boundary. $\theta \in [0, 2\pi]$ in panel (b) is an angular coordinate that spans the inclusion's surface from the positive x_n , anticlockwise. This coordinate is used to plot the sensitivities $S^{(1)}$, $S^{(2)}$ and the magnitude of the normal deformation β along $\partial\mathbb{M}$.

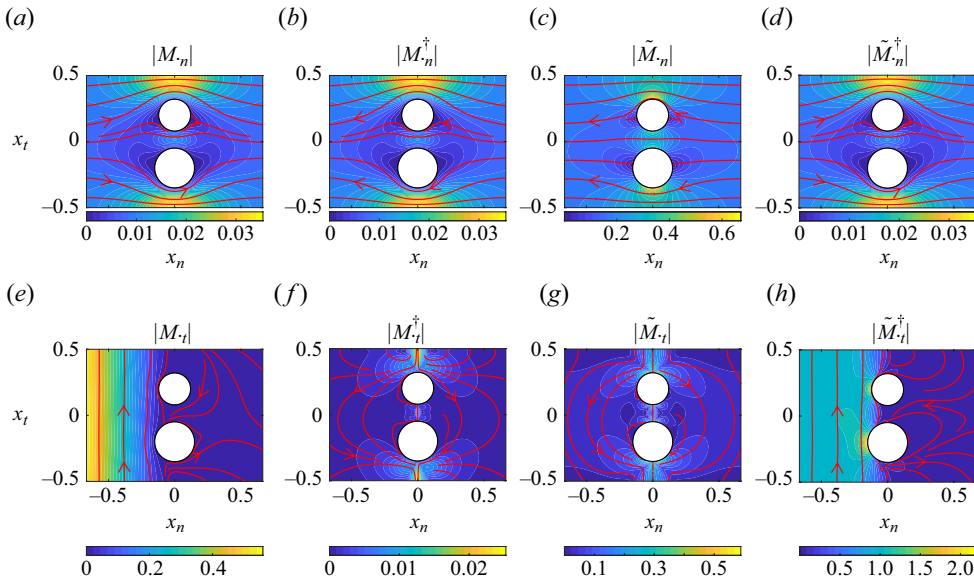


Figure 4. Solution of the (a, e) direct microscopic problems and (b–d, f–h) adjoint microscopic problems in the geometric configuration shown in figure 3 with $R_A = 0.12$, $R_B = 0.15$, $x_t^A = 0.2$ and $x_t^B = -0.2$. Contour of magnitude $\sqrt{M_{nn}^2 + M_{tt}^2}$ and streamlines (red) for the fields (a) (M_{nn}, M_{tn}) , (b) $(M_{nn}^\dagger, M_{tn}^\dagger)$, (c) $(\tilde{M}_{nn}, \tilde{M}_{tn})$, (d) $(\tilde{M}_{nn}^\dagger, \tilde{M}_{tn}^\dagger)$, (e) (M_{nt}, M_{tt}) , (f) $(M_{nt}^\dagger, M_{tt}^\dagger)$, (g) $(\tilde{M}_{nt}, \tilde{M}_{tt})$, (h) $(\tilde{M}_{nt}^\dagger, \tilde{M}_{tt}^\dagger)$ are shown.

condition on $\partial\mathbb{M}$. We now use these quantities to predict variations in the Navier tensors induced by small amplitude shape modifications.

3.1. Radial shape perturbations of a circular solid inclusion

We let the radius R_A of inclusion A vary while keeping the radius of inclusion B constant. Figure 5(a–f) shows the first and second-order sensitivities of the different tensor components evaluated on three different reference geometries with $R_A = 0.054$ (red), 0.120 (green) or 0.186 (blue). In this section, we modify the radius R_A only, which means that the normal deformation β of the solid boundary $\partial\mathbb{M}$ is constant with θ .

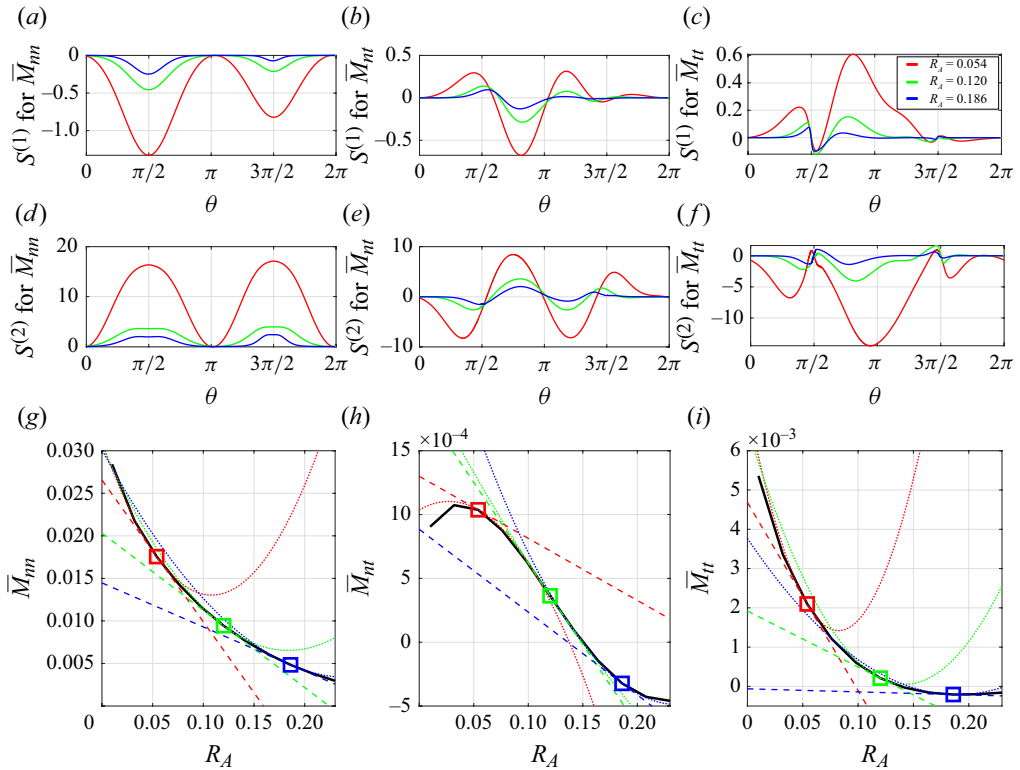


Figure 5. Effect of a modification of the radius of inclusion A on the Navier tensors representing the membrane microstructure macroscopically. Panels (a,d,g), (b,e,h) and (c,f,i) refer to a single Navier tensor component. The sensitivities for each Navier tensor are shown in (a,d), (b,e) and (c,f). Each colour except black refers to one reference geometry used to compute these sensitivities. Reference geometry: $x_i^A = 0.2$, $x_i^B = -0.2$, $R_A = [0.054, 0.120, 0.186]$ (corresponding to red, green and blue) and $R_B = 0.15$ (cf. figure 3a). (a–c) First-order and (d–f) second-order sensitivities of $\bar{M}_{nn}$, $\bar{M}_{nt}$ and $\bar{M}_{tt}$ on the boundary of inclusion A. (g–i) Here $\bar{M}_{nn}$, $\bar{M}_{nt}$ and $\bar{M}_{tt}$ recomputed with the modified geometry (black solid line) and predicted from first-order (dashes) and second-order (dots) shape sensitivities. Coloured squares represent evaluation points of the sensitivities. Since M_{in} is antisymmetric with respect to the x_n axis, its average $\bar{M}_{in}$ is zero and $N_{ij} = -\bar{M}_{ij}$.

We notice in figure 5(a,d) that the maxima (in absolute value) of $\bar{M}_{nn}$ shape sensitivity are attained in $\theta = \pi/2$ and $\theta = 3\pi/2$ or in a neighbourhood of these values. We saw in § 2.1.4 that $\bar{M}_{nn}$ has the physical meaning of a permeability coefficient. Now we can conclude that the membrane permeability is more sensitive to geometry changes in the pore between inclusions A and B (i.e. for example between the bottom part of inclusion A and the top part of inclusion B in figure 3a) than on the upward or downward sides of the inclusion (i.e. their rightmost and leftmost portions in figure 3a). This is visually confirmed (note the adjacency of yellow and blue zone) in figure 4(a–d), where the direct and adjoint fields all show steeper wall-normal gradients (which are quantities determining the sensitivities) in $\theta = \pi/2$ and $3\pi/2$ than in $\theta = 0$ and π , for example. The opposite stands for $\bar{M}_{tt}$ (figure 5c, f), whose shape sensitivity has a maximum in $\theta = \pi$, corresponding to the side of the solid inclusion facing the tangential boundary stress. On the other side ($\theta = 0$), the sensitivity is close to zero, as wall-normal derivatives of the direct and adjoint fields are negligible (figure 4e–h). We conclude that the slip coefficient is more sensitive to shape modifications of the upward or downward sides of the membrane than to its pore shapes. A mixed situation is found in the case of normally directed flow caused by tangential stress

($\bar{M}_{nt}$, cf. figure 5*b,e*) since the most relevant values of the shape sensitivities are found for θ near odd multiples of $\pi/4$. The sensitivity maps in this case suggest that, if a larger $\bar{M}_{nt}$ is desired, one should ‘pull-and-push’ the solid boundary at alternating odd multiples of $\pi/4$, creating a solid geometry that is asymmetric about the x_n axis. In figure 5(*g-i*), we compare the curves representing the direct computations of the $\bar{M}_{ij}$ components (black solid lines) with the predictions based on $S^{(1)}$ only (red, green and blue dashes) and with the predictions based on both $S^{(1)}$ and $S^{(2)}$ (red, green and blue dots). The reference geometries used for predicting each coloured curve correspond to the squares of the same colour. The dashed lines representing the first-order predictions are tangent to the black solid line at the reference points (i.e. the squares), while the dotted parabolas have the same concavity as the solid black lines at the reference points.

The adjoint-based predictions and the direct evaluations of $\bar{M}_{ij}$ agree beyond the theoretical limit of infinitesimal deformations. In the presented cases, the worst second-order prediction corresponds to $\bar{M}_{tt}$ for the reference radius $R_A = 0.054$ (red dots in figure 5*i*). For example, this prediction has a 17.5 % error when R_A increases by ~ 50 % to 0.075. If R_A is further increased, the error increases. The variation of $\bar{M}_{tt}$ between the case with $R_A = 0.054$ and $R_A = 0.075$ is approximately -32 %. The best case corresponds to $\bar{M}_{nn}$ for a reference radius of $R_A = 0.186$ (blue dots in figure 5*g*), where the second-order prediction is in good agreement with the direct solutions in a range of deformations between -95 % and $+24$ %, with a maximum error of ~ 11 % at $R_A = 0.054$ (a -71 % deformation, corresponding to a ~ 263 % variation in $\bar{M}_{nn}$ with respect to the reference case). In the considered cases, there always exists a range of R_A in which second-order predictions are more accurate than first-order ones.

3.2. Displacement of the centre of a circular solid inclusion

In this section, we consider a more general deformation of the solid boundaries, obtained by shifting by a quantity Δ (cf. figure 3*c*) the position of the centre of a circular solid inclusion x_t^A with respect to another, centred at x_t^B (cf. figure 3). The geometry parameters for this configuration are $R_A = 0.125$, $R_B = 0.075$ and $x_t^B = -0.2$. Figure 6(*a-c*) shows some distributions of sensitivity for the reference geometry with $x_t^A = 0.218$ (green squares in figure 6*e-g*). A shift of the inclusion of a quantity Δ causes a distribution of the normal deformation β as shown in figure 6(*d*). The local maxima (in absolute value) of β are located in $\theta = \pi/2, 3\pi/2$, except for $\Delta = R_A$, where we observe a plateau in the range $\theta \in [\pi, 2\pi]$. Indeed, when $\Delta = R_A$ (lighter grey line corresponding to $\Delta = R_A = 0.125$), the image of half of the original inclusion reduces to a single point of the displaced inclusion. It is thus mathematically inconsistent to consider the case $\Delta > R_A$ since some points of the original inclusion have no image on the displaced inclusion through a normal deformation. Note also that the function β in figure 6(*d*) passes by zero twice in its domain $\theta \in (0, 2\pi)$. However, any displacement $\Delta \neq 0$ of the centre causes all points on the circle to move of Δ . The existence of zeros in β is a consequence of its definition as normal displacement. This means that there exist points which change position, but this movement has zero component along the normal to the reference geometry, thus $\beta = 0$ in those points. In figure 6(*e-g*), we compare the actual (black line) and predicted value of $\bar{M}_{ij}$ with first-order (dashes) and second-order (dots) sensitivities computed using three base points (squares). Since β is not constant along $\partial\mathbb{M}$, the first-order predictions are not lines and the second-order ones are not parabolas. The notion of slope and concavity used to assess the performance of the prediction in figure 5 cannot be used in this case and we can visually rely only on how close the predictions and the actual values are.

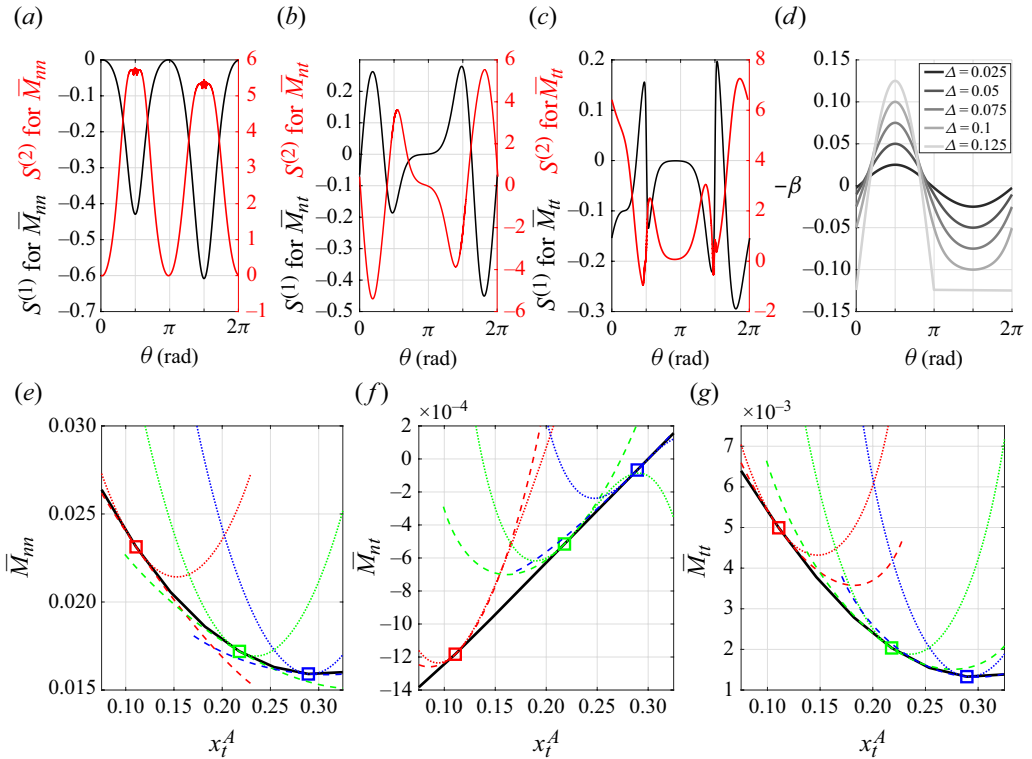


Figure 6. Effect of a displacement Δ of inclusion A along x_I in terms in the Navier tensors representing the membrane microstructure macroscopically. First-order (black) and second-order (red) sensitivities of (a) $\bar{M}_{nm}$, (b) $\bar{M}_{nt}$ and (c) $\bar{M}_{tt}$ on the boundary of inclusion A in the reference configuration $x_I^A = 0.218$, $x_I^B = -0.2$, $R_A = 0.125$ and $R_B = 0.075$ (cf. figure 3a), corresponding to the green square in panels (e–f). (d) Examples of normal deformation β induced by a displacement Δ of inclusion A (colour legend) at each location θ along the solid inclusion. (e–f) Here $\bar{M}_{nm}$, $\bar{M}_{nt}$ and $\bar{M}_{tt}$ recomputed with the modified geometry (black solid line) and predicted from first-order (green dashes) and second-order (green dots) shape sensitivities. First-order (dashes) and second-order (dots) predictions for two additional reference locations x_I^A are shown in red and blue. Coloured squares represent evaluation points of the sensitivities.

We notice that we have a good agreement only for infinitesimal perturbations and most of the second-order predictions do not perform well for sensible deformations.

In conclusion, displacements of $\partial\mathbb{M}$ having a strong tangential-to-the-reference-geometry component are more difficult to predict than those dominated by normal deformation. This condition is embedded in the hypothesis under which (2.20) is valid. However, for small displacements (i.e. $\Delta \ll R_A$ in this case), the first-order prediction can be trusted.

3.3. Application: efficient handling of parametric studies

In § 3.2, we considered a microscopic case constituted by a REV containing two solid inclusions. However, the adjoint procedure presented in this work does not depend on the choice of the REV. In the following section, we consider a REV containing a single solid inclusion. This geometrical configuration was used in Ledda *et al.* (2021) to create a map of permeability and slip coefficients associated with a membrane formed by the periodic repetition of an elliptical solid inclusion. The map, obtained by interpolating a

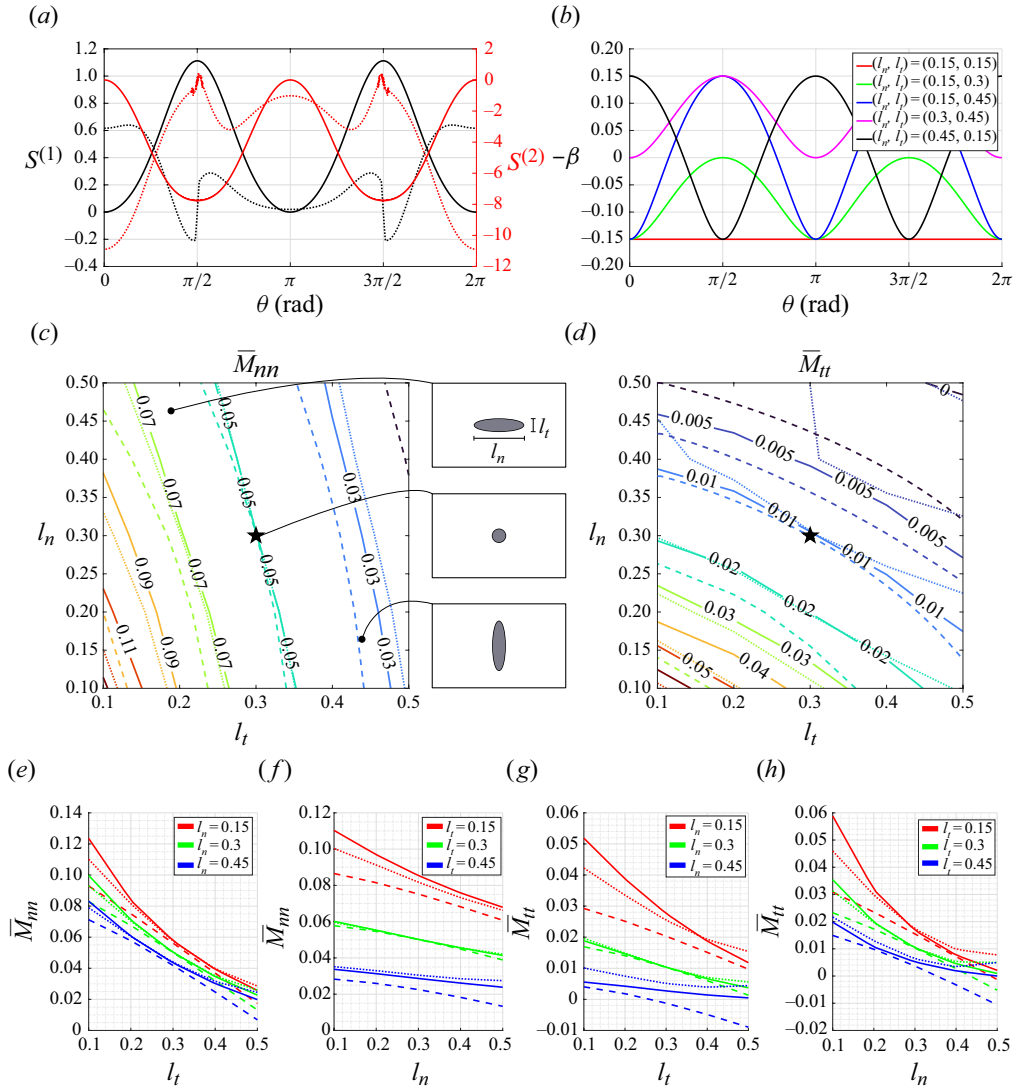


Figure 7. Effect of a modification of the axis l_n and l_t of a single elliptic inclusion on the $\bar{M}_{ij}$ tensor (geometry shown in the insets of panel c). Reference geometry: circular solid inclusion ($l_n = l_t = 0.3$; black stars in panels c, d only). (a) First-order (black) and second-order (red) shape sensitivities of $\bar{M}_{nn}$ (solid lines) and $\bar{M}_{tt}$ (dotted lines) along $\partial\mathbb{M}$ as parametrised by θ (cf. figure 3b). (b) Example of normal deformation β between the base circle with $l_n = l_t = 0.3$ and sample ellipses (l_n, l_t) in the legend. (c, d) Contours of permeability $\bar{M}_{nn}$ and slip $\bar{M}_{tt}$ computed with a direct approach (solid lines) and with first-order (dashes) or second-order (dots) sensitivity. (e-h) Sample of the surfaces in (c, d) at constant l_t (e, g) or l_n (f, h). Colours correspond to ellipse semiaxes values as shown in the legend of each panel.

set of direct microscopic solutions, was used to optimise the flow around a porous thin membrane. Obtaining such a map involves a non-negligible computational cost.

The objective of this section is to replicate a subset of the results obtained by Ledda *et al.* (2021) using a single direct and adjoint microscopic solution. We consider an elliptic, isolated, solid inclusion of axes l_n and l_t , aligned with the (x_n, x_t) axes, respectively. We solve the direct microscopic problem around this geometry for a range of (l_n, l_t) values, obtaining the maps in solid line in figure 7(c, d). We consider a base geometry for

the adjoint computations constituted by a circle $l_n = l_t = 0.3$ (black star). The sensitivity distribution obtained in this configuration is shown in [figure 7\(a\)](#), while [figure 7\(b\)](#) shows some distributions of the normal deformation β as a function of the ellipse semiaxes. Changes in permeability $\bar{M}_{nn}$ or slip $\bar{M}_{tt}$ can be estimated via (2.36) with products involving the normal deformation beta and the sensitivities $S^{(1)}$ and $S^{(2)}$. These predictions of first order (dashes) and second order (dots) are plotted on the same isocontours obtained using the direct solutions for comparison ([figure 7c,d](#)). There is a general agreement between the actual and predicted values of permeability and slip, confirmed also by the local sections of the maps, shown in [figure 7\(e–h\)](#). Overall, second-order predictions improve over the first-order ones: in the (l_n, l_t) space considered, the root mean square of the difference between the direct evaluation and the first- and second-order predictions are (0.0084, 0.0047) for $\bar{M}_{nn}$ and (0.0078, 0.0048) for $\bar{M}_{tt}$, respectively. Local oscillations near $\theta = \pi/2$ and $3\pi/2$ are due to numerical noise caused by the Dirac delta function. Their influence on the final solution is negligible, as shown in [appendix C](#).

We conclude that not only the method proposed in this paper is computationally lighter compared with the parametric study proposed in [Ledda et al. \(2021\)](#), but also it allows for displacements of the solid boundaries of general shape. The numerical resolution has been carried out with the tools specified in [appendix C](#). Using the same computer, the direct evaluation of $\bar{M}_{nn}$ and $\bar{M}_{tt}$ requires in this case approximately 2.5 hr with a step in l_n and l_t of 0.02, whereas the sensitivity-based prediction takes approximately 6 min.

4. Comparison between macroscopic and full-scale solutions

In this section, we use the developed sensitivity-based procedure to predict the flow around a non-periodic porous membrane in a computationally efficient way. We compare full-scale solutions of the flow against macroscopic solutions (2.12) obtained by solving a microscopic problem for each solid inclusion and macroscopic solutions obtained by solving a single microscopic direct and adjoint problem and predicting the effect of the real geometry using shape sensitivities. We propose two complementary test cases: (i) the flow around and across a membrane whose solid inclusions are not periodic because of a small random perturbation and (ii) the flow across a membrane obstructing a channel, whose solid inclusions have a systematic deformation pattern, consisting of a linear variation of the inclusion radius. Notice that the macroscopic flows are normalised with the outer scales as in (2.4).

4.1. Membrane with random small perturbations of the solid inclusion

As a first test case, we consider a periodic 2-D membrane constituted by 20 circles of radius $R = 0.0125$ (i.e. $\epsilon = 0.05$). The i th circle is centred at $(x_1^i, x_2^i) = (-\epsilon(i - 0.5)/\sqrt{2}, \epsilon(i - 0.5)/\sqrt{2})$. The membrane is placed in a vertical channel of size 5×2 . It is oriented at 45° to the horizontal axis and traversed by a fluid flow which obeys Stokes equations (cf. sketch in [figure 8](#)). Dirichlet conditions $(u_1, u_2) = (0, 1)$ apply on the bottom side and $u_i = 0$ on the lateral sides and on the membrane solid inclusions. The Neumann condition $\sum_{ij} n_j = 0$ applies on the top side. For convenience in the notation, we introduce a curvilinear coordinate $\xi = \sqrt{x_1^2 + x_2^2}$, as shown in [figure 8\(a\)](#). We radially perturb the surface of each solid inclusion using a Fourier series such that the i th deformed solid boundary has a radius

$$R^i = R + \alpha_0^i + \sum_{j=1}^N \alpha_j^i \cos(j\theta) + \gamma_j^i \sin(j\theta), \quad (4.1)$$

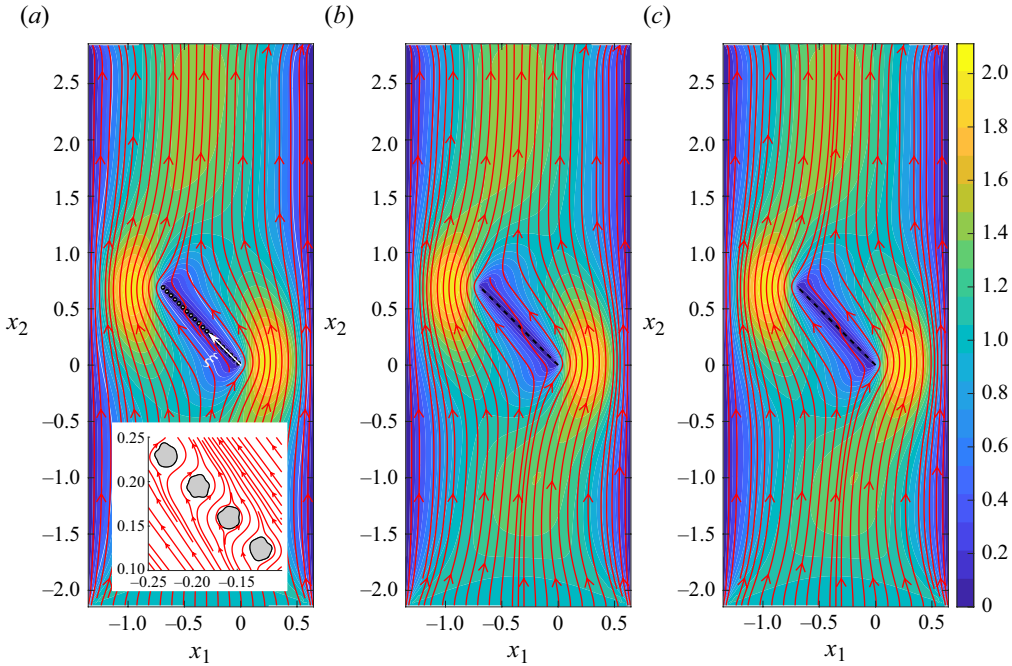


Figure 8. Full-scale and macroscopic simulations around an aperiodic membrane. (a) Contours of velocity magnitude and streamlines (red) for the full-scale simulation. The centre of each solid inclusion (grey obstacles) is located at $(x_1^i, x_2^i) = (-\epsilon(i - 0.5)/\sqrt{2}, \epsilon(i - 0.5)/\sqrt{2})$, thus at the curvilinear coordinate $\xi^i = \sqrt{x_{1,i}^2 + x_{2,i}^2} = (i - 0.5)\epsilon$ along $\mathbb{C}$, while the inset shows the typical streamline pattern in the proximity of the solid inclusions. (b) Macroscopic simulation with $\bar{M}_{ij}$ and $\bar{N}_{ij}$ computed using REV containing only one inclusion and (c) macroscopic simulation with $\bar{M}_{ij}$ and $\bar{N}_{ij}$ predicted using the shape sensitivities computed around a circle of radius 0.25ϵ and multiplying them for the β describing the difference between the considered solid inclusion and the reference circular one. The fictitious interface representing the membrane in panels (b) and (c) is denoted by the black dashes. The flow enters from the bottom of the domain with a unit velocity in the vertical direction. The lateral sides are no-slip walls and at the outlet (top boundary), $\Sigma_{ij} n_j = 0$.

where $\theta \in [0, 2\pi]$, $N = 6$ and α_j^i, γ_j^i are randomly sampled coefficients from a uniform distribution in the range $[-0.005\epsilon, 0.005\epsilon]$ and collected in the Supplementary material. These solid inclusions are visualised in figure 9 (black lines, as opposed to the green lines, representing the reference geometry) and the full-scale solution of system (2.1) is visualised in figure 8(a).

In the macroscopic simulation, we solve (2.5) with (2.12), which requires $\bar{M}_{ij}$ and $\bar{N}_{ij}$. For the microscopic problems, we choose a REV containing a single solid inclusion at a time along the membrane (Ledda *et al.* 2021) and average one by one the microscopic direct problems on each of the 20 inclusion geometries. The tensors obtained in this case are used to compute the macroscopic fluid flow presented in figure 8(b). The computational cost of this operation is that of solving 80 Stokes problems (2.15). Equivalently, this means solving 20 times (one for each inclusion) (2.10), which contains two components for $\bar{M}_{ij}$ and another two for $\bar{N}_{ij}$.

We now consider the macroscopic solution obtained using the sensitivity-based workflow. To obtain $\bar{M}_{ij}$ and $\bar{N}_{ij}$, we solve the direct problem (2.15) and adjoint problems (2.30, 2.40, 2.42) around a circular solid inclusion of radius R , finding the shape

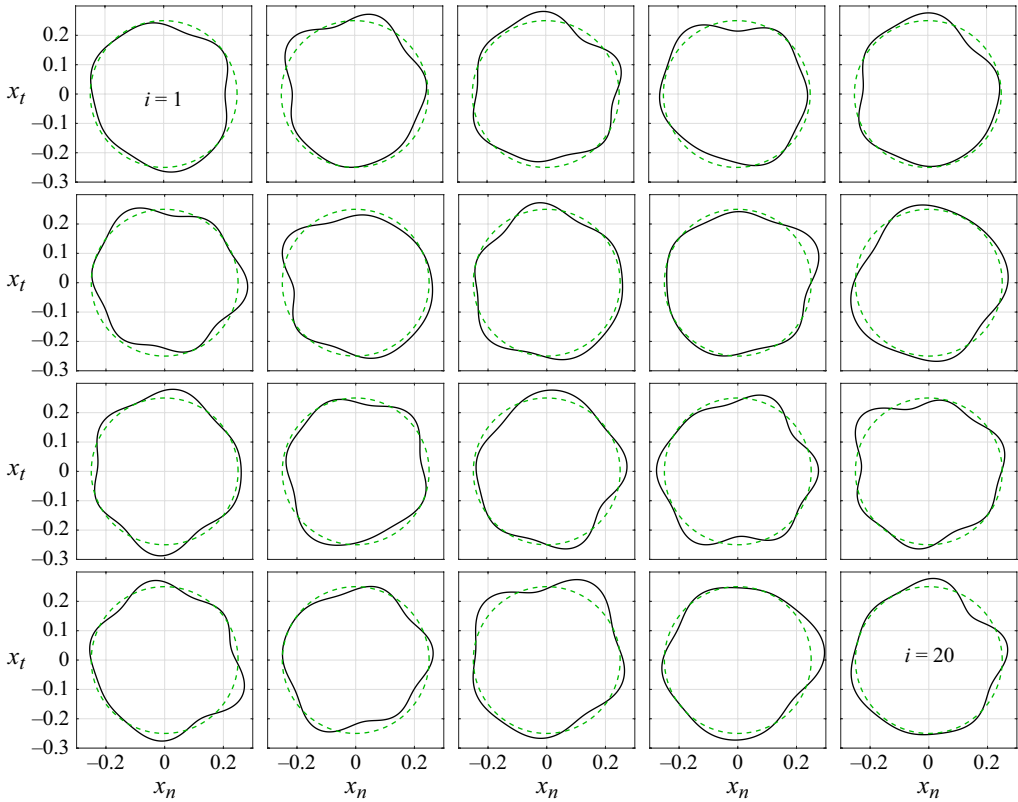


Figure 9. Details of the inclusions in the aperiodic membrane of figure 8. The boundaries of the original circular inclusions are sketched in dashed green line while the actual geometry is sketched in solid black line. Index i increases from top to bottom and from left to right.

sensitivities $S^{(1)}$ and $S^{(2)}$ for all $\bar{M}_{ij}$ and $\bar{N}_{ij}$ components. We then evaluate (2.36) with the normal displacement

$$\beta^i(\theta) = \alpha_0^i + \sum_{j=1}^N \alpha_j^i \cos(j\theta) + \gamma_j^i \sin(j\theta), \quad (4.2)$$

from the reference circular inclusion, obtaining an estimate for the variation of $\bar{M}_{ij}$ and $\bar{N}_{ij}$ caused by the shape modification. The computational cost of this operation is 12 Stokes problems (i.e. four for the direct solution and two for the first adjoint problem to find $S^{(1)}$ and another six to find $S^{(2)}$), regardless of the number of inclusions (and neglecting potential tensor symmetries, which would possibly reduce this cost). The macroscopic fluid flow obtained with these estimates is visualised in figure 8(c) by means of streamlines and isocontours of velocity magnitude.

Figure 10(a,b) compares the velocity profiles on the membrane centreline for the full-scale solution (black lines, average values as dots), direct macroscopic solution (blue) and shape sensitivity-based prediction (red). The agreement of both macroscopic solutions (direct and adjoint) with the average full-scale solution is excellent. For reference, green dots represent the macroscopic solution obtained by computing $\bar{M}_{ij}$ and $\bar{N}_{ij}$ with the base (undeformed) circular inclusions. The values of the $\bar{M}_{ij}$ and $\bar{N}_{ij}$ tensors computed using

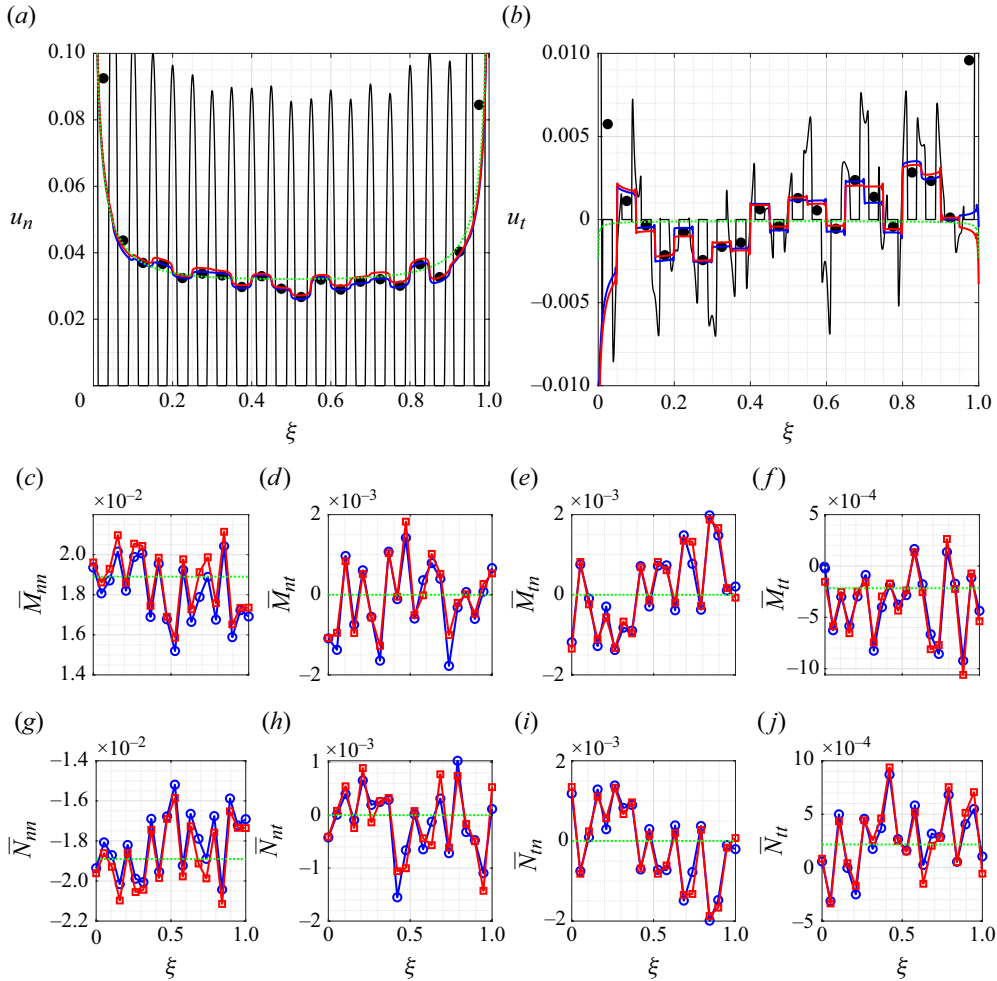


Figure 10. Velocity and Navier tensors on the centreline $\mathbb{C}$ of the aperiodic membrane of figures 8 and 9. (a) Normal- and (b) tangential-to-the-membrane velocity components. Black line, full-scale solution without averaging; black dots, averaged full-scale solution; blue line, macroscopic solution with $\bar{M}_{ij}$ and $\bar{N}_{ij}$ computed cell-by-cell; red line, sensitivity-based predictions on the reference, undeformed geometry (circular inclusion). Additionally, the green line shows the macroscopic solution computed with undeformed circular inclusions, to highlight the differences caused by the geometry modification. Panels (c–j) show the tensors values along the membrane: (c) $\bar{M}_{nn}$, (d) $\bar{M}_{nt}$, (e) $\bar{M}_{tn}$, (f) $\bar{M}_{tt}$, (g) $\bar{N}_{nn}$, (h) $\bar{N}_{nt}$, (i) $\bar{N}_{tn}$, (j) $\bar{N}_{tt}$. Values directly computed via (2.15) are depicted in blue while the values predicted using shape sensitivities (2.36) are in red. The values associated with the reference circular geometry are in green.

the direct (blue) and adjoint (red) procedures are shown in figure 10(c–j). Interestingly, although the geometric modifications may seem small (figure 9), the corresponding microscopic tensor values significantly vary. These variations cause peaks of tangential velocity, which are absent for the undeformed, circular inclusions. We can ascribe these differences entirely to the anisotropic nature of the deformed inclusions. The sensitivity-based prediction proves nearly as accurate as the direct solution, with a considerably lower computational cost. Indeed, the relative error on the membrane velocity magnitude with respect to the average full-scale solution (excluding the first and last REV) is 2.77 % for the macroscopic direct simulation and 2.90 % for the macroscopic adjoint-aided

prediction, while the computational cost of the adjoint-aided simulation is approximately 6.7 times lower. In this section, we expressed the computational cost in terms of Stokes problems because the microscopic direct and adjoint problems are a set of Stokes problems which can be solved in a cascade. To translate this cost in computational time, consider that the computational time associated with a single Stokes solution is approximately 50 s on a laptop with 32 GB RAM and one INTEL i 9–10900HK CPU with eight cores.

4.2. Membrane with large systematic deformations of the solid inclusions

The developed procedure can handle small random geometry variations of the solid inclusions, resulting in membrane velocity profiles with random peaks. However, one may argue that the effect on the macroscopic flow of such modifications is captured – on average – by the green profile in [figure 10\(a,b\)](#) (corresponding to a periodic membrane of base circles) and thus that the effect of these geometry modifications is not significant at the macroscale. We emphasise that the present method can capture macroscopic flow modifications. We consider the flow across a membrane constituted by 20 inclusions of radii $R^i = 0.2\epsilon^2(i - 1/1 - \epsilon) + 0.15\epsilon$ and evenly spaced centres. The average radius, used for the computation of the shape sensitivities is thus the same as in [figure 9](#). The associated normal displacement of the solid boundary about the average radius reaches peak values of $\pm 40\%$ at the membrane extremes. The so-constituted membrane obstructs a 2-D channel of unit height, as shown in [figure 11\(a\)](#). The flow enters from the left-hand side of the domain horizontally with unit speed and exits from the right-hand side with zero stress, and the top and bottom sides are no-slip walls. Contrary to the previous case, where the fluid could flow around the membrane, it is now forced to flow across it. The fluid prefers to flow in the lower-half of the channel where the porosity of the membrane is larger. The flow is hence asymmetric about the centreline $x_2 = 0.5$. Similarly to the previous case, we compare the full-scale solution ([figure 11a](#)) with a macroscopic solution of the flow past a membrane with all circular inclusions having the same radius 0.25ϵ ([figure 11b](#)) and with space-varying microscopic geometry whose tensors are calculated using the direct ([figure 11c](#)) and adjoint ([figure 11d](#)) approach. For the adjoint case, the sensitivity is calculated with a circular solid inclusion of radius 0.25ϵ as reference geometry. The values of $\bar{M}_{nn}$ and $\bar{M}_{tt}$ used to compute the solutions in frames [figure 11\(b,c,d\)](#) are represented in [figure 11\(f,g\)](#) by green, blue and red lines, respectively.

The velocity magnitude contours between the full-scale ([figure 11a](#)), macroscopic direct (c) and sensitivity-based (d) simulations are in good agreement. The differences with respect to the flow through a periodic, unperturbed membrane (cf. [figure 11b](#), where the flow is symmetric with respect to the $x_2 = 0.5$ axis) are important. This is confirmed by the velocity magnitude profiles along the membrane ([figure 11e](#)), where we adopted the same colour code as in [figure 10\(a,b\)](#). The green line is indeed symmetric about $x_2 = 0.5$, while the full-scale flow is not. As in the previous flow configuration, the full-scale average fields are correctly predicted both in the direct and sensitivity-based simulations, with minor differences, and at a much-reduced cost for the latter.

The two examples presented in this section show complementary applications of the proposed model: in the former, the fluid can flow around the membrane and the random geometry modifications locally change the flow along the membrane, while in the latter, the membrane obstructs a channel, forcing the flow through its pores, whose geometric properties globally alter the macroscopic flow. The present model handles both cases, offering an advantageous trade-off between accuracy and computational cost.

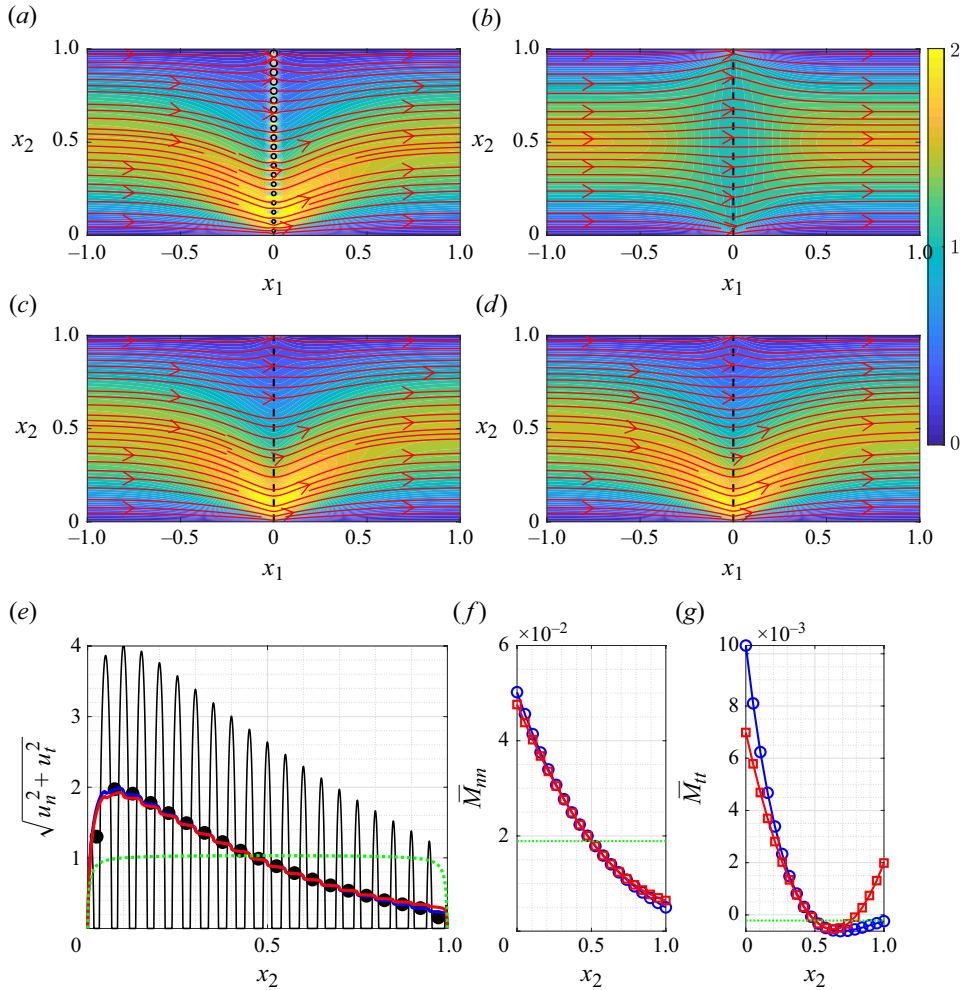


Figure 11. Full-scale and macroscopic flow past an aperiodic membrane constituted by 20 circular inclusions (i.e. $\epsilon = 0.05$). The radii linearly vary between 0.15ϵ (lowermost inclusion) and 0.35ϵ (uppermost inclusion). The centre of the n th inclusion is located in $(x_1^n, x_2^n) = (0, (n - 1/2)\epsilon)$. In panels (a–d) the contours of velocity magnitude and streamlines (red) are shown: (a) full-scale solution; (b) macroscopic solution past a periodic membrane formed by circular inclusions of radius 0.25ϵ ; (c) macroscopic solution with $\bar{M}_{ij}$ and $\bar{N}_{ij}$ computed using REV containing only one inclusion; (d) macroscopic solution with $\bar{M}_{ij}$ and $\bar{N}_{ij}$ predicted using the shape sensitivities computed around a circular inclusion of radius 0.25ϵ . The fictitious interface representing the membrane in panels (b, c) and (d) is denoted by the black dashes. The flow enters from the left of the domain with a unit velocity in the horizontal direction. The top and bottom of the panels are no-slip walls and at the outlet $\Sigma_{ijn} = 0$. (e) Velocity magnitude at the membrane centreline (colour code as in figure 10a,b). (f, g) Non-zero $\bar{M}_{ij}$ components along the membrane (colour code as in figure 10c–j). By symmetry, $\bar{N}_{ij} = -\bar{M}_{ij}$ and $\bar{M}_{ij} = 0$ if $i \neq j$.

5. Conclusions

In the present paper, we considered the problem of computing the fluid flow across a thin, aperiodic porous membrane in an efficient way, coupling the homogenisation technique developed by Zampogna & Gallaire (2020) with a second-order shape-sensitivity approach. We introduced the concept of REV in the model developed in Zampogna & Gallaire (2020) to account for the aperiodic porous microstructure. Using the separation

of scales between the pore- and membrane-level flows, we wrote the macroscopic velocity field on the membrane as a linear combination of the stresses acting on the two sides of the membrane itself. The coefficients of the linear combination, the Navier tensors $\bar{M}_{ij}$ and $\bar{N}_{ij}$, stem from the solution of solvability conditions at the REV scale, the microscopic problems, after an averaging step. While $\bar{M}_{ij}$ and $\bar{N}_{ij}$ only need to be computed once for a periodic microstructure, this is not possible for aperiodic geometries. Indeed, several direct microscopic solutions are needed only to find the proper REV size. The cost of this direct tensor evaluation scales with the number of pores/inclusions and quickly annihilates the computational gain of the homogeneous, macroscopic model.

Consequently, we developed an adjoint-based technique to account for geometrical modifications of the pore-scale microstructure starting from some reference geometry and in the limit of infinitesimal deformations. The computational cost of such an operation is constant with respect to the number of pores/inclusions, only requiring a small set of linear problems to be solved at the pore scale, the adjoint problems. We validated this procedure against direct solutions of the microscopic problems and found that it can predict the effect of moderately small geometric perturbations of the solid inclusions. To conclude our analysis, we considered a full-scale membrane of randomly perturbed microstructure and a membrane of circular inclusions of linearly increasing radius. We compared our model with a direct solution, finding a significant improvement in efficiency for a similar accuracy. Indeed, in § 4.2, we found that the sensitivity-based homogeneous solution was approximately 6.7 times faster than the direct homogeneous solution and the relative error (based on the average full-scale solution) on the velocity at the membrane centreline was 2.77 % for the direct solution and 2.90 % for the sensitivity-based one.

The present work introduces an efficient methodology to relate the Navier tensors to modifications of the membrane microstructure about some reference configuration. In particular, this work is complementary to the optimisation routine proposed by Ledda *et al.* (2021), enabling a truly efficient exploration of many microscopic geometries without requiring large parametric studies.

Further developments towards the analysis of flows through non-periodic membranes should handle large and irregular deformations of the reference inclusion geometry. Describing these situations will require integrating the sensitivity-based approach (formally valid for infinitesimal geometrical deformations) with data-based methods to efficiently explore large deformations using a Newton algorithm. Minimizing the number of Newton iterations through data-based approaches will be crucial in keeping the method computationally convenient when large deformations are considered. Already existing examples of data-aided homogenisation approaches are Karimi & Bhattacharya (2024a) and Wittkowski *et al.* (2024), which efficiently handled inertial flows in bulk porous media and thin permeable membranes, respectively. Exploring the use of such techniques in the present framework opens perspectives for future work.

Supplementary material. Supplementary material is available at <https://doi.org/10.1017/jfm.2025.277>.

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Declaration of interests. The authors report no conflict of interest.

Data availability. A sample code used to produce the results in the present manuscript is publicly available at the following DOI: [10.5281/zenodo.14046643](https://doi.org/10.5281/zenodo.14046643).

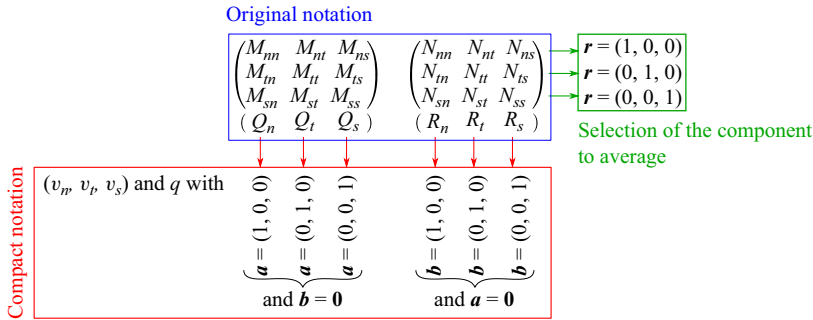


Figure 12. Schematic visualisation of the compact notation and averaging when $\mathbf{n} = (1, 0, 0)$, $\mathbf{t} = (0, 1, 0)$, $\mathbf{s} = (0, 0, 1)$: the M_{ij} and N_{ij} tensors are decomposed column by column into a sequence of six independent problems for (v_i, q) . The rowwise selection of the ‘observed’ component of v_i (i.e. the component whose average is considered) in the computation of the first-order Lagrangian (2.21) is done via the unitary vector $\mathbf{r}$.

Appendix A. Details about the compact notation and averaging

In § 2, we compacted (2.10) as

$$\begin{cases} -\partial_i q + \partial_{kk}^2 v_i = 0 & \text{in } \mathbb{F}, \\ \partial_i v_i = 0 & \text{in } \mathbb{F}, \\ \Sigma_{ij}(v, q)n_j = a_i & \text{on } \mathbb{U}, \\ \Sigma_{ij}(v, q)n_j = -b_i & \text{on } \mathbb{D}, \\ v_i = 0 & \text{on } \partial\mathbb{M}, \\ v_i, q & \text{periodic along } t_i, s_i, \end{cases} \quad (\text{A1})$$

where

$$a_i = (1, 0, 0), \quad b_i = 0 \text{ for } M_n, Q_n, \quad a_i = 0, \quad b_i = (1, 0, 0) \text{ for } N_n, R_n, \quad (\text{A2})$$

$$a_i = (0, 1, 0), \quad b_i = 0 \text{ for } M_t, Q_t, \quad a_i = 0, \quad b_i = (0, 1, 0) \text{ for } N_t, R_t, \quad (\text{A3})$$

$$a_i = (0, 0, 1), \quad b_i = 0 \text{ for } M_s, Q_s, \quad a_i = 0, \quad b_i = (0, 0, 1) \text{ for } N_s, R_s, \quad (\text{A4})$$

and the unitary vector r_i is used to select the i th component of M_{ij} or N_{ij} to be averaged,

$$r_i = (1, 0, 0) \quad \text{to select } \bar{M}_n \text{ or } \bar{N}_n, \quad (\text{A5})$$

$$r_i = (0, 1, 0) \quad \text{to select } \bar{M}_t \text{ or } \bar{N}_t, \quad (\text{A6})$$

$$r_i = (0, 0, 1) \quad \text{to select } \bar{M}_s \text{ or } \bar{N}_s, \quad (\text{A7})$$

as shown in the schematic figure 12.

We clarify the meaning of the compact notation in a 2-D domain where $n_i = (1, 0)$ and $t_i = (0, 1)$:

(i) to find (M_{nn}, M_{tn}) and Q_n we solve

$$\begin{cases} -\partial_i q + \partial_{kk}^2 v_i = 0 & \text{in } \mathbb{F}, \\ \partial_i v_i = 0 & \text{in } \mathbb{F}, \\ \Sigma_{ij}(v, q)n_j = (1, 0) & \text{on } \mathbb{U}, \\ \Sigma_{ij}(v, q)n_i = 0 & \text{on } \mathbb{D}, \\ v_i = 0 & \text{on } \partial\mathbb{M}, \\ v_i, q & \text{periodic along } t_i, \end{cases} \quad \text{equivalent to} \quad \begin{cases} -\partial_i Q_n + \partial_{kk}^2 M_{in} = 0 & \text{in } \mathbb{F}, \\ \partial_i M_{in} = 0 & \text{in } \mathbb{F}, \\ \Sigma_{hj}(M_n, Q_n)n_j = (1, 0) & \text{on } \mathbb{U}, \\ \Sigma_{hj}(M_n, Q_n)n_j = 0 & \text{on } \mathbb{D}, \\ M_{in} = 0 & \text{on } \partial\mathbb{M}, \\ M_{in}, Q_n & \text{periodic along } t_i, \end{cases} \quad (\text{A8})$$

which, respectively, means

$$\left\{ \begin{array}{l} -\partial_i q + \partial_{nn}^2 v_n + \partial_{tt}^2 v_n = 0 \quad \text{in } \mathbb{F}, \\ -\partial_i q + \partial_{nn}^2 v_t + \partial_{tt}^2 v_t = 0 \quad \text{in } \mathbb{F}, \\ \partial_n v_n + \partial_t v_t = 0 \quad \text{in } \mathbb{F}, \\ -q + 2\partial_n v_n = -1 \quad \text{on } \mathbb{U}, \\ \partial_n v_t + \partial_t v_n = 0 \quad \text{on } \mathbb{U}, \\ -q + 2\partial_n v_n = 0 \quad \text{on } \mathbb{D}, \\ \partial_n v_t + \partial_t v_n = 0 \quad \text{on } \mathbb{D}, \\ v_n, v_t = 0 \quad \text{on } \partial\mathbb{M}, \\ v_n, v_t, q \quad \text{periodic along } (1, 0), \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} -\partial_i Q_n + \partial_{nn}^2 M_{nn} + \partial_{tt}^2 M_{nn} = 0 \quad \text{in } \mathbb{F}, \\ -\partial_i Q_n + \partial_{nn}^2 M_{tn} + \partial_{tt}^2 M_{tn} = 0 \quad \text{in } \mathbb{F}, \\ \partial_n M_{nn} + \partial_t M_{tn} = 0 \quad \text{in } \mathbb{F}, \\ -Q_n + 2\partial_n M_{nn} = -1 \quad \text{on } \mathbb{U}, \\ \partial_n M_{tn} + \partial_t M_{nn} = 0 \quad \text{on } \mathbb{U}, \\ -Q_n + 2\partial_n M_{nn} = 0 \quad \text{on } \mathbb{D}, \\ \partial_n M_{tn} + \partial_t M_{nn} = 0 \quad \text{on } \mathbb{D}, \\ M_{nn}, M_{tn} = 0 \quad \text{on } \partial\mathbb{M}, \\ M_{nn}, M_{tn}, Q_n \quad \text{periodic along } (1, 0); \end{array} \right. \quad (\text{A9})$$

(ii) to find (M_{nt}, M_{tt}) and Q_t we solve

$$\left\{ \begin{array}{l} -\partial_i q + \partial_{kk}^2 v_i = 0 \quad \text{in } \mathbb{F}, \\ \partial_i v_i = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{ij}(v, q)n_j = (0, 1) \quad \text{on } \mathbb{U}, \\ \Sigma_{ij}(v, q)n_i = 0 \quad \text{on } \mathbb{D}, \\ v_i = 0 \quad \text{on } \partial\mathbb{M}, \\ v_i, q \quad \text{periodic along } t_i, \end{array} \right. \quad \text{equivalent to} \quad \left\{ \begin{array}{l} -\partial_i Q_t + \partial_{kk}^2 M_{it} = 0 \quad \text{in } \mathbb{F}, \\ \partial_i M_{it} = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{hj}(M_t, Q_t)n_j = (0, 1) \quad \text{on } \mathbb{U}, \\ \Sigma_{hj}(M_t, Q_t)n_j = 0 \quad \text{on } \mathbb{D}, \\ M_{it} = 0 \quad \text{on } \partial\mathbb{M}, \\ M_{it}, Q_t \quad \text{periodic along } t_i, \end{array} \right. \quad (\text{A10})$$

which, respectively, mean

$$\left\{ \begin{array}{l} -\partial_i q + \partial_{nn}^2 v_n + \partial_{tt}^2 v_n = 0 \quad \text{in } \mathbb{F}, \\ -\partial_i q + \partial_{nn}^2 v_t + \partial_{tt}^2 v_t = 0 \quad \text{in } \mathbb{F}, \\ \partial_n v_n + \partial_t v_t = 0 \quad \text{in } \mathbb{F}, \\ -q + 2\partial_n v_n = 0 \quad \text{on } \mathbb{U}, \\ \partial_n v_t + \partial_t v_n = -1 \quad \text{on } \mathbb{U}, \\ -q + 2\partial_n v_n = 0 \quad \text{on } \mathbb{D}, \\ \partial_n v_t + \partial_t v_n = 0 \quad \text{on } \mathbb{D}, \\ v_n, v_t = 0 \quad \text{on } \partial\mathbb{M}, \\ v_n, v_t, q \quad \text{periodic along } (1, 0), \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} -\partial_i Q_t + \partial_{nn}^2 M_{nt} + \partial_{tt}^2 M_{nt} = 0 \quad \text{in } \mathbb{F}, \\ -\partial_i Q_t + \partial_{nn}^2 M_{tt} + \partial_{tt}^2 M_{tt} = 0 \quad \text{in } \mathbb{F}, \\ \partial_n M_{nt} + \partial_t M_{tt} = 0 \quad \text{in } \mathbb{F}, \\ -Q_t + 2\partial_n M_{nt} = 0 \quad \text{on } \mathbb{U}, \\ \partial_n M_{tt} + \partial_t M_{nt} = -1 \quad \text{on } \mathbb{U}, \\ -Q_t + 2\partial_n M_{nt} = 0 \quad \text{on } \mathbb{D}, \\ \partial_n M_{tt} + \partial_t M_{nt} = 0 \quad \text{on } \mathbb{D}, \\ M_{nt}, M_{tt} = 0 \quad \text{on } \partial\mathbb{M}, \\ M_{nt}, M_{tt}, Q_t \quad \text{periodic along } (1, 0); \end{array} \right. \quad (\text{A11})$$

(iii) to find (N_{nn}, N_{tn}) and R_n we solve

$$\left\{ \begin{array}{l} -\partial_i q + \partial_{kk}^2 v_i = 0 \quad \text{in } \mathbb{F}, \\ \partial_i v_i = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{ij}(v, q)n_j = 0 \quad \text{on } \mathbb{U}, \\ \Sigma_{ij}(v, q)n_i = (-1, 0) \quad \text{on } \mathbb{D}, \\ v_i = 0 \quad \text{on } \partial\mathbb{M}, \\ v_i, q \quad \text{periodic along } t_i, \end{array} \right. \quad \text{equivalent to} \quad \left\{ \begin{array}{l} -\partial_i R_n + \partial_{kk}^2 N_{in} = 0 \quad \text{in } \mathbb{F}, \\ \partial_i N_{in} = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{hj}(N_n, R_n)n_j = 0 \quad \text{on } \mathbb{U}, \\ \Sigma_{hj}(N_n, R_n)n_j = (-1, 0) \quad \text{on } \mathbb{D}, \\ N_{in} = 0 \quad \text{on } \partial\mathbb{M}, \\ N_{in}, R_n \quad \text{periodic along } t_i; \end{array} \right. \quad (\text{A12})$$

(iv) to find (N_{nt}, N_{tt}) and R_t we solve

$$\left\{ \begin{array}{l} -\partial_i q + \partial_{kk}^2 v_i = 0 \quad \text{in } \mathbb{F}, \\ \partial_i v_i = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{ij}(v, q)n_j = 0 \quad \text{on } \mathbb{U}, \\ \Sigma_{ij}(v, q)n_i = (0, -1) \quad \text{on } \mathbb{D}, \\ v_i = 0 \quad \text{on } \partial\mathbb{M}, \\ v_i, q \quad \text{periodic along } t_i, \end{array} \right. \quad \text{equivalent to} \quad \left\{ \begin{array}{l} -\partial_i R_t + \partial_{kk}^2 N_{it} = 0 \quad \text{in } \mathbb{F}, \\ \partial_i N_{it} = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{hj}(N_t, R_t)n_j = 0 \quad \text{on } \mathbb{U}, \\ \Sigma_{hj}(N_t, R_t)n_j = (0, -1) \quad \text{on } \mathbb{D}, \\ N_{it} = 0 \quad \text{on } \partial\mathbb{M}, \\ N_{it}, R_t \quad \text{periodic along } t_i. \end{array} \right. \quad (\text{A13})$$

We now provide an explicit example of how we can calculate the shape sensitivities for the Navier tensor component $\bar{M}_{nn}$. We produced figure 5(a,d,g) by solving the equations provided in the present appendix in a 2-D domain with a circular solid inclusion of radius R_A . The remaining tensor components follow the nomenclature provided in schematic figure 12.

To find how a change in shape β affects $\bar{M}_{nn}$, we need to evaluate (2.36) with $v_i = M_{in}$ and $\mathbf{r} = (1, 0)$, i.e.

$$\delta \bar{M}_{nn} = \int_{\partial\mathbb{M}} \beta S^{(1)} + \frac{1}{2} \beta^2 S^{(2)} dS, \quad (\text{A14})$$

where, on a 2-D circular inclusion such as the one in figure 3(a), $dS = R_A d\theta$ and the sensitivities $S^{(1)}$ and $S^{(2)}$ are specialised for M_{in} , i.e.

$$S^{(1)} = \frac{\partial M_{in}^\dagger}{\partial n} \frac{\partial M_{in}}{\partial n}, \quad (\text{A15})$$

$$S^{(2)}(x) = \left(\frac{\partial}{\partial n} + H \right) \left(\frac{\partial M_{in}^\dagger}{\partial n} \frac{\partial M_{in}}{\partial n} \right) + \frac{\partial \tilde{M}_{in}}{\partial n} \frac{\partial M_{in}}{\partial n} + \frac{\partial \tilde{M}_{in}^\dagger}{\partial n} \frac{\partial M_{in}^\dagger}{\partial n}. \quad (\text{A16})$$

These fields are found by solving the direct and adjoint problems, i.e.

$$\left\{ \begin{array}{l} -\partial_i Q_n + \partial_{kk}^2 M_{in} = 0 \quad \text{in } \mathbb{F}, \\ \partial_i M_{in} = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{hj}(M_n, Q_n)n_j = (1, 0) \quad \text{on } \mathbb{U}, \\ \Sigma_{hj}(M_n, Q_n)n_j = 0 \quad \text{on } \mathbb{D}, \\ M_{in} = 0 \quad \text{on } \partial\mathbb{M}, \\ M_{in}, Q_n \quad \text{periodic along } t_i, \end{array} \right. \quad \left\{ \begin{array}{l} -\partial_i Q_n^\dagger + \partial_{kk}^2 M_{in}^\dagger = -\delta(x_n - x_n^C)\delta_{in} \quad \text{in } \mathbb{F}, \\ \partial_i M_{in}^\dagger = 0 \quad \text{in } \mathbb{F}, \\ \Sigma_{pq}^\dagger(M_n^\dagger, Q_n^\dagger)n_q = 0 \quad \text{on } \mathbb{U}, \mathbb{D}, \\ M_{in}^\dagger = 0 \quad \text{on } \partial\mathbb{M}, \\ M_{in}^\dagger, Q_n^\dagger \quad \text{periodic along } t_i, s_i, \end{array} \right. \quad (\text{A17})$$

$$\left\{ \begin{array}{l} -\partial_i \tilde{Q}_n + \partial_{kk}^2 \tilde{M}_{in} = 0 \quad \text{in } \mathbb{F}, \\ \partial_i \tilde{M}_{in} = 0 \quad \text{in } \mathbb{F}, \\ \tilde{\Sigma}_{pq}(\tilde{M}_n, \tilde{Q}_n)n_q = 0 \quad \text{on } \mathbb{U}, \mathbb{D}, \\ \tilde{M}_{in} = -\frac{\partial M_{in}^\dagger}{\partial n} \quad \text{on } \partial\mathbb{M}, \\ \tilde{M}_{in}, \tilde{Q}_n \quad \text{periodic along } t_i, s_i, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{l} -\partial_i \tilde{Q}_n^\dagger + \partial_{kk}^2 \tilde{M}_{in}^\dagger = 0 \quad \text{in } \mathbb{F}, \\ \partial_i \tilde{M}_{in}^\dagger = 0 \quad \text{in } \mathbb{F}, \\ \tilde{\Sigma}_{pq}^\dagger(\tilde{M}_n^\dagger, \tilde{Q}_n^\dagger)n_q = 0 \quad \text{on } \mathbb{U}, \mathbb{D}, \\ \tilde{M}_{in}^\dagger = -\frac{\partial M_{in}}{\partial n} \quad \text{on } \partial\mathbb{M}, \\ \tilde{M}_{in}^\dagger, \tilde{Q}_n^\dagger \quad \text{periodic along } t_i, s_i, \end{array} \right. \quad (\text{A18})$$

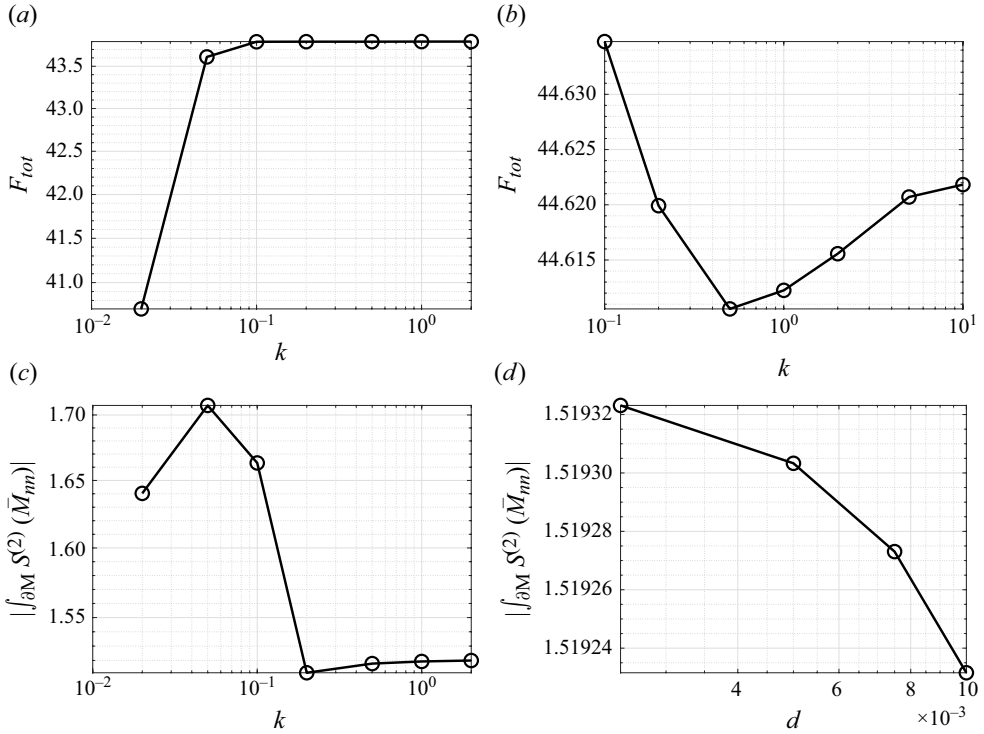


Figure 13. Mesh independence study. Total force $F_{tot} = |\int_{\partial M} \Sigma_{ij} n_j|$ exerted by the fluid on the membrane in the full-scale simulation (a) and in the macroscopic simulation (b) as a function of the mesh factor k . The integral of the second-order shape sensitivity of $\bar{M}_{nn}$ as a function of the mesh factor k (c) and the numerical Dirac delta function amplitude d (d) in the microscopic simulation.

on a reference configuration, e.g. $R_A = 0.12$, $R_B = 0.15$, $x_t^A = 0.2$ and $x_t^B = -0.2$, as in figure 4(a–d), corresponding to the green curves of figure 5(a,d). Now we can reconstruct the green dotted lines in figure 5(g) by simply evaluating (B14) with $\beta = \Delta R_A$ (the variation in radius R_A from the reference configuration) and summing $\delta \bar{M}_{nn}$ to the $\bar{M}_{nn}$ of the reference configuration (i.e. the average solution of the first problem in (B17)).

Appendix B. Numerical implementation and mesh independence study

In the present study, we carried out simulations using the finite-element software COMSOL Multiphysics. We employed P3-P2 elements (for velocity and pressure, respectively) in all the microscopic simulations, and P2-P1 elements in the macroscopic and full-scale simulations. Elements are quadrilaterals in the boundary layers and triangles everywhere else. The mesh independence in the microscopic simulations was tested for the microscopic domain size, the amplitude of the numerical Dirac delta function and the mesh thickness. The study regarding the microscopic domain size shows the same trends as Zampogna & Gallaire (2020), thus it will not be repeated here. The Dirac delta function has been modelled using a Gaussian function

$$\delta(x - x_0) = \frac{1}{\sqrt{2\pi}d} e^{-\frac{(x-x_0)^2}{2d^2}}, \quad (C1)$$

discretised with 10 mesh elements in the normal direction. In the present simulations, we found that $d = 0.005$ is a good compromise between cost and accuracy, as shown

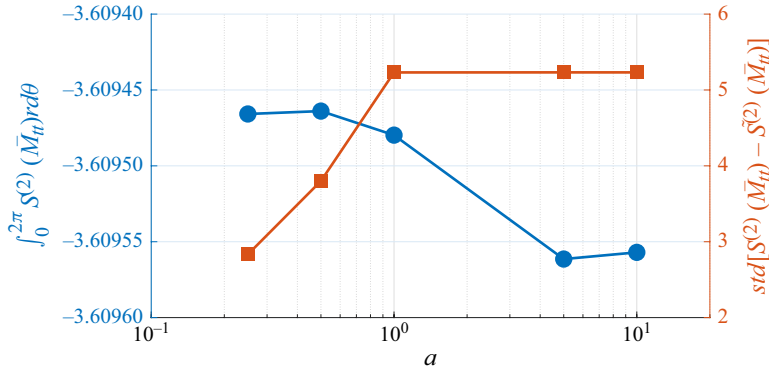


Figure 14. Integral of the second order sensitivity $S^{(2)}$ for the component $\bar{M}_{tt}$ along the solid inclusion (left-hand axis, blue) and its standard deviation with respect to a low-pass filtered signal $\tilde{S}^{(2)}$ (right-hand axis, red) in the window $\theta \in [\pi/2 - d/(2r), \pi/2 + d/(2r)]$, for a range of the mesh size parameter a . The low-pass filter has a step response at a wavelength of $d/2$, to eliminate the oscillations caused by the Dirac delta function.

in figure 13(d). The convergence with respect to the mesh refinement has been studied considering a mesh having typical sizes of $0.001l$ on the solid inclusion, as well as eight quadrilateral layers, and $0.03l$ far from it. This mesh has been modified by dividing these sizes by a factor of k . Figure 13(c) shows that for $k = 1$ the mesh-related error concerning the integral value of the second-order sensitivity on the solid inclusion is smaller than 1 % between two subsequent meshes. The influence of the mesh in the full-scale and macroscopic simulations has been studied similarly, as shown in figure 13(a,b). In this case, the mesh sizes corresponding to $k = 1$ are

- (i) for the full-scale simulation: 5×10^{-4} on the solid inclusions and 0.05 far from them, with an enclosure around the membrane having a typical mesh size of 0.01;
- (ii) for the macroscopic simulation: 0.0025 on the interface and 0.05 far from it.

In both cases, for $k = 1$, the module of the force exerted on the membrane F_{tot} changes between two subsequent meshes less than 1 %.

Appendix C. About the oscillations of the second-order sensitivity

In this section, we discuss the influence of the oscillations around the locations $\theta = \pi/2$ and $3\pi/2$ of the second order sensitivity $S^{(2)}(\bar{M}_{tt})$ in figures 7(a) and 6(a,c). To show their numerical nature, we consider the geometry corresponding to the black stars in figure 7(c,d) (i.e. $l_n = l_t = r = 0.15$) and a base mesh whose sizing is

- (i) 0.001 inside a zone large $d = 0.01$ around $x_n = 0$ and on the solid inclusion;
- (ii) 0.02 far from the solid inclusion;

and change only the discretisation in the zone of amplitude d including the numerical Dirac delta function by multiplying the mesh sizes by a factor a . In figure 14, we compare the integral of the second-order sensitivity and its standard deviation with respect to a low-pass filtered signal $\tilde{S}^{(2)}$ for $a \in [0.25, 10]$. The oscillations of the second order sensitivity decrease in amplitude as the mesh is refined (lower a) and its integral value along $\partial\mathbb{M}$ has relative variations below 0.01 %. We conclude that these oscillations can be suppressed with high mesh refinement, however, they do not influence the conclusions drawn in § 3.

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