Thèse

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Synthèse de microstructures par optimisation topologique, et optimisation de forme d'un problème d'interaction fluide-structure

Soutenue le 20 Décembre 2021 devant le jury composé de

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Résumé

Cette thèse de mathématiques appliquées à la mécanique à pour objet la conception optimale de matériaux. Elle porte sur l'étude d'outils théoriques et numériques qui permettent la synthèse de nouveaux matériaux aux propriétés émergentes. Ce travail se décompose en deux parties distinctes.

La première partie concerne la synthèse de matériaux architecturés périodiques, par l'utilisation d'une méthode d'optimisation topologique. Le but est de concevoir des matériaux périodiques ayant des propriétés du second gradient importantes, en optimisant la forme et la distribution de matière de la cellule périodique constitutive de ce matériau. Ces propriétés sont définies à partir de *tenseurs homogénéisés*.

La méthode que nous appliquons nécessite dans un premier temps une étude théorique de la sensibilité de ces tenseurs homogénéisés, par rapport à une perturbation infinitésimale de la géométrie de la cellule périodique. Cette information s'appelle la *dérivée topologique* des tenseurs homogénéisés, et son étude est l'objet du chapitre 1. En particulier, nous calculons la dérivée topologique du tenseur du second gradient.

Puis dans le chapitre 2, nous utilisons la dérivée topologique calculée précédemment en l'incorporant dans une procédure numérique d'optimisation topologique. Ainsi, nous obtenons des topologies nouvelles à l'échelle de la cellule périodique qui permettent la conception de matériaux périodiques ayant des propriétés de second gradient prononcées.

La seconde partie concerne l'étude théorique de l'optimisation d'un problème d'interaction fluide-structure. Elle est l'objet du chapitre 3. Nous cherchons à optimiser la forme d'un matériau élastique plongé dans un fluide visqueux et incompressible, afin d'améliorer une fonctionnelle abstraite qui dépend des solutions de ce problème d'interaction, dont nous montrons l'existence et l'unicité. Pour cela, nous calculons la dérivée de forme de la fonctionnelle, en appliquant la méthode appelée *méthode des vitesses* (ou méthode d'Hadamard).

Summary

This thesis of mathematics applied to mechanics deals with the optimal design of materials. It focuses on the study of theoretical and numerical tools that allow the synthesis of new materials with emerging properties. This work is divided in two distinct parts.

The first part concerns the synthesis of periodic materials by using a topological optimization method. The goal is to design periodic materials with important second gradient properties, by optimizing the shape and the distribution of the periodic cell constituting this material. These properties are defined from *homogenized tensors*.

The method we apply requires first a theoretical study of the sensitivity of these homogenized tensors, with respect to an infinitesimal perturbation of the geometry of the periodic cell. This information is called the *topological derivative* of the homogenized tensors, and its study is the subject of Chapter 1. In particular, we compute the topological derivative of the second gradient tensor.

Then in Chapter 2, we use the topological derivative computed previously by incorporating it into a numerical procedure of topological optimization. Thus, we obtain new topologies at the scale of the periodic cell that allow the design of periodic materials with pronounced second gradient properties.

The second part concerns the theoretical study of the optimization of a Fluid Structure Interaction problem. We seek to optimize the shape of an elastic material immersed in a viscous and incompressible fluid, in order to improve an abstract shape functional which depends on the solutions of this interaction problem, whose existence and uniqueness are shown. For this purpose, we compute the shape derivative of the shape functional, by applying the so-called *speed method* (or Hadamard's method).

Sommaire

Introduction (français)

La fabrication additive et l'optimisation topologique ont suscité un regain d'intérêt pour l'étude des *matériaux architecturés* au cours des deux dernières décennies. Ces progrès technologiques sont en partie dus à l'émergence des imprimantes 3D, permettant une production rapide et peu onéreuse d'échantillons pour l'expérimentation, et à l'amélioration des méthodes et de la puissance en calculs numériques. Les matériaux architecturés sont des matériaux dont les propriétés macroscopiques sont dues à l'organisation de leur microstructure interne, ainsi que leur structure à plus grande échelle. Ils sont aussi appelés *matériaux composites.* Bien que les microstructures non périodiques ou quasi-périodiques aient également été amplement étudiées, les matériaux architecturés sont souvent basés sur un arrangement périodique de cellules unitaires. Dans cette thèse, nous nous intéressons plus particulièrement aux matériaux périodiques.

Les matériaux architecturés sont largement utilisés en ingénierie en raison de leurs propriétés remarquables, comme la légèreté, la résistance, l'absorption d'énergie, l'isolation acoustique. Ils permettent de concevoir des matériaux artificiels que l'on trouve difficilement dans la nature, aussi appelés *métamatériaux.* On peut citer par exemple la conception de *matériaux auxétiques*, dont les bénéfices en terme de capacité de résistance au choc et à l'impact, isolation acoustique, absorption des vibrations, grande capacité de changement d'aire ou de volume, ont été largement soulignés dans la littérature depuis plusieurs décennies (voir par exemple, [Alm85]). Un matériau auxétique est un matériau qui se dilate transversalement lorsqu'un étirement uniaxial est appliqué sur celui-ci.

Un autre exemple que l'on peut citer parmi les nombreux métamatériaux concerne les réseaux *tétrachiraux* (voir Figure 1). Un matériau chiral est un matériau qui ne possède pas la symétrie miroir (son image par symétrie dans un miroir ne lui est pas superposable). Un matériau tétrachiral est un cas particulier de matériau chiral, qui reste inchangé lorsqu'il est tourné d'un angle de $2\pi/4$. La structure tétrachirale périodique étudiée dans [Kar+20] et reproduite Figure 1, présente des déformations en élongation couplées à des rotations. Sous les forces de traction, la structure se courbe vers le haut. Cette structure est intéressante par exemple pour la conception de ponts, afin de compenser la flexion due à leur poids (voir Figure 1).

Bien souvent la taille de la période ou des hétérogénéités est petite par rapport à la taille de la structure macroscopique d'un matériau architecturé. Des simulations numériques peuvent être réalisées afin de prédire le comportement global d'un tel matériau. Mais, du fait de la taille de la microstructure, une analyse directe est très coûteuse en temps de calcul. Ainsi le matériau microstructuré peut être approché par un matériau homogène. La théorie décrivant les propriétés macroscopiques (appelées aussi propriétés *homogénéisées* ou *effectives*) d'un matériau à partir de l'analyse de sa microstructure est appelée *homogénéisation.* Nous introduisons le

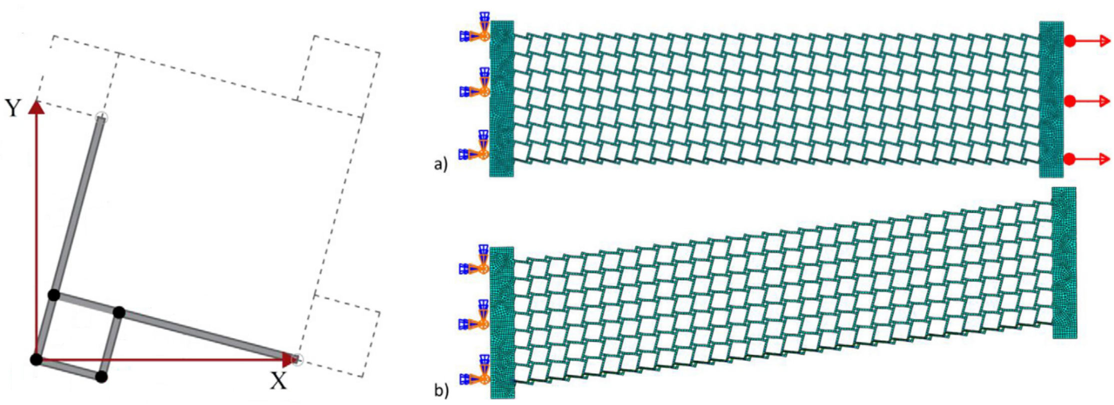

Figure 1: Cellule unitaire tétrachirale (à gauche), et réponse d'une structure périodique composée de cette cellule périodique, lorsqu'elle est soumise à des forces de traction horizontales (à droite) (Figure de [Kar+20]).

concept d'homogénéisation dans la section 1.2 du chapitre 1.

L'homogénéisation permet d'obtenir un modèle macroscopique de Cauchy du premier ordre décrivant un matériau architecturé. Nous appelons *homogénéisation du premier ordre* une telle description d'un matériau architecturé. Un matériau de Cauchy du premier ordre est un matériau pour lequel seul le premier gradient du champ de déplacement est utilisé pour mesurer les déformations, et tous les gradients de déplacement d'ordre supérieur sont négligés. Les modèles de Cauchy du premier ordre sont valides sous une hypothèse de séparation d'échelle : la taille des hétérogénéités doit être infiniment petite par rapport à la dimension caractéristique macroscopique de la structure. Ainsi, une telle hypothèse doit être satisfaite dans le cas d'une homogénéisation du premier ordre, à savoir dans le cas d'un matériau périodique, que la taille de la cellule périodique doit être infiniment petite par rapport à la taille macroscopique de la structure.

En pratique, cette hypothèse n'est jamais vérifiée puisque les matériaux architecturés ont des cellules périodiques de taille finie. Ainsi, la théorie de l'élasticité de Cauchy pour l'homogénéisation doit être parfois enrichie afin de prédire avec précision les effets d'échelle du matériau. Il existe deux manières d'améliorer ce modèle.

La première approche concerne les modèles dits *d'ordre supérieur*. Ils reposent sur l'ajout de degrés de liberté dans le modèle. Alors qu'un matériau de Cauchy a pour seul degré de liberté le champ de déplacement, un *matériau de Cosserat* par exemple, a pour degrés de liberté le champ de déplacement et un champ de micro-rotation. Un matériau dit *micromorphe* sera lui doté d'une nouvelle variable de microdéformation, un tenseur d'ordre deux.

La seconde approche concerne les modèles dit *de degré supérieur*. Ces modèles incluent comme variable un gradient d'ordre supérieur de la variable cinématique (le déplacement ou la déformation). Par exemple, un *modèle de second gradient* a comme variable non seulement le gradient du déplacement, mais aussi son second gradient. Ainsi, le second gradient du champ de déplacement est pris en compte dans la densité d'énergie de déformation, alors que dans un modèle de Cauchy, seul son premier gradient est pris en compte. Nous appelons *homogénéisation du second gradient* la procédure qui calcule un modèle macroscopique du second gradient pour un matériau hétérogène. On appelle aussi *modèle à gradient de déformation*, un modèle qui fait intervenir le gradient du champ de déformation à la place du second gradient du déplacement.

Par exemple, nous avons calculé dans le chapitre 2 de cette thèse la forme d'une cellule périodique par une procédure d'optimisation topologique, afin de maximiser des effets macroscopiques de second gradient. Un échantillon de matériau constitué de cette cellule périodique, présenté sur la Figure 2, a été étudié par Baptiste Durand lors de sa thèse au laboratoire Navier (École des Ponts ParisTech, Université Gustave Eiffel, thèse en cours), et présente des effets de second gradient.

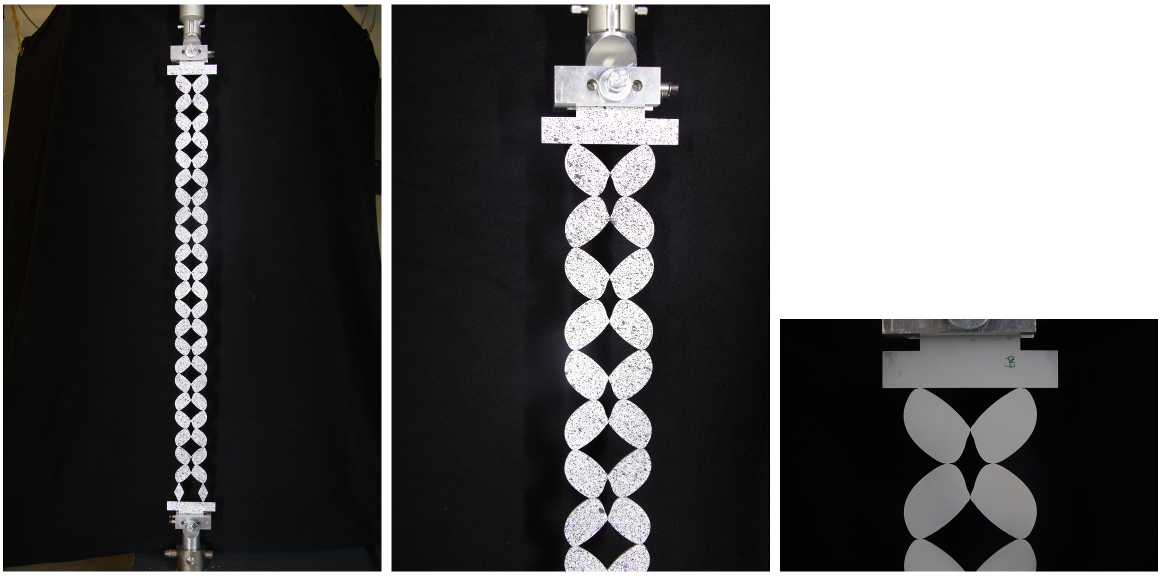

Figure 2: Échantillon d'un matériau constitué d'une cellule périodique de type pantographique. Ces images proviennent d'expériences menées par Baptiste Durand dans le laboratoire Navier (École des Ponts ParisTech, Université Gustave Eiffel).

Les matériaux architecturés ont d'excellentes propriétés. Ceci est en partie dû à la possibilité d'ajuster leur microstructure, soit par la distribution de matière à l'échelle microscopique, soit par leur topologie, afin d'atteindre les propriétés souhaitées à l'échelle macroscopique. Les techniques d'optimisation de forme et de la topologie permettent d'obtenir des formes originales qui ne sauraient être imaginées par les concepteurs de matériaux émergents.

L'objectif de cette thèse est d'étudier et d'appliquer des techniques d'optimisation topologique afin de synthétiser de nouveaux matériaux architecturés dans le cadre des matériaux continus homogénéisés en 2D.

L'analyse de la sensibilité du tenseur d'élasticité homogénéisé du second ordre par rapport aux changements topologiques de sa microstructure est menée. La cellule unitaire constitutive du matériau est topologiquement perturbée par la nucléation d'une petite inclusion circulaire d'un matériau aux propriétés différentes du matériau sous jacent. Cette analyse conduit au calcul de la *dérivée topologique* du tenseur d'élasticité homogénéisé, qui est donnée par un champ de tenseur d'ordre 6 défini sur la cellule unitaire. Cette dérivée topologique mesure comment le tenseur d'élasticité homogénéisé d'ordre 2 change lorsqu'une petite inclusion circulaire est introduite dans sa cellule périodique. Cette étude fait l'objet du chapitre 1.

Dans le chapitre 2, les dérivées topologiques des tenseurs homogénéisés précédemment obtenues sont utilisées dans une méthode numérique d'optimisation forme et de topologie des microstructures. Cette optimisation a pour objet la synthèse et la conception optimale de métamatériaux, qui présentent des effets du second gradient très prononcés en regard de l'élasticité de Cauchy et en raison d'un effet de microstructure, ce qui n'est pas le cas de la plupart des matériaux rencontrés en ingénierie.

Le chapitre 3 de cette thèse est consacré à une étude qui ne s'inscrit pas dans le cadre de l'homogénéisation et des matériaux architecturés, mais qui est liée à l'optimisation de structures. Cette étude est consacrée à l'optimisation de forme d'un problème d'Interaction Fluide Structure. On cherche à optimiser la forme d'un matériau élastique plongé dans un fluide, en calculant la dérivée de forme d'une fonctionnelle de forme abstraite, afin de trouver une direction de descente pour faire évoluer cette forme avec la méthode dite des vitesses.

Présentation de la thèse

J'ai commencé ma thèse en octobre 2018, dans le cadre du projet ArchiMatHOS[1] financé par l'*Agence Nationale de la Recherche*. Ce projet rassemble des chercheurs de laboratoires de Mathématiques et de Mécanique pour explorer les comportements élastiques non standard des matériaux architecturés, afin de trouver et de synthétiser de tels matériaux. Jean-François Scheid (Maître de conférences à l'Institut Élie Cartan de Lorraine (IECL), Université de Lorraine, Nancy, France) et Jean-François Ganghoffer (Professeur au Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux, Université de Lorraine, Metz- Nancy, France) ont supervisé ma thèse.

Je tiens à souligner que cette thèse est le fruit de nombreuses collaborations enrichissantes. En plus de mes superviseurs, j'ai travaillé avec André Novotny (Laboratório Nacional de Computação Científica LNCC/MCT, Petrópolis, RJ, Brazil), Jan Sokołoswski (Institut Élie Cartan de Lorraine (IECL), Université de Lorraine, Nancy, France), Arthur Lebée (Laboratoire Navier, École des Ponts, Université Gustave Eiffel, CNRS, Marne-la-Vallée, France), Ilaria Lucardesi (Institut Élie Cartan de Lorraine (IECL), Université de Lorraine, Nancy, France), Baptiste Durand (Laboratoire Navier, École des Ponts, Université Gustave Eiffel, CNRS, Marne-la-Vallée, France) et Nicolas Auffray (Laboratoire Modélisation et Simulation Multi Échelle, MSME UMR 8208 CNRS, Université Paris-Est, 5 bd Descartes, 77454 Marne-la-Vallée, France).

Détaillons le contenu du manuscrit.

Dans le chapitre 1, nous calculons les dérivées topologiques des tenseurs homogénéisés d'ordre supérieur d'un matériau périodique, par rapport à une perturbation topologique de la cellule périodique constituant ce matériau. La dérivée topologique donne le comportement d'une grandeur mécanique affectée à la cellule d'une structure périodique d'un matériau composite, lorsque celle-ci est soumise à une perturbation infinitésimale de sa topologie. Cette information est intéressante du point de vue de l'optimisation, car elle indique s'il est avantageux ou non de changer la topologie de la cellule de base du composite. De plus, la dérivée topologique permet l'émergence de géométries nouvelles et non

[1] Matériaux architecturés conçus avec une homogénéisation d'ordre supérieur, `https://anr.fr/Project-ANR-17-CE08-0039`

triviales qui répondent à des défis majeurs, sans avoir besoin d'une grande précision sur la topologie initiale.

Nous commençons par introduire le cadre dans lequel nous travaillons : l'homogénéisation. La théorie de l'homogénéisation est un domaine à la fois des mathématiques et de la physique, qui aborde les modèles qui contiennent des effets de taille. En général, ces modèles comportent différentes échelles de longueur, en la présence d'au moins une échelle microscopique et une échelle macroscopique. Des outils pertinents doivent être utilisés afin de prendre en compte les effets de l'interaction de ces différentes échelles, et de prédire quelle sera l'influence de la microstructure sur le comportement macroscopique du système étudié.

Dans la section 1.2, après une introduction à la théorie de l'homogénéisation, nous présentons un schéma d'homogénéisation utilisé pour explorer les matériaux élastiques périodiques pour lesquels la taille de la cellule périodique est petite. Ce schéma nous permet de définir des tenseurs dits homogénéisés, qui incorporent des informations relatives aux propriétés macroscopiques de ce matériau. Une fois ces tenseurs définis, nous étudions leur sensibilité topologique.

Le concept de dérivée topologique est présenté dans la section 1.3, puis nous décrivons ce qu'est une perturbation topologique du problème. Nous ajoutons une petite inclusion de taille ε dans la cellule périodique, qui a pour effet de modifier légèrement les valeurs des tenseurs homogénéisés. Ainsi nous calculons les dérivées topologiques de ces tenseurs, et pour cela, nous avons besoin d'introduire des états dits *adjoints*. Ces états sont définis grâce à la *méthode adjointe* que nous présentons dans cette section. Nous renvoyons à l'annexe 1.5 contenant quelques lemmes utiles et les preuves des estimations des champs topologiquement perturbés utilisés pour définir les tenseurs homogénéisés.

Dans le chapitre 2, nous abordons un problème numérique d'optimisation topologique, basé sur les résultats obtenus au chapitre 1. Le but est d'optimiser les propriétés macroscopiques d'un matériau périodique. Ainsi la fonction coût de notre problème d'optimisation est une fonction qui dépend uniquement des tenseurs homogénéisés. Nous commençons par une brève revue des différentes méthodes numériques existantes pour l'optimisation de forme et topologique.

Ensuite, nous présentons dans la section 2.2 la méthode que nous avons adoptée, à savoir une méthode topologique de type gradient couplée à une représentation level-set du domaine. Nous la décrivons dans le cadre de l'homogénéisation, et nous donnons les détails techniques de la procédure algorithmique que nous avons implémentée avec Matlab. L'algorithme fonctionne comme suit. Pour une distribution donnée de la cellule périodique, nous calculons les tenseurs homogénéisés, évaluons la fonctionnelle de coût, et calculons la dérivée topologique associée. Puis nous actualisons l'architecture interne de la cellule de base grâce à la dérivée topologique.

Dans la section 2.3, nous analysons un problème d'optimisation topologique dans le cas où la cellule périodique est composée d'un mélange de deux matériaux, l'un rigide et l'autre mou, c'est à dire que le module d'Young du premier et significativement plus grand que ce lui du second. Nous appelons *contraste* le rapport entre ces modules d'Young. Nous définissons dans une première étape, des fonctionnelles de coût naïves, définies avec des longueurs intrinsèques obtenues comme rapport entre les coefficients des tenseurs homogénéisés du second et du premier ordre, que nous optimisons. Nous étudions également la sensibilité de l'algorithme au maillage, aussi bien pour sa composante d'homogénéisation que pour sa composante d'optimisation topologique. Nous terminons cette section par l'étude d'une cellule de type pantographique que nous avons obtenu en amont.

À partir de là, nous nous intéressons dans la section 2.4 au cas où le matériau mou imite du vide, ce qui signifie que l'on fait tendre son module d'Young vers zéro. Nous observons que dans cette situation, nous améliorons certaines des longueurs caractéristiques précédentes. En particulier, nous parvenons à rendre certaines jonctions matérielles de plus en plus fines, améliorant du même coup les effets d'ordre supérieur.

Enfin, nous étudions un problème d'optimisation pour lequel la fonctionnelle de coût dépend des invariants des tenseurs homogénéisés du premier et du second ordre dans la section 2.5.

L'optimisation de la forme d'un problème d'interaction fluide-structure (FSI) est étudiée dans le dernier chapitre. Après une introduction aux problèmes FSI, ainsi qu'aux travaux récents concernant leur optimisation topologique et de forme, nous présentons dans la section 3.2 le modèle qui nous intéresse, à savoir, un corps élastique incompressible bidimensionnel immergé dans un fluide de Stokes incompressible. Une partie de sa frontière est attachée à un rivet rigide et fixe, tandis que l'autre partie est en interaction avec le fluide. Les forces surfaciques fluides s'appliquent au corps élastique, le déformant, et les équations fluides sont posées dans le domaine défini à partir du déplacement du corps élastique.

A partir de là, le problème posé est de connaître et de calculer la forme optimale du corps élastique initial, qui permet d'optimiser une fonctionnelle de forme abstraite (par exemple l'énergie). Pour répondre à cette question, nous commençons par donner un résultat d'existence et d'unicité pour le système IFS dans la section 3.3, en appliquant une procédure de point fixe.

Puis dans la section 3.4, nous calculons la dérivée de forme de la fonctionnelle de forme au moyen de la *méthode des vitesses*. Nous introduisons cette méthode dans la section 3.4.1 . Nous l'appliquons au problème IFS dans les sections 3.4.2 et 3.4.3, afin de calculer les problèmes de valeurs aux limites des dérivées matérielles de la solution IFS dans la section 3.4.4, et la dérivée de forme de la fonctionnelle dans la section 3.4.5.

Enfin, nous simplifions la dérivée de forme de la fonctionnelle avec une méthode adjointe, aussi appelée *méthode de Céa*.

Introduction (English)

The additive manufacturing and topological optimization sparked a renewed interest in the study of *architectured materials* over the past two decades. These technological progress are partly due to the emergence of 3D printers, enabling fast and affordable sample production, and the improvement of the computational methods and power. Architectured materials are materials for which the macroscopic properties are due to the organization of their inner microstructure, including composition and internal structure, not only at microlevel, but also at larger length scales, up to the size of a sample or structural member. They are also called *composite material*. Although non-periodic or quasi-periodic microstructures has also been widely studied, architectured materials are often based on periodic unit cell arrangement. In this thesis we are in particular interested in periodic materials.

Architectured materials are extensively used in engineering in virtue of their remarkable properties such as low weight, strength, energy absorption, acoustic insulation. They make it possible to design artificial materials that can hardly be found in nature, also called *metamaterials*. For example *auxetic materials* can be obtained, whose benefits in terms of shock and impact resistance, acoustic insulation, vibration absorption, high capacity of area or volume change, have been widely underlined in the literature for several decades (see e.g., [Alm85]). An auxetic material is a material expanding transversely when an uniaxial stretch load is applied on it.

Another example which can be cited among the numerous metamaterials concerns *tetrachiral* lattices (see Figure 3). A chiral material has a lack of symmetry when it is subjected to a mirror transformation (its image by symmetry in a mirror is not superimposable with itself). A tetrachiral material is a particular case of chiral material, which stays unchanged when it is rotating by an $2\pi/4$ angle. The periodic tetrachiral structure studied in [Kar+20] and presented Figure 3 has bulk deformations being coupled to rotations. This creates a so-called normal to shear strain coupling. Under traction forces, the structure bends upwards. This could be interesting for the design of a bridge, in order to compensate for the bending due to the weight of the bridge (see Figure 3).

Quite often the size of the period or the one of the inhomogeneities is small in comparison to the size of the macroscopic structure of an architectured material. Numerical simulations can be performed in order to predict the overall behaviour of such a material. But because of the size of the microstructure, a direct analysis is very costly in terms of computation time, which is cumbersome for an application point of view. Thus the microstructured material is approximated by a homogeneous material. The theory describing macroscopic (also called *homogenized* or *effective*) properties of a material from the analysis of its microstructure is called *homogenization*. We introduce the concept of

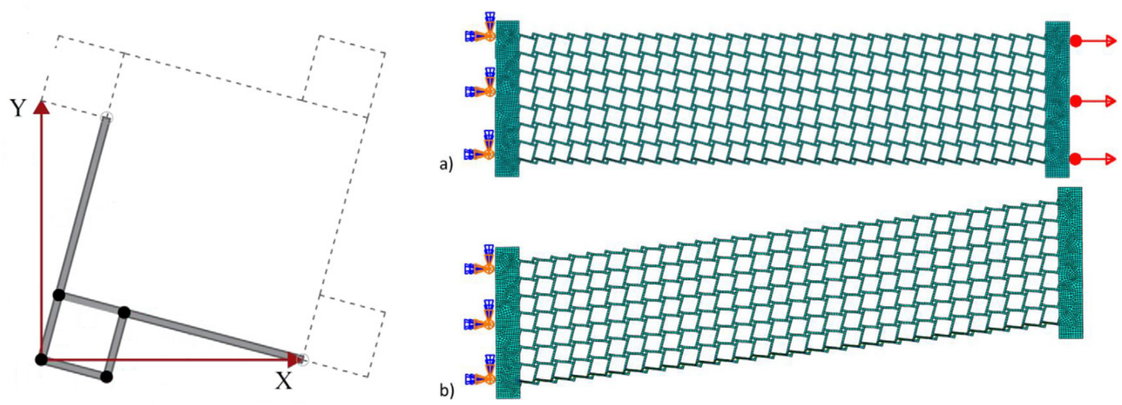

Figure 3: Tetrachiral unit cell (left), and response of a periodic structure composed with this periodic unit cell, when it is subjected to horizontal traction forces (right) (Figure from [Kar+20]).

homogenization in Section 1.2 of Chapter 1.

The homogenization allows to obtain a first-order Cauchy macroscopic model describing an architectured material. We call *first order homogenization* such a description of an architectured material. A first-order Cauchy material is a material for which the sole first gradient of the displacement field is used for measuring the deformations, and all higher-order displacement gradients are neglected. First-order Cauchy models are valid under an hypothesis of scale separation: the size of the inhomogeneities has to be infinitely small in comparison to the macroscopic characteristic dimension of the structure Thus, such an hypothesis need to be satisfied in the case of first order homogenization, namely in the case of a periodic material, where the size of the periodic cell needs to be infinitely small in comparison to the macroscopic size of the structure.

However, in practice, this hypothesis is never satisfied since the architectured materials have finite size periodic cell. Thus, the Cauchy theory of elasticity for homogenization needs sometimes to be enriched in order to predict accurately scale effects of the material. The are two ways to improve this model.

The first one concerns the so-called higher order models. They rely on the addition of degree of freedom in the model. While a Cauchy material only has the displacement field as only degree of freedom, a *Cosserat material* has the displacement field and a micro rotation field as degrees of freedom, and a *micromorphic material* has a new microstrain variable, a second order tensor.

The second one concerns higher gradient models. These models include higher order gradient of the kinematic variable (the displacement or the strain) as variable. For example a *second gradient model* includes not only the gradient of the displacement, but also its second gradient. Thus the second gradient of the displacement field goes into the strain energy density, while in a Cauchy model, only its first gradient goes into it. We call *second gradient homogenization* the procedure offering a macroscopic second gradient model for a heterogeneous material. We also call *strain gradient model*, a model which involves the gradient of the strain field, in place of the second gradient of the displacement.

For example, we have calculated in Chapter 2 of this thesis the shape of a periodic cell through an topological optimization procedure, in order to maximize homogenized second gradient effects. A sample of material constituted with this periodic cell, presented in

Figure 4, has been studied by Baptiste Durand during his thesis in the laboratory Navier (École des Ponts ParisTech, Université Gustave Eiffel), and shows up second gradient effects.

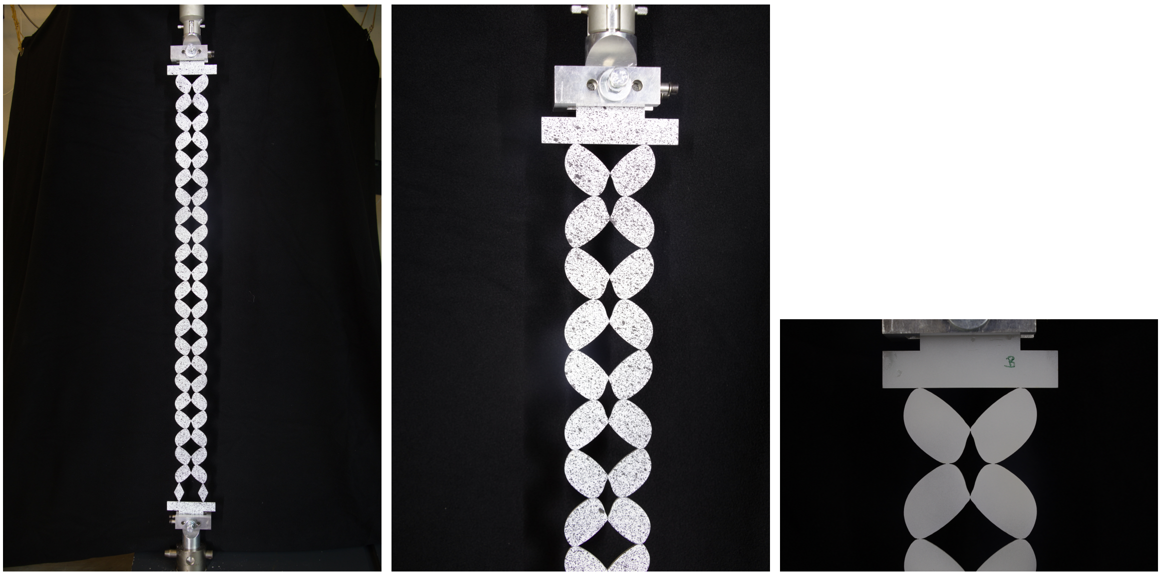

Figure 4: Sample of a material constituted with a pantographic like periodic cell. These pictures come from experiments conducted by Baptiste Durand in the laboratory Navier (École des Ponts ParisTech, Université Gustave Eiffel).

The architectured materials have excellent properties. This is in part due to the possibility to adjust their microstructure, either the distribution of matter at the microscopic scale, or the topology, in order to reach desired properties at the macroscopic scale. Designers of emerging materials are limited by their imagination. Shape and topological optimization techniques can be put at the service of the imagination.

The objective of this thesis is to study and apply topological optimization techniques in order to synthesize new architectured materials in the framework of homogenized continuous materials in 2D.

The sensitivity analysis of second order homogenized elasticity tensor to topological microstructural changes is performed. The microstructure is topologically perturbed by the nucleation of a small circular inclusion of weak material that allows for deriving the sensitivity in closed form. The resulting topological derivative is given by a sixth order tensor field over the microstructural domain, which measures how the second order homogenized elasticity tensor changes when a small circular inclusion is introduced at the microscopic level. This study is the object of Chapter 1.

In Chapter 2, the obtained topological derivatives of second order homogenized tensors are used within a numerical method of shape and topology optimization of microstructures. This method aims to design optimal metamaterials having very pronounced second gradient effects with respect to the Cauchy elasticity due to a microstructure effect, which is not the case for most materials encountered in engineering.

This thesis ends with a study which is not in the scope of homogenization and architectured materials, but which is related to structural optimization. Chapter 3 devoted to the shape optimization of a Fluid Structure Interaction problem. We want to optimize the shape of an elastic material immersed in a fluid, by calculating the shape derivative of an abstract shape functional, in order to find a direction of descent to make this shape evolve with the so-called *velocity method*.

Presentation of the thesis

I started my thesis in October 2018, in the framework of the project ArchiMatHOS[2] funded by the french *Agence Nationale de la Recherche*. This project gathers researchers from Mathematics and Mechanics laboratories to explore non-standard elastic behaviours of architectured materials, in order to find and synthesize such materials. Jean-François Scheid (Associate Professor at the Institut Élie Cartan de Lorraine (IECL), University of Lorraine, Nancy, France) and Jean-François Ganghoffer (Professor at the Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux, University of Lorraine, Metz-Nancy, France) supervised my thesis.

I would like to emphasise that this thesis is the result of numerous enriching collaborations. In addition to my supervisors, I worked with André Novotny (Laboratório Nacional de Computação Científica LNCC/MCT, Petrópolis, RJ, Brazil), Jan Sokołoswski (Institut Élie Cartan de Lorraine (IECL), Université de Lorraine, Nancy, France), Arthur Lebée (Laboratoire Navier, École des Ponts, Université Gustave Eiffel, CNRS, Marne-la-Vallée, France), Ilaria Lucardesi (Institut Élie Cartan de Lorraine (IECL), Université de Lorraine, Nancy, France), Baptiste Durand (Laboratoire Navier, École des Ponts, Université Gustave Eiffel, CNRS, Marne-la-Vallée, France) et Nicolas Auffray (Laboratoire Modélisation et Simulation Multi Échelle, MSME UMR 8208 CNRS, Université Paris-Est, 5 bd Descartes, 77454 Marne-la-Vallée, France).

Let us detail the content of the present manuscript.

In Chapter 1, we calculate the topological derivatives of the higher order homogenized tensors of a periodic material, with respect to a topological perturbation of the periodic cell constituting this material. The topological derivative gives the behaviour of a mechanical quantity assigned to the cell of a periodic structure of a composite material, when the latter is subjected to an infinitesimal perturbation of its topology. This information is interesting from the optimization point of view, because it indicates whether it is beneficial or not to change the topology of the cell of the composite. Furthermore, the topological derivative has been quite used throughout numerical topological optimization scheme, and it allows the emergence of novel and non trivial geometries that meet major challenges, without the need for great precision on the initial topology.

In Section 1.2, we start by introducing the framework of microstructure optimization, that we associate directly with the concept of homogenization. The homogenization theory is a field of both mathematics and physics, which tackles the models that contain large size effects. In general this models consist of different length scales, at least a microscopic and a macroscopic one. Relevant tools need to be used in order to take into account this scales effect, and in some sense, to predict what will be the influence of the microstructure on the macroscopic behaviour of the system studied.

[2]Architectured materials designed with higher-order homogenization, `https://anr.fr/Project-ANR-17-CE08-0039`

In Section 1.2, after an introduction to the homogenization theory, we present an homogenization scheme used to explore periodic elastic materials for which the size of the periodic cell is very small. This scheme allows us to define so-called homogenized tensors, which encapsulate information about the macroscopic properties of this material. Once these tensors are defined, we study their topological sensitivity.

The topological derivative concept is presented in Section 1.3. Then we describe what we call a topological perturbation of the problem. Actually, we add a small inclusion of size ε in the periodic cell, which has the effect of slightly modifying the values of the homogenized tensors. Thus we compute the topological derivatives of these tensors, and for that we need to introduce states called *adjoints*. These adjoint states are defined thanks to the so-called *adjoint method* that we introduce in this section. After this, we perform the direct calculation of the topological derivatives, relegating to Appendix 1.5 some useful lemmas, together with the proofs of the estimates of the topological counterparts of the fields used to define the homogenized tensors.

In Chapter 2, we lead a numerical topology optimization problem based on the results obtained in Chapter 1. We start by a brief review of the different exiting numerical methods for shape and topological optimization.

Then the method that we have adopted is presented in Section 2.2, namely a topological gradient-type method coupled with a level-set representation of the domain. We describe it within the framework of homogenization, and we give the technical details of the algorithmic procedure we have have implemented with MATLAB. The algorithm works as follows. For a given distribution of the periodic cell, we compute the homogenized tensors, evaluate the cost functional (which we can define with a symbolic expression as any smooth function depending on the homogenized tensors), and calculate the associated topological derivative. Then we update the internal architecture of the unit cell using the topological derivative.

In Section 2.3, we perform a topological optimization problem in the case where the periodic cell is composed with a mixture of two materials, one being stiff and the other one being soft, that is to say that the Young's modulus of the first is significantly greater than that of the second. We call *contrast* the ratio between these Young's moduli. We define some naive cost functionals with intrinsic lengths obtained as the ratios between the coefficients of the second and the first order homogenized tensors. We also study the sensitivity of the algorithm with the mesh. We end this section with the study of an obtained pantographic like cell.

From there we are interesting in the case where the soft material mimic voids, throughout Section 2.4. We observe that in this situation, we improve some of the previous characteristic lengths. In particular, we manage to make the material connections more and more fine, improving at the same time the higher order effects.

Finally, we investigate a optimization problem for which the cost functional depends on invariants of the first and the second order homogenized tensors in Section 2.5.

A shape optimization of a Fluid Structure Interaction (FSI) problem is studied in the last chapter. After an introduction to FSI problems, and to the recent works regarding their topological and shape optimization, we present in Section 3.2 the model we are interesting in. Namely, a two-dimensional incompressible elastic body is immersed in an incompressible Stokes fluid. A part of its boundary is attached to rigid and fixed rivet from , while the other part is in interaction with this fluid. Fluid surface forces apply to the elastic body, and the fluid equations are posed on the domain defined from the elastic body displacement: this is a two-way coupling system. The elastic body is deformed, because of this interaction with the fluid.

From there, we wonder what is the optimal shape of the initial elastic body, in order to optimize an abstract volume shape functional (for example the energy). To answer this question, we start by giving an existence and uniqueness result for the FSI system in Section 3.3, by application of a fixed point procedure.

Then in Section 3.4 we compute the shape derivative of the shape functional by means of the *velocity method*. In Section 3.4.1 we introduce this method. Then we apply it to the FSI problem in Sections 3.4.2 and 3.4.3, in order to compute the boundary value problems of the material derivatives of the FSI solution in Section 3.4.4, and the shape derivative of the shape functional in Section 3.4.5.

Finally, we simplify the shape derivative of the functional with an adjoint method, also called *Céa's method*.

Chapter 1

Sensitivity of the second order homogenized elasticity tensor to topological microstructural changes

1.1 Introduction

The study of synthesis and design of materials involving multiscale effects gave rise to a wide interest in Engineering, Mechanics, and Mathematics during the two past decades, and it broadened the application scope, among others structural mechanics, biomechanics, aerospace engineering, wave propagation in solids, and acoustics. The research works on this subject have increased with the emergence of recent experimental and manufacturing techniques, computational methods and tools, and theoretical developments. The various length scales of this type of materials allow the elaboration of multiscale constitutive theories, the so-called *theory of homogenization*, in order to explain, more accurately than standard phenomenological approaches, their macroscopic response under loading for example. The first developments has been made for periodic structures [BLP11; GNS83; HS63; Hil65; MMS99; MSS99; San80; Suq87], and since then the framework has not stop expanding to fit more general and complex models. We propose in Section 1.2 a short introduction to homogenization theory.

In this context, the design of the microstructure is a major issue for a mixture of different materials, and also for a material perforated with void areas. For example, in [Alm85] and [Lak87] microstructural topologies that produce negative macroscopic Poisson's ratio are obtained with a relaxation-based technique. A material having a negative Poisson's ratio, called *auxetic*, is a material that unfolds in the direction transverse to the loading direction.

Most of the works in the literature devoted to microstructures exhibiting such unusual behaviors have been found recoursing to a rather heuristic approach, underlining the need for a more systematic methodoloy for their design. To find out new microstructures producing these kinds of non classical behaviours at the macroscopic scale, different methods have been developed in the last two decades; we can cite the use of classical shape optimization method (see e.g., [HP06; SZ92]), based on shape gradient of the desired criterion, with respect to a smooth variation of the boundary. This approach depends deeply on the initial guess for the microstructure, because it does not allow for topology changes. More recently, the combination of shape gradient concept and level-set method (investigated in [OS88]), has produced interesting results in structural optimization; the reader can see for instance [AJ05; AJT04; Bur03; OS01; SW00; WWG03]. Relaxed formulations based on homogenization theory have been developed in [All02; AK93; All+97a; BK88], and provide topology variations in certain cases. In Section 2.1, the different methods of structure optimization are presented in more details.

Another strategy is based on the concept of *topological derivative*, which was rigorously introduced in [SŻ99]. The idea is to produce a new microstructure which is the result of an optimization problem. For improving a selected optimization criterion yielding such a microstructure, the strategy adopted is to compute a topological asymptotic expansion of this criterion with respect to an infinitesimal topological perturbation of the domain. The reader may find the use of this concept in topology optimization in [AJT04; AA06; BHR04]. In the framework of the development of homogenized models of elastic materials, the topological derivative of the first order homogenized elasticity tensor has been calculated in [GNS10; Giu+09a] in the case of void and soft inclusion, respectively, and in [Ams+10] in the case of a soft material inclusion, completed with a numerical investigation. More recently the topological derivative of the second-order macroscopic model associated with scalar waves in periodic media has been evaluated in [BCG18], making use of integral equations together with the periodic Green's function.

Our goal is to produce new microstructures which aim to optimize the macroscopic properties of a material, with the use of a topological optimization procedure relying on the higher order homogenized tensors of this material. In the present chapter, the elasticity system in plane stress in two-dimensional periodic media is considered, so that the microstructure we aim to optimize is the periodic unit cell constituting this material. Concretely, we want to investigate the following kind of problems:

$$\min_{\mathcal{Y}} \left\{ \mathcal{J}(\boldsymbol{\mathcal{H}}_{\mathcal{Y}}) \right\}, \tag{1.1}$$

where $\mathcal{Y}$ is the periodic unit cell of the material, and $\mathcal{J}$ is a functional depending of a higher order homogenized tensor $\boldsymbol{\mathcal{H}}_{\mathcal{Y}}$, itself depending on the unit cell $\mathcal{Y}$. In this chapter we give no clue concerning the nature of $\mathcal{J}$, which we consider as an abstract smooth functional. We will explicit it in Chapter 2.

For tackling this topological optimization problem, we compute the topological derivatives of its higher order homogenized tensors. These topological derivatives measure how the homogenized tensors change when a small circular inclusion is introduced at the microscale level. This information is crucial for the synthesis and optimal design of microsctructures having a macroscopic behaviour depending on higher order derivatives of the average displacement.

This chapter is organized as follows. We start, after an introduction to the theory of homogenization, by describing in Section 1.2.1 a homogenization scheme in the framework of periodic media (see [SC00]). We consider a material which is paved with a periodic *unit cell*, itself being weighted by a size ratio τ meant to vanish. Namely we have a periodic material for which the domain is of finite size, with a periodic unit cell of decreasing size. We use the *asymptotic expansion method* in order to compute an asymptotic expansion of the macroscopic energy of the material $\mathscr{E}^h$ with respect to the parameter τ. For this we need to compute in Section 1.2.2 the solutions of auxiliary problems posed on the unit cell, called *correctors*. Next, different truncations in the asymptotic expansion of the energy lead to the formal definition of so-called *higher-order homogenized tensors*. These homogenized tensors are defined in Sections 1.2.3 and 1.2.4, and are constructed with the help of so-called correctors. In order to produce microstructure improving certain macroscopic behaviours in Chapter 2, we choose to optimize functional depending on these homogenized tensors, through a topological optimization procedure. For this purpose we need to compute the topological derivatives of these homogenized tensors.

We undertake in Section 1.3 a perturbation of the unit cell. After an introduction to the *topological derivative* concept through Section 1.3.1, we define what is the topological perturbation we perform in Section 1.3.2. The microstructure of the underlying material is topologically perturbed by the nucleation of a small circular inclusion endowed with different material properties from the background material. We give the estimations of the perturbed correctors, that is the solutions of the auxiliary problems defined on the unit cell we have topologically perturbed. Together with these estimations, an *adjoint method* is need for the computation of the topological derivatives. We present this method in Section 1.3.3. We recall in Section 1.3.4 the formula of the topological asymptotic of the classical first-order homogenized tensor derived in [Ams+10; GNS10; Giu+09a], and we calculate the topological derivative associated with a simple higher-order homogenized tensor for introducing the method. In Section 1.3.5 we finally derive in details the topological derivative of the second-order homogenized tensor.

The chapter ends with some concluding remarks in Section 1.4. The proofs of certain lemmas are moved to Appendix 1.5.

This work and its context was initiated by Arthur Lebée[1] and Jan Sokołowski[2]. Then I worked in a close collaboration with Antonio André Novotny[3], with the help and the advices of my supervisors Jean-François Scheid and Jean-François Ganghoffer. This resulted in the publication of an article in the Journal of Elasticity [Cal+21].

1.2 Homogenization

Many problems coming from the Physics, or other fields, which are modeled by partial differential equations involving specific quantities together with boundary or limit conditions, come across different intrinsic scales. For example we can imagine a medium with a characteristic length, in which waves with far longer wave-length propagate. Another situation is that of a plate constituted of a multitude of small unit cells. In such problems we can see emerging scale effects, resulting directly from the multi-scale character of the problem. We at least distinguish two different scale, the microscopic and the macroscopic one, although we could imagine more than two length-scales being involved (see Figure 5).

Generally speaking, *homogenization theory* consists in the study of the macroscopic behaviour of a system which possesses microscopic heterogeneities. Thus the idea is somehow to average a heterogeneous medium, characterized by microscopic properties, in order to replace it with a homogeneous medium, being in some sense a good approximation of the original one, and from which derive so-called *homogenized*, or *effective* (or even *macroscopic*) properties. For example we can imagine heterogeneous media for which we calculate effective thermal or electrical conductivity. Even if this theory was notably first developed in mechanics, the term *homogenization* comes most likely from nuclear engineering and the study of neutron transport in networks, and the definition

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of the diffusion coefficient of a network by representing it with an homogeneous medium with the same averaged characteristics [Ben64].

To illustrate this introduction, we consider a diffusion type boundary value problem posed on a fixed domain D, with a source term f, and homogeneous Dirichlet condition. This domain as a whole represents the macroscopic scale. And we consider a problem characterised by the parameter τ representing the ratio of a microscopic characteristic size of heterogeneities to a macroscopic dimension (see Figure 5). This is expressed by a diffusion matrix A^τ depending on this parameter. For example the matrix A^τ fluctuates rapidly from a wave length of τ. The solution of the problem is a scalar field denoted by u_τ, satisfying the following problem.

$$\begin{cases} -\operatorname{div}(A^\tau \nabla u_\tau) = f & \text{in D}, \\ u_\tau = 0 & \text{on } \partial\mathrm{D}. \end{cases} \tag{1.2}$$

The idea of homogenization is to replace the problem (1.2) by an approximated homogeneous problem:

$$\begin{cases} -\operatorname{div}(A^* \nabla u) = f & \text{in D}, \\ u = 0 & \text{on } \partial\mathrm{D}, \end{cases} \tag{1.3}$$

homogeneous in the sense that A^* is constant or it varies slowly.

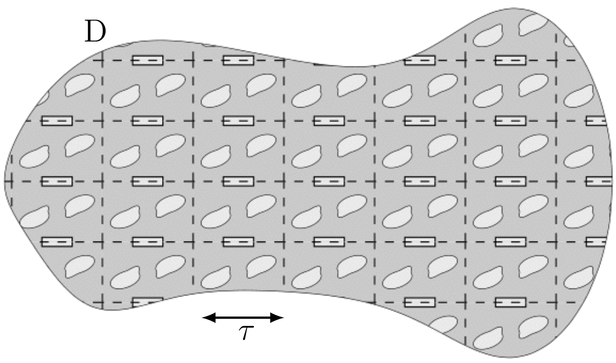

Figure 5: The domain D constituted with a microstructure of microscopic characteristic size τ.

There are different ways of thinking homogenization. From the physical, or mechanical point of view, the idea is to identify a length-scale on which we compute the average of the true microscopic fields. We deduce from these averaged quantities the definition of the homogenized (or effective) properties. This is often called the Representative Volume Element (RVE) method. For our example problem, it stands for the averaging of the gradient field ∇u_τ on the RVE, denoted by ξ, and the averaging of the flux $A^\tau \nabla u_\tau$, denoted by σ. Then the effective diffusion matrix A^* is deduced from the constitutive relation $\sigma = A^*\xi$. This method is quite efficient to have the intuition of an effective model, but is not always justified from a mathematical point of view. Anyway, we use it in the following section for the definition of the homogenized tensors.

From the mathematical point view, which is quite new in comparison to the physical one, the method is different. The homogeneous model is defined as the limit of a sequence of heterogeneous problems depending on a scale parameters $(\tau_n)_{n\geq 0}$ going to zero. The homogenized or effective properties are defined as the resulting properties of this limit problem. Those are the questions arising from this homogenization method by means of analysis of sequences of boundary value problems:

- Does u_{τ_n} converge to some limit u?
- Is actually u the solution of some limit boundary value problem?
- Is u a good approximation of u_{τ_n}?

One can find the first developments towards answering these scientific questions in the concept of *G-convergence*, developed in [Spa67], [Spa68]. It deals with the convergence of symmetric matrices A^τ for a elliptic Dirichlet problem, through the convergence of Green kernel. One can as well attribute the first developments of the theory of homogenization for the mathematical study of periodic structures to the earlier works [Sán70], [Sán71], and also to [Bab76], where the term homogenization was used for the first time in a mathematical context. Then the concept of G-convergence was generalized to *H-convergence* in [Mur77; MT97], [Tar75], giving a framework for a general theory of homogenization. Since then other theories and methods was developed. For example the *two-scale convergence method*, introduced in [Ngu89], and developed in [All92]. We can also mention the Γ-convergence ([De 84], [Dal93]), which constitutes a variational theory of homogenization, used for studying minimization problems and convergence properties of functionals. Finally, we can also cite stochastic or probabilistic theory of homogenization ([GP83; Koz79; PV81]).

For other general references to homogenization we refer to [San80; BP89] for linearized elasticity, [BLP11; San80] for heat equation, [BLP11] for wave equation. Introductions to homogenization and related mathematical framework can be found in [CD99], [Tar09] or [All02; All07; All12].

In the following, we present the formal homogenization framework introduced in [SC00], which allows to define higher order homogenized tensors in the context of periodic homogenization. In this presentation, τ represent a size ratio between the size of the macroscopic material, and the size of the microscopic periodic cell. In light of what we have introduced before, the higher order tensors act as corrective terms in the approximation of the flux $A^\tau \nabla u_\tau$ by $A^*\xi$, or equivalently of the approximation of the energy $(A^\tau \nabla u_\tau)\cdot \nabla u_\tau$ by $(A^*\xi)\cdot\xi$.

The asymptotic expansion method is used to derive an asymptotic expansion of the macroscopic energy $\mathscr{E}^h$ of the material with respect to the parameter τ. The energy $\mathscr{E}^h$ is actually the average on a cell of the microscopic energy. We give an overview of this procedure in Section 1.2.1, where the macroscopic energy is written in function of the solutions of auxiliary problems named correctors. Then we describe in Section 1.2.2 how the auxiliary problems are obtained. We finally show in Sections 1.2.3 and 1.2.4 how the homogenized tensors are defined from the truncation of the asymptotic expansion of the macroscopic energy.

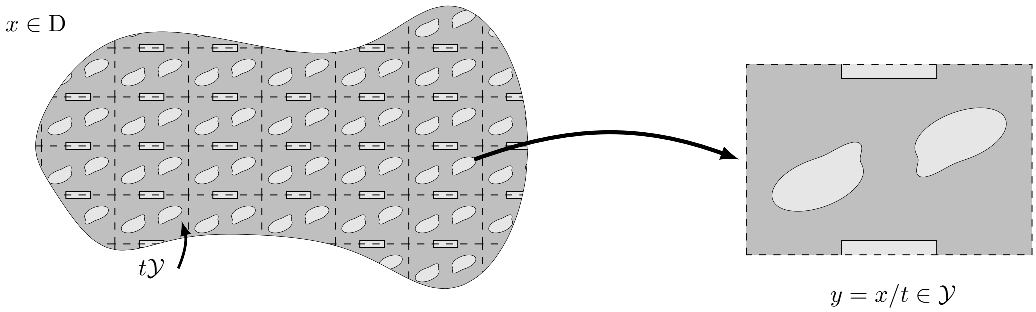

Figure 6: The domain D is paved with the unit cell domain $\mathcal{Y}$, weighted by the length parameter t. The unit cell is composed of two different materials, a light gray and a dark gray.

1.2.1 Smyshlyaev and Cherednichenko homogenization scheme

This section describes the multi-scale method used in [SC00] to identify the homogenized coefficients of an elasticity problem written for a periodic media, in order to calculate their topological sensitivities with respect to a configurational perturbation in the periodic cell.

Let D be a connected bounded regular open subset of $\mathbb{R}^2$ representing an elastic material having, as described bellow, a periodic micro-structure. Furthermore we assume that this material is a *Cauchy material*, completely characterized by its *elasticity tensor*, or *stiffness tensor*. In this manner the periodic structure of this material is in fact given by the periodicity of this elasticity tensor. We first define what periodicity means, and then what the elasticity tensor is. Let $\{\mathrm{e}_1, \mathrm{e}_2\}$ be an orthonormal basis of $\mathbb{R}^2$, and

$$\mathcal{Y} = (0, l_1) \times (0, l_2) \tag{1.4}$$

be an open rectangle of $\mathbb{R}^2$, for $0 < l_1, l_2$. The open set $\mathcal{Y}$ stands for the *unit cell* of the periodic material, and we define $\mathcal{Y}$-periodicity for a function as follows.

Definition 1.1. *Let f be a real-valued function defined a.e. on $\mathbb{R}^2$. We say that the function f is* $\mathcal{Y}$-periodic *iff for all $k \in \mathbb{Z}$, and for all i in $\{1, 2\}$,*

$$f(x + kl_i\mathrm{e}_i) = f(x), \qquad \textit{for a.e. } x \in \mathbb{R}^2. \tag{1.5}$$

Before defining the elasticity tensor, we rely on the convention used in classical tensor calculus (see also Appendix A). Let u and v be two vectors of $\mathbb{R}^2$, A and B be two second order tensors of $\mathbb{R}^2$, and $\mathbf{T}$ be a fourth order tensor of $\mathbb{R}^2$, we write:

$$\mathbf{T}A = \mathbf{T}_{ijkl}A_{kl}\,\mathrm{e}_i \otimes \mathrm{e}_j, \tag{1.6}$$
$$AB = A_{ik}B_{kj}\,\mathrm{e}_i \otimes \mathrm{e}_j, \tag{1.7}$$
$$A \cdot B = A_{ij}B_{ij}, \tag{1.8}$$
$$Au = A_{ij}u_j\,\mathrm{e}_i, \tag{1.9}$$
$$u \cdot v = u_i v_i, \tag{1.10}$$

by using the Einstein summation convention, and where $\mathrm{e}_i \otimes \mathrm{e}_j$ is a matrix such that $(\mathrm{e}_i \otimes \mathrm{e}_j)_{kl} = \delta_{ik}\delta_{jl}$. Now we can define the elasticity tensor characterizing the material

D. For this, we need to defined first the elasticity tensor characterizing the unit cell $\mathcal{Y}$. We consider that the elasticity tensor of the unit cell is given by a fourth order tensor $\mathbf{C} = (\mathbf{C}_{ijkl})_{1\leq i,j,k,l\leq 2}$, such that for all indices $i, j, k, l = 1, 2$ we have:

(i) $\mathbf{C}_{ijkl} \in L^\infty(\mathbb{R}^2)$, and is $\mathcal{Y}$-periodic,

(ii) the following major and minor index symmetries hold:

$$\mathbf{C}_{ijkl} = \mathbf{C}_{jikl} = \mathbf{C}_{klij}, \tag{1.11}$$

(iii) $\mathbf{C}$ is uniformly continuous, that is there exists a real numbers $0 < b$ such that for any second order tensor A:

$$|\mathbf{C}A| \leq b|A|, \tag{1.12}$$

where $|\cdot|$ denotes the following norm for second order tensors:

$$|A|^2 = A_{ij}A_{ij}, \tag{1.13}$$

and $\mathbf{C}$ is uniformly coercive, that is there exists a constant $0 < a$ such that for any symmetric second order tensor A:

$$a|A|^2 \leq \mathbf{C}A \cdot A. \tag{1.14}$$

Let $0 < t$ be a microscopic length parameter describing the length-scale of the microscopic variations of the elasticity tensor and let $0 < T$ be a macroscopic length parameter which can be for example defined by $T = \operatorname{diam}(\mathrm{D})$ (see Figure 6). We denote by τ the ratio

$$\tau = t/T. \tag{1.15}$$

We have assumed that the medium is macroscopically homogeneous, so that the tensor $\mathbf{C}^\tau$ of microscopic moduli does not depend on the macroscale position, but only on the microscale variable. Thus we define the elasticity tensor of the periodic material D, depending on the parameter τ as follows:

$$\mathbf{C}^\tau(x) := \mathbf{C}(x/t). \tag{1.16}$$

This definition can be illustrated as follows. The periodic medium we are interested in, consists of the domain D, which is paved with the *microscopic periodic cell* $t\mathcal{Y}$ (see Figure 6).

We consider for this material a pure displacement problem in plane stress: this material is subjected to *volume forces*, also called *loads*, $f \in L^2(\mathrm{D})$, and the *displacement field* $u^\tau : \mathrm{D} \to \mathbb{R}^2$, which is the unknown of the problem, is fixed on the boundary $\partial\mathrm{D}$ being equal to a Dirichlet data $u_D \in H^{1/2}(\partial\mathrm{D})$. The displacement vector field u^τ is then given by the solution of the following boundary value problem of linearized elasticity

$$\begin{cases} -\operatorname{div}_x(\sigma_x^\tau(u^\tau)) = f & \text{in D}, \\ u^\tau = u_D & \text{on } \partial\mathrm{D}, \end{cases} \tag{1.17}$$

where the second order tensor field $\sigma_x^\tau(u^\tau)$, called the total *stress tensor*, is specified throughout the following constitutive law (1.18), also called the stress-strain relation in the linear regime. Namely $\sigma_x^\tau(u^\tau)$ depends linearly on the total *linearized strain tensor* $e_x(u^\tau)$, defined as the symmetrized first gradient of the displacement:

$$\sigma_x^\tau(u^\tau) := \mathbf{C}^\tau e_x(u^\tau), \tag{1.18}$$

$$e_x(u^\tau) := \nabla_x^s u^\tau := \frac{1}{2}\left(\nabla_x(u^\tau) + \nabla_x(u^\tau)^\top\right), \tag{1.19}$$

where the right lower index of a differential operator denotes the differentiation variable. It is well know that for all $0 < \tau$, the boundary value problem (1.17)-(1.18)-(1.19) has a unique solution u^τ in the Sobolev space $H^1(\mathrm{D})$ (see e.g., [Cia88] Section 6.3). For having a good numerical approximation of u^τ, it is usual to make use of Finite Element Method (FEM) to solve (1.17) in discretized spaces. But when τ turns to be really small, and this is the case we are interested in, then the size of the elements of the FEM has to be small enough to take into account the microscopic variations of $\mathbf{C}^\tau$ – namely we need at least several elements inside each microscopic cells $t\mathcal{Y}$. Such a fine discretization could be computationally heavy for small τ. Thus we want to find a *homogenized model*, or *effective model*, which does not depend on the microscopic oscillations of the true model. For this we apply the *multiple-scale method* (see e.g., [CD99] Chapter 7).

We define

$$y = x/t \quad \text{and} \quad Y = x/T, \tag{1.20}$$

respectively the normalized micro and macro variables, for all $x \in \mathrm{D}$ (see Figure 6). Let the vector field $u^\tau(x) \in \mathbb{R}^2$ be the displacement, solution of the elasticity system (1.17)-(1.18)-(1.19) in D. We assume that u^τ can be expanded as

$$u^\tau(x) = T\left[u_0\left(\frac{x}{T},\frac{x}{t}\right) + \tau u_1\left(\frac{x}{T},\frac{x}{t}\right) + \cdots + \tau^n u_n\left(\frac{x}{T},\frac{x}{t}\right) + \cdots\right], \tag{1.21}$$

where the functions $u_i(Y, y)$ are $\mathcal{Y}$-periodic with respect to the y-variable for all $i \geq 0$. Using this expansion in the equilibrium (1.17) and constitutive equations (1.18)-(1.19), we obtain a family of auxiliary problems, that we are going to explicit in the following section 1.2.2. The solutions of these auxiliary equations are a family of tensor fields $(H^{(i)}(y))_{i\geq 0}$ called *correctors*, each of these tensors being a tensor of order $i+2$. We can see in [SC00] that u^τ can be then asymptotically developed in function of terms depending on the one hand on these correctors fields, and on the other hand on a sequence of macroscopic vector fields $(U^{(i)}(Y))_{i\geq 0}$ assumed to be constant within a cell. For $0 \leq i$ and $1 \leq j$ fixed, and for a given macroscopic vector field $U^{(i)}(Y)$, the corrector $H^{(j)}(y)$ of order $j+2$ acts on the tensor $\nabla^{j-1}\nabla_Y^s U^{(i)}(Y)$ of order $j+1$ to give a vector field as follows:

$$(H^{(j)}(y)\nabla^{j-1}\nabla_Y^s U^{(i)}(Y))_{p_1} = (H^{(j)}(y))_{p_1 p_2 \cdots p_{j+2}}(\nabla^{j-1}\nabla_Y^s U^{(i)}(Y))_{p_2\cdots_{+j+2}}. \tag{1.22}$$

This gives the following expansion for u^τ:

$$\begin{aligned} T^{-1}u^\tau(x) = {} & U^{(0)}(x/T) & (1.23)\\ & + \tau\left(U^{(1)}(x/T) + H^{(1)}(x/t)\nabla_Y^s U^{(0)}(x/T)\right) \\ & + \tau^2\left(U^{(2)}(x/T) + H^{(1)}(x/t)\nabla_Y^s U^{(1)}(x/T) + H^{(2)}(x/t)\nabla_Y\nabla_Y^s U^{(0)}(x/T)\right) \\ & + \tau^3\Big(U^{(3)}(x/T) + H^{(1)}(x/t)\nabla_Y^s U^{(2)}(x/T) + H^{(2)}(x/t)\nabla_Y\nabla_Y^s U^{(1)}(x/T) \\ & \qquad + H^{(3)}(x/t)\nabla_Y^2\nabla_Y^s U^{(0)}(x/T)\Big) + \cdots . & (1.24) \end{aligned}$$

By writing formally

$$U(Y) = \sum_{i=0}^{\infty} \tau^i U^{(i)}(Y), \tag{1.25}$$

the above expansion suggests to seek approximations of u^τ in the form of truncations with respect to different orders of τ of the following form

$$T^{-1}u^\tau(x) = U(x/T) + \tau H^{(1)}(x/t)\nabla_Y^s U(x/T) + \cdots + \tau^k H^{(k)}(x/t)\nabla^{k-1}\nabla_Y^s U(x/T), \quad \text{for } k \geq 0. \tag{1.26}$$

Therefore, we seek the total field u^τ as the sum of a macroscopic displacement field U and its i-th derivative weighted by τ^i and a corrector field, for $1 \leq i \leq k$.

From this, we define the macroscopic energy $\mathscr{E}^h$ as being the average of the microscopic elastic energy $\mathscr{E}_\mu$ on the unit cell domain $\mathcal{Y}$, where $\mathscr{E}_\mu$ is defined by

$$\mathscr{E}_\mu = \frac{1}{2}\sigma_x(u^\tau) \cdot e_x(u^\tau), \tag{1.27}$$

so that

$$\mathscr{E}^h = \frac{1}{V}\int_{\mathcal{Y}} \frac{1}{2}\sigma_x(u^\tau) \cdot e_x(u^\tau)\, dy, \tag{1.28}$$

where $V = |\mathcal{Y}|$ denotes the area of the unit cell, $|\mathcal{Y}|$ being the Lebesgue measure of $\mathcal{Y}$. Calculating the macroscopic energy induced by truncation (1.26), we obtain such a development with respect to τ

$$\mathscr{E}^h = \mathscr{E}_0 + \tau\mathscr{E}_1 + \tau^2\mathscr{E}_2 + \cdots + \tau^k\mathscr{E}_k, \tag{1.29}$$

where $\mathscr{E}_i$ does not depend on τ, for $0 \leq i \leq k$.

In Section 1.2.3 and 1.2.4, we are going to show how to compute the successive terms of the energy expansion (1.29) for $k = 1$ and $k = 2$, and how we can identify the homogenized tensors from this expression. Before we recall in the next paragraph how to obtain formally the auxiliary equations and the corrector fields in the framework of the multi-scale method (see e.g., [CD99; SC00; For06; JS20]).

1.2.2 Auxiliary equations

Let us write the auxiliary problems in their strong formulations. We have that for any $\alpha = 1, 2$, the total derivative with respect to the x variable in the direction e_i is given by the following double scale derivative formula:

$$\partial_{x_\alpha} = \frac{1}{T}\left(\partial_{Y_\alpha} + \frac{1}{\tau}\partial_{y_\alpha}\right). \tag{1.30}$$

From now on, we set $T = 1$ for convenience. In view of *Ansatz* (1.21), we can formally write

$$e_x(u^\tau) = \tau^{-1}\nabla_y^s u_0 + \sum_{i=0}^{\infty} \tau^i e^{(i)}, \tag{1.31}$$

where

$$e^{(i)} := \nabla_Y^s u_i + \nabla_y^s u_{i+1}. \tag{1.32}$$

Let us define in the same way

$$\sigma^{(i)} := \mathbf{C}e^{(i)}. \tag{1.33}$$

Introducing expansion (1.21) of u^τ in the equilibrium equation (1.17), we obtain a sequence of equations at the successive order of τ:

$$\begin{aligned}
&\nabla_y^s u_0 = 0, && && \text{(a)}\\
&\operatorname{div}_y(\sigma^{(0)}) = 0, && && \text{(b)}\\
&\operatorname{div}_y(\sigma^{(1)}) + \operatorname{div}_Y(\sigma^{(0)}) + f = 0, && && \text{(c)}\\
&\operatorname{div}_y(\sigma^{(i+1)}) + \operatorname{div}_Y(\sigma^{(i)}) = 0, && \text{for } i \geq 1, && \text{(d)}
\end{aligned} \tag{1.34}$$

where (a), (b) and (c) are respectively the equations of order τ^{-2}, τ^{-1} and τ^0, and (d) stands for equations of order τ^i, for all $i \geq 1$. Each of these equations is written on a unit cell $\mathcal{Y}$, with the $\mathcal{Y}$-periodicity of u_i as boundary condition. The corresponding boundary value problems, also named auxiliary problems, can be solved by induction. In the sequel, we just solve the three first auxiliary equations (a), (b), and (c) in (1.34), because we only need the correctors deriving for these equations for the expression of the truncation (1.26) for $k = 1, 2$.

1. The first equation (1.34(a)) determines that the displacement $u_0(Y, y)$ does not depend on the microscopic variable y. From now on we will write

$$u_0(Y, y) = U^{(0)}(Y). \tag{1.35}$$

2. Let us rewrite the second equation (1.34(b)), reminding that $\sigma^{(0)}$ is given by (1.33), and setting

$$E^{(0)} := \nabla_Y^s U^{(0)}, \tag{1.36}$$

we find

$$\operatorname{div}_y\left(\mathbf{C}\nabla_y^s u_1 + \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j)E_{ij}^{(0)}\right) = 0, \tag{1.37}$$

where we recall that $E^{(0)}$ can be written as

$$E^{(0)} = E_{ij}^{(0)}(\mathrm{e}_i \otimes_s \mathrm{e}_j), \tag{1.38}$$

with

$$a \otimes_s b := \frac{a \otimes b + b \otimes a}{2}, \tag{1.39}$$

for all vectors $a, b \in \mathbb{R}^2$. By linearity of the problem (1.37) we can write

$$u_1(Y, y) = U^{(1)}(Y) + \tilde{u}_{ij}(y)E_{ij}^{(0)}(Y), \tag{1.40}$$

where the vector field $\tilde{u}_{ij}$, called the *first order corrector*, is the solution of the $\mathcal{Y}$-periodic boundary value problem posed on the unit cell $\mathcal{Y}$ for the first auxiliary equation:

$$\operatorname{div}_y\left(\mathbf{C}\nabla_y^s \tilde{u}_{ij} + \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j)\right) = 0. \tag{1.41}$$

We choose this notation for the first order corrector for the sake of readability of the calculations we are going to lead in Section 1.3. For a comparison with the generic notation we have introduced in the previous Section, recalling that $\tilde{u}_{ij}$ is a vector field and $H^{(1)}$ is a 3 order tensor, we have

$$(\tilde{u}_{ij}(y))_k = (H^{(1)}(y))_{ijk}. \tag{1.42}$$

3. Before solving the third auxiliary problem, let us evaluate the average on the unit cell of equation (1.34(c)). We assume that $f = T^{-1}F(Y)$. This gives us that:

$$\mathrm{div}_Y(\langle \sigma^{(0)} \rangle) + F = 0, \tag{1.43}$$

where for all tensor fields A, we define the *volume averaging* of A

$$\langle A \rangle := \frac{1}{V} \int_{\mathcal{Y}} A(y)dy, \tag{1.44}$$

where $V = |\mathcal{Y}|$ denotes the area of the unit cell. From (1.32) and (1.33), we have

$$\langle \sigma^{(0)} \rangle = \langle \mathbf{C} \nabla^s_Y u_0 \rangle + \langle \mathbf{C} \nabla^s_y u_1 \rangle. \tag{1.45}$$

We have that $E^{(0)} = \nabla^s_Y u_0$ where $u_0 = U^{(0)}$ depends only on the macroscopic variable, thus from equation (1.38) we have $\langle \mathbf{C} \nabla^s_Y u_0 \rangle = \langle \mathbf{C} \mathrm{e}_i \otimes \mathrm{e}_j \rangle E^{(0)}_{ij}$. By definition of u_1 given in (1.40), we have $\langle \mathbf{C} \nabla^s_y u_1 \rangle = \langle \mathbf{C} \nabla^s_y \tilde{u}_{ij} \rangle E^{(0)}_{ij}$. Finally, by defining the following the vector field

$$u_{ij}(y) := (\mathrm{e}_i \otimes_s \mathrm{e}_j)y + \tilde{u}_{ij}(y), \tag{1.46}$$

we can relate the average stress to the average strain through the relation

$$\langle \sigma^{(0)} \rangle = \langle \mathbf{C} \nabla^s_y u_{ij} \rangle E^{(0)}_{ij}. \tag{1.47}$$

Now let us rewrite the equation (1.34(c)) setting

$$E^{(1)} := \nabla^s_Y U^{(1)}, \quad \text{and} \quad K^{(0)} := \nabla_Y E^{(0)}, \tag{1.48}$$

and taking into account (1.43). We find

$$\mathrm{div}_y \left(\mathbf{C} \nabla^s_y u_2 \right) + \mathrm{div}_y(\mathbf{C} E^{(1)}) + [\mathrm{div}_y(\mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)) + (\mathbf{C} \nabla^s_y u_{ij} - \langle \mathbf{C} \nabla^s_y u_{ij} \rangle)\mathrm{e}_k] K^{(0)}_{ijk} = 0. \tag{1.49}$$

Once again by linearity we can write the solution u_2 in the following way

$$u_2(Y, y) = U^2(Y) + \tilde{u}_{ij}(y) E^{(1)}_{ij}(Y) + \tilde{\tilde{u}}_{ijk}(y) K^{(0)}_{ijk}(Y), \tag{1.50}$$

where the vector field $\tilde{\tilde{u}}_{ijk}$, called the *second order corrector*, is the solution of the $\mathcal{Y}$-periodic boundary value problem on the unit cell $\mathcal{Y}$ for the second auxiliary equation:

$$\mathrm{div}_y \left(\mathbf{C} \nabla^s_y \tilde{\tilde{u}}_{ijk} \right) + \mathrm{div}_y \left(\mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \right) + (\mathbf{C} \nabla^s_y u_{ij} - \langle \mathbf{C} \nabla^s_y u_{ij} \rangle)\mathrm{e}_k = 0. \tag{1.51}$$

As before, we notice that we have the following connexion with the previous notation

$$(\tilde{\tilde{u}}_{ijk}(y))_l = (H^{(2)}(y))_{ijkl}. \tag{1.52}$$

Now since we have calculated the first and second order correctors, we can compute the macroscopic energy. We consider for this a truncation (1.26) of the displacement u^τ for $k = 1$. This is done in the next section.

1.2.3 First-order truncation

We recall that $Y = x/T$, $y = x/t$ and $\tau = t/T$, with $x \in \mathbb{R}^2$, and we set $T = 1$. Motivated by expansion (1.26), we introduce the macroscopic displacement field $U(Y) \in \mathbb{R}^2$, and the macroscopic deformation is defined as

$$E(Y) = \nabla^s U(Y). \tag{1.53}$$

We write $\tilde{u}(Y, y) = \tilde{u}_{ij}(y) E_{ij}(Y)$, where

$$E_{ij}(Y) = E(Y) \cdot (\mathrm{e}_i \otimes_s \mathrm{e}_j). \tag{1.54}$$

Then introduce the expansion

$$u^\tau(Y, y) = U(Y) + \tau\, \tilde{u}(Y, y). \tag{1.55}$$

The displacement fields $\tilde{u}_{ij}$ are solutions of the following canonical set of variational problems

$$\tilde{u}_{ij} \in \mathcal{V} \ : \ \int_{\mathcal{Y}} \sigma_y(\tilde{u}_{ij}) \cdot e_y(\eta) + \int_{\mathcal{Y}} \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot e_y(\eta) = 0, \quad \forall \eta \in \mathcal{W}, \tag{1.56}$$

where $\sigma_y(\tilde{u}_{ij}) = \mathbf{C} e_y(\tilde{u}_{ij})$ and the spaces $\mathcal{W}$ and $\mathcal{V}$ are defined as follows

$$\mathcal{W} := H^1_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^2)/\mathbb{R}, \tag{1.57}$$

$$\mathcal{V} := \left\{ \eta \in H^1_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^2) \ \mid \langle \eta \rangle = 0 \right\}, \tag{1.58}$$

where $H^1_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^2)$ is the completion in $H^1(\mathcal{Y}; \mathbb{R}^2)$ of the space of functions in $C^\infty(\mathbb{R}^2, \mathbb{R}^2)$ which are $\mathcal{Y}$-periodic. From these elements, we have

$$e_x(u^\tau) = e_Y(u^\tau) + \frac{1}{\tau} e_y(u^\tau) = \left(e_y(u_{ij}) E_{ij} + \tau (\tilde{u}_{ij} \otimes_s \nabla_Y E_{ij}) \right), \tag{1.59}$$

where

$$u_{ij} := (\mathrm{e}_i \otimes_s \mathrm{e}_j) y + \tilde{u}_{ij}, \tag{1.60}$$

with $\tilde{u}_{ij}$ solutions to the set of canonical variational problems (1.56).

Then we calculate the macroscopic energy $\mathscr{E}^h$, being the average of the microscopic elastic energy $\frac{1}{2}\sigma_x(u^\tau) \cdot e_x(u^\tau)$ on the unit cell domain $\mathcal{Y}$, in order to identify the homogenized elasticity tensors. We find using (1.59) with (1.28):

$$\begin{aligned} \mathscr{E}^h &= \frac{1}{2V} \int_{\mathcal{Y}} \sigma_x(u^\tau) \cdot e_x(u^\tau) \\ &= \frac{1}{2V} \int_{\mathcal{Y}} \{ E_{kl} \sigma_y(u_{kl}) \cdot e_y(u_{ij}) E_{ij} \\ &\qquad + \tau \left(E_{kl} \sigma_y(u_{kl}) \cdot (\tilde{u}_{ij} \otimes_s \nabla_Y E_{ij}) + E_{ij} \sigma_y(u_{ij}) \cdot (\tilde{u}_{kl} \otimes_s \nabla_Y E_{kl}) \right) \\ &\qquad + \tau^2 \left(\tilde{u}_{ij} \otimes_s \nabla_Y E_{ij} \right) \cdot \mathbf{C} (\tilde{u}_{kl} \otimes_s \nabla_Y E_{kl}) \} . \end{aligned} \tag{1.61}$$

We set

$$K(Y) := \nabla E(Y) \tag{1.62}$$

which can be written in the canonical basis of third order tensors $K(Y) = K_{ijk}(Y)\mathrm{e}_i \otimes \mathrm{e}_j \otimes \mathrm{e}_k$. Thus we obtain

$$\mathscr{E}^h = \mathscr{E}^h(E, K) = \frac{1}{2}E_{ij}\mathbf{C}^h_{ijkl}E_{kl} + \tau\frac{1}{2}E_{ij}\mathbf{E}^\sharp_{ijpqr}K_{pqr} + \tau^2\frac{1}{2}K_{ijk}\mathbf{D}^\sharp_{ijkpqr}K_{pqr} + o(\tau^2), \quad (1.63)$$

which defines the three following homogenized elasticity tensors: the fourth order tensor $\mathbf{C}^h = (\mathbf{C}^h_{ijkl})_{1\leq i,j,k,l\leq 2}$, the fifth order tensor $\mathbf{E}^\sharp = (\mathbf{E}^\sharp_{ijpqr})_{1\leq i,j,p,q,r\leq 2}$, and the sixth-order tensor $\mathbf{D}^\sharp = (\mathbf{D}^\sharp_{ijkpqr})_{1\leq i,j,k,p,q,r\leq 2}$, given by

$$\mathbf{C}^h_{ijkl} := \frac{1}{V}\int_{\mathcal{Y}} \sigma_y(u_{ij}) \cdot e_y(u_{kl}), \quad (1.64)$$

$$\mathbf{E}^\sharp_{ijpqr} := \frac{2}{V}\int_{\mathcal{Y}} \sigma(u_{ij}) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r), \quad (1.65)$$

and

$$\mathbf{D}^\sharp_{ijkpqr} := \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r). \quad (1.66)$$

The macroscopic energy density (1.63) corresponds well to a strain gradient model. However the terms of order τ and τ^2 in the expression (1.63) of the macroscopic energy $\mathscr{E}^h$ are not complete. The higher-order tensors $\mathbf{E}^\sharp$ and $\mathbf{D}^\sharp$ do not contain all contributions from the order τ and τ^2 provided by the full asymptotic expansion of u^τ (1.21). It is shown in [SC00] and [Dur+20] that these tensors cannot be used as a correct estimate of strain gradient effects. For encapsulating all the contributions of order τ and τ^2, we nee to go further in the truncation of the displacement (1.26) and consider the second order truncation, for $k = 2$.

1.2.4 Second-order truncation

We introduce the expansion up to the second order of the small-scale parameter:

$$u^\tau(Y, y) = U(Y) + \tau\,\tilde{u}(Y, y) + \tau^2\,\tilde{\tilde{u}}(Y, y), \quad (1.67)$$

where $\tilde{\tilde{u}}(Y, y) = \tilde{\tilde{u}}_{ijk}(y)K_{ijk}(Y)$, with $K_{ijk}(Y) = K(Y)\cdot(\mathrm{e}_i\otimes\mathrm{e}_j\otimes\mathrm{e}_k)$ and $K(Y) = \nabla E(Y)$. The displacement fields $\tilde{\tilde{u}}_{ijk}$ are solutions of the following canonical set of variational problems

$$\tilde{\tilde{u}}_{ijk} \in \mathcal{V} \;:\; \int_{\mathcal{Y}} \sigma_y(\tilde{\tilde{u}}_{ijk}) \cdot e_y(\eta) + \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot e_y(\eta) = \int_{\mathcal{Y}} (\sigma_y(u_{ij}) - \mathbf{C}^h(\mathrm{e}_i \otimes_s \mathrm{e}_j))\mathrm{e}_k \cdot \eta, \quad \forall \eta \in \mathcal{W}, \quad (1.68)$$

where $\mathcal{V}$ and $\mathcal{W}$ are defined in (1.58) and (1.57). Let us calculate the strain tensor induced by u^τ:

$$e_x(u^\tau) = e_y(u_{ij})E_{ij} + \tau(\tilde{u}_{ij} \otimes_s \mathrm{e}_k + e_y(\tilde{\tilde{u}}_{ijk}))K_{ijk} + \tau^2(\tilde{\tilde{u}}_{ijk} \otimes_s \mathrm{e}_l)\partial_{Y_l}K_{ijk}. \quad (1.69)$$

Same as before, we need to calculate $\frac{1}{2}\sigma_x(u^\tau) \cdot e_x(u^\tau)$ in order to evaluate the average of the elastic energy on the cell and then identify the macroscopic energy law. Performing a formal macroscopic integration by parts on D in order to transform the coupled terms $E_{ij}\partial_{y_k}K_{pqr}$ into $K_{ijk}K_{pqr}$ (see [SC00]), we calculate

$$\mathscr{E}^h = \frac{1}{2}E_{ij}\mathbf{C}^h_{ijkl}E_{kl} + \tau\frac{1}{2}E_{ij}\mathbf{E}^h_{ijpqr}K_{pqr} + \tau^2\frac{1}{2}K_{ijk}\mathbf{D}^h_{ijkpqr}K_{pqr} + o(\tau^2), \quad (1.70)$$

where $\mathbf{E}^h = (\mathbf{E}^h)_{1\le i,j,p,q,r\le 2}$ and $\mathbf{D}^h = (\mathbf{D}^h_{ijkpqr})_{1\le i,j,k,p,q,r\le 2}$ are the homogenized fifth and sixth-order tensor given in index format by

$$\mathbf{E}^h_{ijpqr} := \frac{2}{V}\int_{\mathcal{Y}} \sigma(u_{ij}) \cdot (e(\tilde{\tilde{u}}_{pqr}) + \tilde{u}_{pq} \otimes_s \mathrm{e}_r), \tag{1.71}$$

and

$$\mathbf{D}^h_{ijkpqr} := \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k + e_y(\tilde{\tilde{u}}_{ijk})) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r + e_y(\tilde{\tilde{u}}_{pqr})) \\ - \frac{1}{V}\int_{\mathcal{Y}} \left(\sigma_y(u_{ij}) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) + \sigma_y(u_{pq}) \cdot (\tilde{\tilde{u}}_{ijk} \otimes_s \mathrm{e}_r)\right). \tag{1.72}$$

By setting $\eta = \tilde{\tilde{u}}_{pqr}$ as test function in (1.68), we obtain the following equality

$$\int_{\mathcal{Y}} \sigma_y(\tilde{\tilde{u}}_{ijk}) \cdot e_y(\tilde{\tilde{u}}_{pqr}) + \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot e_y(\tilde{\tilde{u}}_{pqr}) = \int_{\mathcal{Y}} (\sigma_y(u_{ij}) - \mathbf{C}^h(\mathrm{e}_i \otimes_s \mathrm{e}_j))\mathrm{e}_k \cdot \tilde{\tilde{u}}_{pqr}, \tag{1.73}$$

which allows to write (1.72) as

$$\mathbf{D}^h_{ijkpqr} = \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k + e_y(\tilde{\tilde{u}}_{ijk})) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) \\ - \frac{1}{V}\int_{\mathcal{Y}} \left(\mathbf{C}^h(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) + \sigma_y(u_{pq}) \cdot (\tilde{\tilde{u}}_{ijk} \otimes_s \mathrm{e}_r)\right), \tag{1.74}$$

since $\sigma_y(u_{ij})\mathrm{e}_k \cdot \tilde{\tilde{u}}_{pqr} = \sigma_y(u_{ij}) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k)$. Finally we also define

$$\mathbf{F}^h_{ijkpqr} = \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k + e_y(\tilde{\tilde{u}}_{ijk})) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r + e_y(\tilde{\tilde{u}}_{pqr})), \tag{1.75}$$

which represents the second order homogenized tensor computed without the macroscopic integration by parts. We point out that $\mathbf{F}^h$ is positive definite contrary to $\mathbf{D}^h$.

Remark 1. *In the case of a centrosymmetric unit cell, the tensor $\mathbf{E}^h$ turns to be equal to zero (see e.g. [SC00]). In Chapter 2, we are going to investigate unit cell which are centrosymmetric. Thus in a first step we are not interested in the tensor $\mathbf{E}^h$. Nevertheless, its topological derivative could be interesting for a future study, that is why we compute it in Appendix B.*

So far, we have defined the homogenized tensors $\mathbf{C}^h$, $\mathbf{E}^\sharp$, $\mathbf{E}^h$ $\mathbf{D}^\sharp$, $\mathbf{F}^h$, and $\mathbf{D}^h$. As we explained in the introduction, we are interested in the optimization of the topology of the microstructure of a material, in our case the unit cell, in order to improve some of its macroscopic properties. For this purpose, we choose functionals based on the homogenized tensors as optimization criteria.

In the following section, we compute the topological derivatives of these tensors. We start by a presentation of the concept of topological derivative, then we define what is the perturbation of the unit cell that we undertake. Before exploring the behaviour of the homogenized tensors regarding the size of such a perturbation, that is to say before computing their topological derivatives, we present the adjoint method needed for these computations.

1.3 Topological Sensitivity

1.3.1 The topological derivative concept

We are interested in the behaviour of the homogenized tensors $\mathbf{C}^h$ and $\mathbf{D}^h$ with respect to the size of the topological perturbation of the unit cell of a periodic material. For this purpose, we will use the concept of *topological derivative*. It has been rigorously introduced in [SŻ99] in the context of heat conduction and elasticity problems. Developments of the theory have been led the past two decades in among others [Ams06; AN11; ANV14; BT10a; BT10b; Bon06; Bon09; BD13; Fei+03; GGM01; GB04; Khl+09; LS03; NS06; Nov13; NS16; SŻ03; SŻ05; Toa11]. Furthermore, the topological derivative was applied in many fields, such as topology optimization [AA06; AN10; Nov+07], inverse problems [CLN14; GB06; HLN12; Jac+02; MPS05], and image processing [AMB07; Bel+08; HL09]. Let us briefly introduce the topological derivative concept, while we refer to [NS13], [NSŻ19], and [NS20] for a complete introduction.

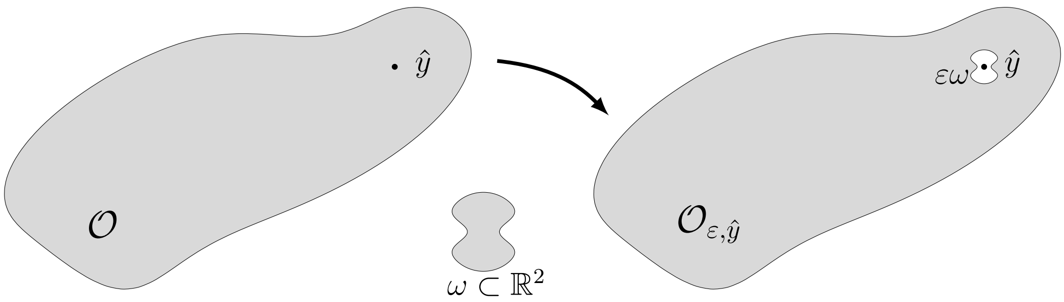

Figure 7: Nucleation of hole with the shape ω, with diameter ε, centered at $\hat{y}$.

Let $\mathcal{O}$ be a bounded subset of $\mathbb{R}^n$, and ω be a bounded simply connected open subset of $\mathbb{R}^n$, with $2 \leq n$, which contains the origin. We change the domain $\mathcal{O}$ by removing a small region

$$\omega_\varepsilon(\hat{y}) := \hat{y} + \varepsilon\omega, \tag{1.76}$$

for an arbitrary point $\hat{y} \in \mathcal{O}$ and $0 < \varepsilon$ small enough that $\omega_\varepsilon(\hat{y}) \subset\subset \mathcal{O}$. This gives rise to the definition of the topologically perturbed domain (see Figure 7)

$$\mathcal{O}_{\varepsilon,\hat{y}} := \mathcal{O} \setminus \overline{\omega_\varepsilon(\hat{y})}. \tag{1.77}$$

Now we consider a shape functional defined on a class of admissible domains $\mathcal{O} \in \mathcal{U}_{\text{ad}} \mapsto \mathcal{J}(\mathcal{O}) \in \mathbb{R}$. We are interested in the behaviour of the shape functional $\mathcal{J}(\mathcal{O})$ associated to the topologically perturbed domain $\mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}})$ in comparison with the shape functional associated to the unperturbed domain $\mathcal{J}(\mathcal{O})$, with respect to the location of the perturbation $\hat{y}$. Thus, for a given location of perturbation $\hat{y}$, we study the behaviour of the shape functional with respect to the size of the perturbation ε and we define – when it exists – the topological derivative field as being the *first order correction term* in the expansion of $\mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}})$ with respect to ε. This leads to the definition bellow.

Definition 1.2 ([NS13]). *Let $\mathcal{J}$ be a shape functional. We assume that the following* topological asymptotic expansion *holds true*

$$\mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}}) = \mathcal{J}(\mathcal{O}) + g(\varepsilon)\mathcal{D}_T\mathcal{J}(\hat{y}) + o(g(\varepsilon)), \tag{1.78}$$

where g is positive, is such that $g(\varepsilon) \to 0$ and $o(g(\varepsilon))/g(\varepsilon) \to 0$ with $\varepsilon \to 0$. Then the function

$$\hat{y} \in \mathcal{O} \longmapsto \mathcal{D}_T\mathcal{J}(\hat{y}) \tag{1.79}$$

is called the **geometric topological derivative** *of $\mathcal{J}$ at $\hat{y}$.*

We notice that this definition of the topological derivative implies that we consider a shape functional which is at least continuous with respect to the size of the perturbation: that is $\lim_{\varepsilon\to 0} \mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}}) = \mathcal{J}(\mathcal{O})$. Let us give a very simple example of calculation of topological derivative.

Example 2. (Area of a two-dimensional domain). *Let $\mathcal{J}(\mathcal{O})$ be the shape functional defined as the area of a domain $\mathcal{O}$ of $\mathbb{R}^2$:*

$$\mathcal{J}(\mathcal{O}) := |\mathcal{O}|, \tag{1.80}$$

where $|\mathcal{O}|$ is the Lebesgue measure of $\mathcal{O}$. By defining the topologically perturbed domain $\mathcal{O}_{\varepsilon,\hat{y}}$ as in (1.77)-(1.76)*, we have*

$$\mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}}) = \mathcal{J}(\mathcal{O}) - \varepsilon^2|\omega|, \tag{1.81}$$

where $|\omega|$ is the Lebesgue measure of ω. Indeed

$$|\omega_\varepsilon(\hat{y})| = |\omega_\varepsilon(0)| = \int_{\omega_\varepsilon(0)} 1\, dx = \int_\omega \varepsilon^2\, dx. \tag{1.82}$$

By setting $g(\varepsilon) = \varepsilon^2$ in (1.81)*, we obtain*

$$D_T\mathcal{J}(\hat{y}) = -|\omega|, \quad \forall \hat{y} \in \mathcal{O}. \tag{1.83}$$

In the case where the perturbation shape is the unit ball B_1, we have that the topological derivative is equal to $-\pi 1^2$. It appears that we face an arbitrary ingredient in the definition of the topological derivative. Indeed we have a choice regarding the positive constant we put in the definition of $g(\varepsilon)$. If we had chosen for example in the definition of the topological perturbation the unit domain 2ω instead of ω, for the same $g(\varepsilon) = \varepsilon^2$, then the topological derivative would have been equal to $-4|\omega|$ instead of $-|\omega|$. This underlines that the topological derivative is not a quantitative information by its own, and that we are mainly interested in its sign. But putting in $g(\varepsilon)$ the area of the unit shape, we obtain that for any perturbation shape, the topological derivative of $\mathcal{J}$ is -1. Thus even for more complex cases, we will normalize the first order function $g(\varepsilon)$ by the volume of the unit perturbation shape ω.

Furthermore the sign of the topological derivative indicates whether it is interesting or not regarding the considered criterion $\mathcal{J}$ to add a small hole into the material at the point $\hat{y}$. As we said in introduction, we are interested in a shape optimization problem of the microstructure of a periodic media, with the aim of improving a criterion $\mathcal{J}$ depending on the homogenized tensors we have just defined. To this end, we will calculate the topological derivative of the homogenized tensors in the next section.

Before this, we extend the definition of topological derivative to a more general framework. Indeed we gave above the definition in the case where the perturbation is a geometric perturbation of the domain $\mathcal{O}$. We made a small hole in $\mathcal{O}$ and thus changed its topology. But we can consider a more general case in which we do not directly perturb the domain, but we rather perturb a boundary value problem defined on $\mathcal{O}$. We name it a *configurational perturbation* [NS13]. This is quite interesting for the case of PDE constraint optimization, for which the shape function is defined by $\mathcal{J}(\mathcal{O}) = j(\mathcal{O}, u_{\mathcal{O}})$, where $u_{\mathcal{O}}$ is the solution of a boundary value problem defined on $\mathcal{O}$. We do not attempt to give a general definition of what a configurational perturbation is. We prefer to make it simple and clear, even if the following definition could be applied to other kind of problems and perturbations. Let f be a source term and $u_{\mathcal{O}}$ be the solution of

$$\begin{cases} -\Delta u_{\mathcal{O}} = f & \text{in } \mathcal{O}, \\ \quad u_{\mathcal{O}} = 0 & \text{on } \partial\mathcal{O}. \end{cases} \tag{1.84}$$

Let $\omega_\varepsilon(\hat{y})$ and $\mathcal{O}_{\varepsilon,\hat{y}}$ be defined by (1.76) and (1.77) respectively, and let $0 < \gamma \neq 1 < +\infty$. We denote by $u_{\mathcal{O}_{\varepsilon,\hat{y}}}$ the solution of the following problem:

$$\begin{cases} -\operatorname{div}\left((1\chi_{\mathcal{O}_{\varepsilon,\hat{y}}} + \gamma\chi_{\omega_\varepsilon(\hat{y})})\nabla u_{\mathcal{O}_{\varepsilon,\hat{y}}}\right) = f & \text{in } \mathcal{O}, \\ \qquad\qquad\qquad\qquad u_{\mathcal{O}_{\varepsilon,\hat{y}}} = 0 & \text{on } \partial\mathcal{O}, \end{cases} \tag{1.85}$$

where $\chi_{\mathcal{O}_{\varepsilon,\hat{y}}}$ (resp. $\chi_{\omega_\varepsilon(\hat{y})}$) is the characteristic function of $\mathcal{O}_{\varepsilon,\hat{y}}$ (resp. $\omega_\varepsilon(\hat{y})$). This situation can be interpreted as follows. We consider a diffusion equation posed on a medium $\mathcal{O}$ having a diffusion coefficient being equal to 1, and we perturb this media with a small inclusion of a new medium confined in the open set $\omega_\varepsilon(\hat{y})$ and having a diffusion coefficient being equal to γ. Let $\mathcal{J}(\mathcal{O})$ be the shape functional defined for all $0 \leq \varepsilon$ small enough by

$$\mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}}) = j(\mathcal{O}_{\varepsilon,\hat{y}}, u_{\mathcal{O}_{\varepsilon,\hat{y}}}), \tag{1.86}$$

with the convention $\mathcal{O}_{0,\hat{y}} = \mathcal{O}$.

Definition 1.3 ([NS13])**.** *Let $\mathcal{J}$ be the shape functional defined by* (1.86)*. We assume that the following* topological asymptotic expansion *holds true*

$$\mathcal{J}(\mathcal{O}_{\varepsilon,\hat{y}}) = \mathcal{J}(\mathcal{O}) + g(\varepsilon)D_T\mathcal{J}(\hat{y}) + o(f(\varepsilon)), \tag{1.87}$$

where g is positive, is such that $g(\varepsilon) \to 0$, and $o(g(\varepsilon))/g(\varepsilon) \to 0$ with $\varepsilon \to 0$. Then the function

$$\hat{y} \in \mathcal{O} \longmapsto D_T\mathcal{J}(\hat{y}) \tag{1.88}$$

is called the **topological derivative** *of $\mathcal{J}$ at $\hat{y}$.*

For the rest of this chapter, we will work with this framework of configurational perturbation, by considering a small inclusion in the unit cell $\mathcal{Y}$ of a material having different elastic properties from the background material. Before this, we give a simple example of calculation of topological derivative for a configurational perturbation.

Example 3. (Diffusion in a one-dimensional bar). *Let $0 < \gamma$ be a positive parameter called* contrast*, and $F \in \mathbb{R}$ be a constant volume force. We consider a diffusion equation on the rod $(0,1) \subset \mathbb{R}$ for which the diffusion coefficient is equal to* 1*. Let $I_{\varepsilon,\hat{y}} := (\hat{y}-\varepsilon, \hat{y}+\varepsilon)$ be a small interval of $(0,1)$ on which we multiply the diffusion coefficient by γ, where $\hat{y} \in (0,1)$ and $0 < \varepsilon$ is a small size parameter such that $I_{\varepsilon,\hat{y}} \subset\subset (0,1)$. We assume that the volume* *force does not apply to the part $I_{\varepsilon,\hat{y}}$. We look for the solution u_ε of the following problem:*

$$\begin{cases} u''_\varepsilon(x) = F(1-\chi_{I_{\varepsilon,\hat{y}}}(x)), \quad \text{in } \left((0,1)\setminus\overline{I_{\varepsilon,\hat{y}}}\right)\cup I_{\varepsilon,\hat{y}}, \\ u_\varepsilon(0)=0, \\ u'_\varepsilon(1)=1, \\ u_\varepsilon(\hat{y}-\varepsilon)^- = u_\varepsilon(\hat{y}-\varepsilon)^+, \quad u_\varepsilon(\hat{y}+\varepsilon)^- = u_\varepsilon(\hat{y}+\varepsilon)^+, \\ u'_\varepsilon(\hat{y}-\varepsilon)^- = \gamma u'_\varepsilon(\hat{y}-\varepsilon)^+, \quad \gamma u'_\varepsilon(\hat{y}+\varepsilon)^- = u'_\varepsilon(\hat{y}+\varepsilon)^+. \end{cases} \tag{1.89}$$

We are interested in the energy shape functional $\mathcal{J}\left((0,1)\setminus\overline{I_{\varepsilon,\hat{y}}}\right) = j(\hat{y},\varepsilon,u_\varepsilon)$ given by

$$j(\hat{y},\varepsilon,u_\varepsilon) := \int_0^1 \gamma_{\varepsilon,\hat{y}}(x)(u'_\varepsilon(x))^2 dx, \tag{1.90}$$

where

$$\gamma_{\varepsilon,\hat{y}}(x) := (1-\chi_{I_{\varepsilon,\hat{y}}}(x)) + \gamma\chi_{I_{\varepsilon,\hat{y}}}(x). \tag{1.91}$$

The limit problem as $\varepsilon \to 0$ is then

$$\begin{cases} u''(x) = F, \quad \text{in } (0,1) \\ u(0)=0, \\ u'(1)=1, \end{cases} \tag{1.92}$$

whose solution is given for all $x \in (0,1)$ by

$$u(x) = (1-F)x + \frac{F}{2}x^2, \tag{1.93}$$

resulting in

$$j(\hat{y},0,u) = 1 - F + \frac{F^2}{3}. \tag{1.94}$$

The solution of (1.89) is given by

$$u_\varepsilon(x) = \begin{cases} (1-F+2F\varepsilon)x + \frac{1}{2}Fx^2, & \text{if } x \le \hat{y}-\varepsilon, \\ u_\varepsilon(\hat{y}-\varepsilon) + (x-(\hat{y}-\varepsilon))\frac{1}{\gamma}(1-F+F(\hat{y}+\varepsilon)), & \text{if } \hat{y}-\varepsilon < x < \hat{y}+\varepsilon, \\ u_\varepsilon(\hat{y}+\varepsilon) + (1-F)(x-(\hat{y}+\varepsilon)) + \frac{F}{2}(x^2-(\hat{y}+\varepsilon)^2) & \text{if } \hat{y}+\varepsilon \le x, \end{cases} \tag{1.95}$$

where

$$u_\varepsilon(\hat{y}-\varepsilon) = (1-F+2F\varepsilon)(\hat{y}-\varepsilon) + \frac{1}{2}F(\hat{y}-\varepsilon)^2, \tag{1.96}$$

$$u_\varepsilon(\hat{y}+\varepsilon) = u_\varepsilon(\hat{y}-\varepsilon) + 2\varepsilon\frac{1}{\gamma}\left(1-F+F(\hat{y}+\varepsilon)\right). \tag{1.97}$$

This gives

$$\begin{aligned} j(\hat{y},\varepsilon,u_\varepsilon) = 1 - F + \frac{F^2}{3} + \varepsilon &\left[-2(F-1)^2 + \frac{2}{\gamma}(F\hat{y}-F+1)^2\right] \\ &+ \varepsilon^2\left[\frac{4F}{\gamma}(1-\gamma+F(-1+\gamma+\hat{y}))\right] \end{aligned}$$

$$+\varepsilon^3\left[-\frac{2F^2}{3\gamma}(4\gamma-3)\right]. \tag{1.98}$$

Thus the topological derivative is

$$D_T\mathcal{J}(\hat{y}) = -2(F-1)^2 + \frac{2}{\gamma}(F\hat{y}-F+1)^2. \tag{1.99}$$

For the trivial case $F=0$ we obtain, by defining $g(\varepsilon)=\varepsilon$, a constant topological derivative for all $0<\gamma$.

$$D_T\mathcal{J}(\hat{y}) = 2\frac{1-\gamma}{\gamma}. \tag{1.100}$$

For quite simple setting $F = 1.5$, and $\gamma = 0.5$ we obtain the non trivial topological derivative given in Figure 8.

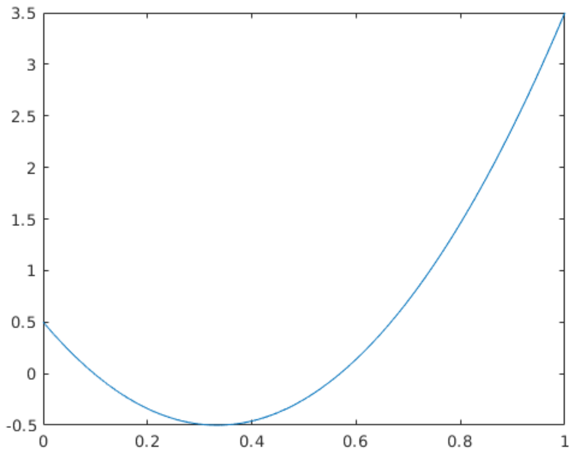

Figure 8: $D_T\mathcal{J}(\hat{y})$ when $\hat{y}$ belongs to $(0,1)$, for the settings $F=1.5$, and $\gamma=0.5$.

1.3.2 Perturbation of the unit cell

Now we return to the topological sensitivity analysis of the homogenized tensors obtained in Section 1.2.4. The topological optimization framework is as follows. The original unit cell $\mathcal{Y}$ defined in (1.4) is composed of two phases of isotropic materials, the first one represented by the domain $\mathcal{Y}_1$, and the second represented by $\mathcal{Y}_\gamma$, such that $\mathcal{Y} = \mathcal{Y}_1 \cup \mathcal{Y}_\gamma \cup \Gamma_\gamma$, where $\Gamma_\gamma = \partial\mathcal{Y}_\gamma \cap \mathcal{Y}$ with $\partial\mathcal{Y}$ and $\partial\mathcal{Y}_\gamma$ being Lipschitz continuous (see Figure 9). These two phases result in a piecewise constant elasticity tensor denoted by $\mathbf{C}$, which is defined as follows. Let

$$\mathbf{C}_0 = 2\mu\mathbb{I} + \lambda\mathrm{I}\otimes\mathrm{I}, \tag{1.101}$$

where the so-called Lamé coefficients $\mu,\lambda\in\mathbb{R}$ are chosen such that $\mathbf{C}_0$ satisfies the conditions *(i)*, *(ii)* and *(iii)* given in Section 1.2.2. The tensor $\mathrm{I} = \mathrm{e}_i\otimes\mathrm{e}_i$ is the identity second order tensor, and $\mathbb{I}$ the fourth order symmetric identity tensor, they are defined by

$$\mathrm{I}_{ij} = \delta_{ij}, \tag{1.102}$$

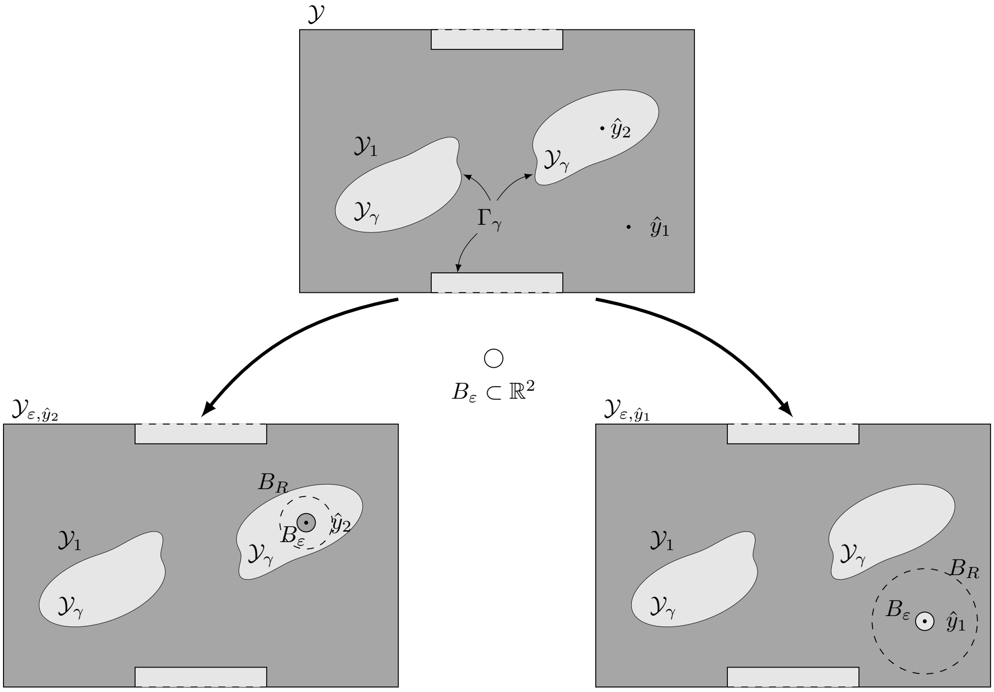

Figure 9: Introduction of an inclusion centered at $\hat{y}_1$ or $\hat{y}_2$ into the domains $\mathcal{Y}_\gamma$ or $\mathcal{Y}_1$ respectively. The resulting domains are denoted by $\mathcal{Y}_{\varepsilon,\hat{y}_1}$ and $\mathcal{Y}_{\varepsilon,\hat{y}_2}$.

$$\mathbb{I}_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{1.103}$$

where δ_{ij} is the Kronecker symbol. Thus we defined $\mathbf{C}$ by

$$\mathbf{C}(y) := \begin{cases} \mathbf{C}_0 & \text{if } y \in \mathcal{Y}_1 \ , \\ \gamma_0 \mathbf{C}_0 & \text{if } y \in \mathcal{Y}_\gamma \ , \end{cases} \tag{1.104}$$

where $0 < \gamma_0 < \infty$ is a parameter characterizing the contrast of elastic properties between the two different materials. We can consider that $\mathcal{Y}_1$ stands for a stiff material, and that $\mathcal{Y}_\gamma$ stands for a soft one in the case where $\gamma_0 < 1$.

From there, $\mathcal{Y}$ is subjected to a perturbation confined in a small circular open set $B_\varepsilon(\hat{y})$ of radius ε and centered at an arbitrary point $\hat{y}$ of $\mathcal{Y}$, such that $\overline{B_\varepsilon(\hat{y})} \subset \mathcal{Y}$, and which does not touch the interface Γ_γ (see Figure 9). Then, the region occupied by $B_\varepsilon(\hat{y})$ is filled by an inclusion with different material property from the background. The material properties of the perturbed domain are characterized by the piecewise constant function γ_ε of the form

$$\gamma_\varepsilon(x) := \begin{cases} 1 & \text{if } x \in \mathcal{Y} \setminus \overline{B_\varepsilon} \ , \\ \gamma(x) & \text{if } x \in B_\varepsilon \ , \end{cases} \tag{1.105}$$

where

$$\gamma(x) := \begin{cases} \gamma_0 & \text{if } x \in \mathcal{Y}_1 \ , \\ \gamma_0^{-1} & \text{if } x \in \mathcal{Y}_\gamma \ . \end{cases} \tag{1.106}$$

Namely if the perturbation B_ε lies in $\mathcal{Y}_1$ (the right case in Figure 9), then we multiply the elasticity tensor being equal to $\mathbf{C}_0$ by the contrast γ_0 in B_ε, so that in B_ε the elasticity tensor is now equal to $\gamma_0\mathbf{C}_0$. If the perturbation lies in $\mathcal{Y}_\gamma$ (the left case in Figure 9), then we multiply the elasticity tensor being equal to $\gamma_0 \mathbf{C}_0$ by γ_0^{-1} in B_ε, so that in B_ε the elasticity tensor is now equal to $\mathbf{C}_0$. In other words we introduce either a small ball of soft material into the stiff one, or a small ball of stiff material into the soft one. Finally the elasticity tensor is given by $\gamma_\varepsilon \mathbf{C}$ in the perturbed domain.

Henceforth we leave the lower indices of differential operators behind, because we only deal with y-variable depending fields. The topologically perturbed counterparts of problems (1.56) and (1.68) are respectively given by

$$\tilde{u}_{ij}^{\varepsilon} \in \mathcal{V} \; : \; \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{u}_{ij}^{\varepsilon}) \cdot e(\eta) = -\int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot e(\eta), \quad \forall \eta \in \mathcal{W}, \tag{1.107}$$

and

$$\begin{aligned} \tilde{\tilde{u}}_{ijk}^{\varepsilon} \in \mathcal{V} \; : \; \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{\tilde{u}}_{ijk}^{\varepsilon}) \cdot e(\eta) = & -\int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\tilde{u}_{ij}^{\varepsilon} \otimes_s \mathrm{e}_k) \cdot e(\eta) \\ & + \int_{\mathcal{Y}} (\gamma_\varepsilon \sigma(u_{ij}^{\varepsilon}) - \mathbf{C}_\varepsilon^h(\mathrm{e}_i \otimes_s \mathrm{e}_j))\mathrm{e}_k \cdot \eta \quad \forall \eta \in \mathcal{W}, \end{aligned} \tag{1.108}$$

where $\mathcal{V}$ and $\mathcal{W}$ are function spaces defined in (1.58) and (1.57) respectively, and as we did in Section 1.2, we can define the topologically perturbed counterparts of the homogenized tensors, denoted as $\mathbf{C}_\varepsilon^h$, $\mathbf{D}_\varepsilon^\sharp$ and $\mathbf{D}_\varepsilon^h$. By setting

$$u_{ij}^{\varepsilon} := (\mathrm{e}_i \otimes_s \mathrm{e}_j) y + \tilde{u}_{ij}^{\varepsilon}, \tag{1.109}$$

this gives

$$(\mathbf{C}_\varepsilon^h)_{ijkl} = \frac{1}{V} \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(u_{ij}^{\varepsilon}) \cdot e(u_{kl}^{\varepsilon}), \tag{1.110}$$

$$(\mathbf{D}_\varepsilon^\sharp)_{ijkpqr} = \frac{1}{V} \int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\tilde{u}_{ij}^{\varepsilon} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq}^{\varepsilon} \otimes_s \mathrm{e}_r), \tag{1.111}$$

$$\begin{aligned} (\mathbf{D}_\varepsilon^h)_{ijkpqr} = & \frac{1}{V} \int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\tilde{u}_{ij}^{\varepsilon} \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}_{ijk}^{\varepsilon})) \cdot (\tilde{u}_{pq}^{\varepsilon} \otimes_s \mathrm{e}_r) \\ & - \frac{1}{V} \int_{\mathcal{Y}} (\mathbf{C}_\varepsilon^h(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot (\tilde{\tilde{u}}_{pqr}^{\varepsilon} \otimes_s \mathrm{e}_k) + \gamma_\varepsilon \sigma(u_{pq}^{\varepsilon}) \cdot (\tilde{\tilde{u}}_{ijk}^{\varepsilon} \otimes_s \mathrm{e}_r)). \end{aligned} \tag{1.112}$$

Proposition 1.4. *Each of the auxiliary variational problems* (1.56)*,* (1.68)*,* (1.107) *and* (1.108) *admit a unique solution in the space* $\mathcal{V}$ *defined in* (1.58)*.*

Proof: Due to Korn's inequality together with the Poincaré-Wirtinger inequality, the space $\mathcal{W}$ endowed with the norm $\|\cdot\|_{\mathcal{W}}$, defined as follows

$$\|\eta\|_{\mathcal{W}} := \left(\int_{\mathcal{Y}} \sigma(\eta) \cdot e(\eta) \right)^{\frac{1}{2}}, \quad \forall \eta \in \mathcal{W}, \tag{1.113}$$

is an Hilbert space. In view of the properties (1.11), (1.12), and (1.14) introduced in Section 1.2.2 and satisfied by the elasticity tensor $\mathbf{C}$, the bilinear form a_ε of these problems, defined for all $u, v \in \mathcal{W}$ and for all $0 \leq \varepsilon$, by

$$a_\varepsilon(u, v) = \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(u) \cdot e(v), \tag{1.114}$$

is symmetric, and uniformly continuous and coercive on $(\mathcal{W}, \|\cdot\|_{\mathcal{W}})$ with respect to ε. Furthermore $\mathcal{W}^*$, the dual space of $\mathcal{W}$, can be identified with the subspace of the dual space $(H^1_{\text{per}}(\mathcal{Y};\mathbb{R}^2))^*$ whose elements $F \in (H^1_{\text{per}}(\mathcal{Y};\mathbb{R}^2))'$ are such that $F(c) = 0$ for all $c \in \mathbb{R}^2$. We can see that for all the problems (1.56), (1.68), (1.107), and (1.108), the linear forms applied to the test functions η belong indeed to $\mathcal{W}^*$. Then according to Lax-Milgram theorem, the existence and uniqueness of the solutions of variational problems on $(\mathcal{W}, \|\cdot\|_{\mathcal{W}})$ are ensured. We finally fix for each problem a solution belonging to $H^1_{\text{per}}(\mathcal{Y};\mathbb{R}^2)$ by choosing the representative element which has a zero mean value over $\mathcal{Y}$ for problems (1.56), (1.68), (1.107), and (1.108), so that $\tilde{u}_{ij}$ and $\tilde{\tilde{u}}_{ijk}$, as well as $\tilde{u}^\varepsilon_{ij}$ and $\tilde{\tilde{u}}^\varepsilon_{ijk}$ belong to $\mathcal{V}$. □

From there, we want to compute the topological derivative $D_T\boldsymbol{\mathcal{H}}$ such that the following expansion holds

$$\boldsymbol{\mathcal{H}}_\varepsilon = \boldsymbol{\mathcal{H}} + g(\varepsilon)D_T\boldsymbol{\mathcal{H}} + o(g(\varepsilon)), \tag{1.115}$$

where $\boldsymbol{\mathcal{H}}$ represents any homogenized tensor we are interested in, such as $\mathbf{C}^h$, $\mathbf{D}^\sharp$ and $\mathbf{D}^h$. In order to lead these calculations for $\mathbf{C}^h$ and $\mathbf{D}^\sharp$ in Section 1.3.4, and for $\mathbf{D}^h$ in Section 1.3.5, we need both:

- estimates of the correctors $\tilde{u}^\varepsilon_{ij}$ and $\tilde{\tilde{u}}^\varepsilon_{ijk}$,
- an *adjoint method*, allowing us to simplify some terms that we cannot simply analyse with the estimations of the correctors.

We will describe in the next Section 1.3.3 what the adjoint method is. Concerning the correctors estimates, let us introduce a truncated domain of the form

$$\mathcal{Y}_R := \mathcal{Y} \setminus B_R(\hat{y}). \tag{1.116}$$

We fix a positive real number R, such that $\overline{B_R(\hat{y})}$ is included in $\mathcal{Y}_1$ if $\hat{y} \in \mathcal{Y}_1$, or included in $\mathcal{Y}_\gamma$ if $\hat{y} \in \mathcal{Y}_\gamma$ (see Figure 9). We consider the small positive parameter ε which attempts to go to zero, with $R > \varepsilon > 0$. Note that $B_R(\hat{y})$ contains the inclusion $B_\varepsilon(\hat{y})$. The existence of the topological derivatives for the components of homogenized tensors is ensured by the following two lemmas. The proofs of these results are postponed to Section 1.5.

Lemma 1.5. *Let $\tilde{u}_{ij}$ and $\tilde{u}^\varepsilon_{ij}$ be the solutions of the original problem* (1.56) *and the perturbed problem* (1.107) *respectively. Then, the following estimates hold true*

$$\|\tilde{u}^\varepsilon_{ij} - \tilde{u}_{ij}\|_{H^1(\mathcal{Y};\mathbb{R}^2)} = O(\varepsilon), \tag{1.117}$$
$$\|\tilde{u}^\varepsilon_{ij} - \tilde{u}_{ij}\|_{L^2(\mathcal{Y};\mathbb{R}^2)} = o(\varepsilon), \tag{1.118}$$
$$\|\tilde{u}^\varepsilon_{ij} - \tilde{u}_{ij}\|_{H^1(\mathcal{Y}_R;\mathbb{R}^2)} = O(\varepsilon^2). \tag{1.119}$$

Lemma 1.6. *Let $\tilde{\tilde{u}}_{ijk}$ and $\tilde{\tilde{u}}^\varepsilon_{ijk}$ be the solutions of the original problem* (1.68) *and the perturbed problem* (1.108) *respectively. Then, the following estimates hold true*

$$\|\tilde{\tilde{u}}^\varepsilon_{ijk} - \tilde{\tilde{u}}_{ijk}\|_{H^1(\mathcal{Y};\mathbb{R}^2)} = O(\varepsilon), \tag{1.120}$$
$$\|\tilde{\tilde{u}}^\varepsilon_{ijk} - \tilde{\tilde{u}}_{ijk}\|_{L^2(\mathcal{Y};\mathbb{R}^2)} = o(\varepsilon), \tag{1.121}$$
$$\|\tilde{\tilde{u}}^\varepsilon_{ijk} - \tilde{\tilde{u}}_{ijk}\|_{H^1(\mathcal{Y}_R;\mathbb{R}^2)} = o(\varepsilon). \tag{1.122}$$

The proof of these estimates relies on the asymptotic expansion of the solutions $\tilde{u}^{\varepsilon}_{ij}$ and $\tilde{\tilde{u}}^{\varepsilon}_{ijk}$ with respect to the parameter ε, expressed with suitable classical *transmission problem* solutions, for which we have an explicit representations in the case where the singular inclusion is a disk [Bar92; NS13]. For a more general shape of the inclusion, we should use the representation of these exterior problem solutions in terms of layer potential [AK04; AK07]. Using the expressions of the asymptotic expansions of the solutions, besides proving the existence of the topological derivate, we are able to write an explicit formula. This formula depends on the gradient of the unperturbed solution, and it is expressed by means of a so-called *Polarization tensor* (notion introduced in [SS49], [PS51], for more details see e.g., [AK07]). In order to derive these expressions, we invoke the following fundamental result.

Let ψ be a constant matrix field of $\mathbb{R}^{2\times 2}$. Let w^{ε} be the solution of the following transmission problem

$$\begin{cases} \operatorname{div}(\gamma_{\varepsilon}\sigma(w^{\varepsilon})) = 0 & \text{in } \mathbb{R}^2 \\ \sigma(w^{\varepsilon}) = \mathbf{C}e(w^{\varepsilon}) & \text{in } \mathbb{R}^2 \\ e(w^{\varepsilon}) = \nabla^s w^{\varepsilon} & \text{in } \mathbb{R}^2 \\ w^{\varepsilon} \to 0 & \text{at } \infty \\ [\![w^{\varepsilon}]\!] = 0 & \text{on } \partial B_{\varepsilon}, \\ [\![\gamma_{\varepsilon}\sigma(w^{\varepsilon})]\!] n = -(1-\gamma)\psi n & \text{on } \partial B_{\varepsilon}, \end{cases} \tag{1.123}$$

where γ_{ε} and γ are defined in (1.105) and (1.106) respectively, n is the inward normal vector on ∂B_{ε}, and $[\![\cdot]\!]$ denotes the jump across the interface of the inclusion:

$$[\![\cdot]\!] = (\cdot)_{\mathcal{Y}\setminus\overline{B_{\varepsilon}}} - (\cdot)_{B_{\varepsilon}} \quad \text{on} \quad \partial B_{\varepsilon}. \tag{1.124}$$

We have the following result.

Theorem 1.7 (Eshelby's Theorem [Esh57; Esh59]). *The stress tensor field σ associated to the solution of the transmission problem* (1.123) *is constant inside the inclusion B_{ε}, and can be written as follows (see e.g., [NS20] Section 5.1.3)*

$$\sigma(w^{\varepsilon}) \mid_{B_{\varepsilon}} = \bar{\mathbb{T}}\psi, \tag{1.125}$$

where $\bar{\mathbb{T}}$ is a fourth order constant tensor given by

$$\bar{\mathbb{T}} = \frac{1-\gamma}{1+\beta\gamma}\left(\beta\mathbb{I} + \frac{1}{2}\frac{\alpha-\beta}{1+\alpha\gamma}\mathrm{I}\otimes\mathrm{I}\right), \tag{1.126}$$

with the constant α and β depending on the Lamé coefficients λ and μ are given by

$$\alpha = \frac{\mu+\lambda}{\mu}, \quad \beta = \frac{3\mu+\lambda}{\mu+\lambda}. \tag{1.127}$$

1.3.3 The adjoint method

For a more detailed and general presentation of the adjoint method, the reader may refer to [GGM01] or [Ams06]. We present herein the method written in such a way that it matches with the calculations led in the two next sections. Let $(\mathcal{W}, \|\cdot\|_{\mathcal{W}})$ be a Hilbert space, and a_ε be a family of symmetric bilinear forms on $\mathcal{W}$, uniformly continuous and coercive on $\mathcal{W}$, depending on $\varepsilon \geq 0$. For all arbitrary multi-index $\mathbf{i}$, aiming to designate indifferently the couple or triplet of indices of the correctors $\tilde{u}_{ij}$ or $\tilde{\tilde{u}}_{ijk}$, let $l_\varepsilon^{\mathbf{i}}$ be a family of continuous linear forms on $\mathcal{W}$. For all $\mathbf{i}$ and for all ε, we denote by $\boldsymbol{X}_\varepsilon^{\mathbf{i}}$ the unique solution of the problem

$$\text{Find } \boldsymbol{X}_\varepsilon^{\mathbf{i}} \in \mathcal{W} \text{ such that:} \quad a_\varepsilon(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{Y}) = l_\varepsilon^{\mathbf{i}}(\boldsymbol{Y}), \quad \forall \boldsymbol{Y} \in \mathcal{W}. \tag{1.128}$$

For all $\mathbf{i}, \mathbf{j}$ multi-indices we define the following functionals depending on ε by:

$$\mathcal{J}^{\mathbf{ij}}(\varepsilon) := j_\varepsilon(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}), \tag{1.129}$$

where for all $0 \leq \varepsilon$, we have that j_ε is a smooth map from $\mathcal{W} \times \mathcal{W}$ to $\mathbb{R}$. We introduce such a shape functional $\mathcal{J}^{\mathbf{ij}}(\varepsilon) := j_\varepsilon(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}})$, because if we go back to the definitions of the coefficients of the homogenized tensor $\mathbf{D}_\varepsilon^\sharp$ given in (1.110) for example, we can see its expression as a bilinear form defined on $\mathcal{W} \times \mathcal{W}$ which is parametrized by ε through γ_ε, and which is evaluated on the functions $(\tilde{u}_{ij}^\varepsilon, \tilde{u}_{pq}^\varepsilon)$. Our goal is to investigate the behaviour of $\mathcal{J}^{\mathbf{ij}}(\varepsilon)$ when ε goes to zero by writing an expansion of the form

$$\mathcal{J}^{\mathbf{ij}}(\varepsilon) = \mathcal{J}^{\mathbf{ij}}(0) + g(\varepsilon) D_T \mathcal{J}^{\mathbf{ij}} + o(g(\varepsilon)), \tag{1.130}$$

where $g(\varepsilon)$ is a positive function going to zero when ε goes to zero. Let us develop

$$\begin{aligned} \mathcal{J}^{\mathbf{ij}}(\varepsilon) - \mathcal{J}^{\mathbf{ij}}(0) &= j_\varepsilon(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}) - j_0(\boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{X}_0^{\mathbf{j}}) \\ &= j_\varepsilon(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}) - j_0(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}) + j_0(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}) - j_0(\boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{X}_0^{\mathbf{j}}) \\ &= (j_\varepsilon - j_0)(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}) + D_1 j_0(\boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{X}_0^{\mathbf{j}})(\boldsymbol{X}_\varepsilon^{\mathbf{i}} - \boldsymbol{X}_0^{\mathbf{i}}) \\ &\qquad + D_2 j_0(\boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{X}_0^{\mathbf{j}})(\boldsymbol{X}_\varepsilon^{\mathbf{j}} - \boldsymbol{X}_0^{\mathbf{j}}) + \mathcal{R}(\varepsilon), \end{aligned} \tag{1.131}$$

where D_1 and D_2 denotes respectively the partial derivatives with respect to the first and the second variables of j_0 or j_ε. Furthermore we assume on the one hand that $\mathcal{R}(\varepsilon) = o(g(\varepsilon))$, and on the other hand that there exists a positive constant $\boldsymbol{\delta} j^{\mathbf{ij}}$ such that

$$(j_\varepsilon - j_0)(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{X}_\varepsilon^{\mathbf{j}}) = g(\varepsilon)\boldsymbol{\delta} j^{\mathbf{ij}} + o(g(\varepsilon)). \tag{1.132}$$

If we consider that we have the estimate $\|\boldsymbol{X}_\varepsilon^{\mathbf{i}} - \boldsymbol{X}_0^{\mathbf{i}}\|_{\mathcal{W}} = O(g(\varepsilon))$, we cannot obtain an expansion as (1.130) because of the presence of the terms $D_1 j_0$ and $D_2 j_0$. To overcome this problem, we introduce what we call *adjoint states*. Let the adjoint state $\boldsymbol{Z}^\alpha$ be the solution of the following problem, for all $\alpha = 1, 2$

$$\text{Find } \boldsymbol{Z}^\alpha \in \mathcal{W} \text{ such that:} \quad a_0(\boldsymbol{Y}, \boldsymbol{Z}^\alpha) = -D_\alpha j_0(\boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{X}_0^{\mathbf{j}})(\boldsymbol{Y}), \quad \forall \boldsymbol{Y} \in \mathcal{W}. \tag{1.133}$$

This allows rewriting

$$\begin{aligned} D_1 j_0(\boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{X}_0^{\mathbf{j}})(\boldsymbol{X}_\varepsilon^{\mathbf{i}} - \boldsymbol{X}_0^{\mathbf{i}}) &= -a_0(\boldsymbol{X}_\varepsilon^{\mathbf{i}} - \boldsymbol{X}_0^{\mathbf{i}}, \boldsymbol{Z}^1), \\ &= -a_0(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{Z}^1) + l_0^{\mathbf{i}}(\boldsymbol{Z}^1), \\ &= (a_\varepsilon - a_0)(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{Z}^1) - a_\varepsilon(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{Z}^1) + l_0^{\mathbf{i}}(\boldsymbol{Z}^1), \\ &= (a_\varepsilon - a_0)(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{Z}^1) + (l_0^{\mathbf{i}} - l_\varepsilon^{\mathbf{i}})(\boldsymbol{Z}^1), \end{aligned} \tag{1.134}$$

and the similar expression for $D_2 j_0$. Now if we assume that we have positive constants $\boldsymbol{\delta} a^{\mathbf{i}\alpha}$ and $\boldsymbol{\delta} l^{i\alpha}$ such that the following estimates hold:

$$(a_\varepsilon - a_0)(\boldsymbol{X}_\varepsilon^{\mathbf{i}}, \boldsymbol{Z}^\alpha) = g(\varepsilon)\boldsymbol{\delta} a^{\mathbf{i}\alpha} + o(g(\varepsilon)),$$

$$(l_0^{\mathbf{i}} - l_\varepsilon^{\mathbf{i}})(\boldsymbol{Z}^\alpha) = g(\varepsilon)\boldsymbol{\delta} l^{\mathbf{i}\alpha} + o(g(\varepsilon)), \tag{1.135}$$

then we could conclude that

$$\mathcal{J}^{\mathbf{ij}}(\varepsilon) = \mathcal{J}^{\mathbf{ij}}(0) + g(\varepsilon)\left(\boldsymbol{\delta} j^{\mathbf{ij}} + \boldsymbol{\delta} a^{\mathbf{i}1} + \boldsymbol{\delta} a^{\mathbf{j}2} + \boldsymbol{\delta} l^{\mathbf{i}1} + \boldsymbol{\delta} l^{\mathbf{j}2}\right) + o(g(\varepsilon)). \tag{1.136}$$

Let us apply this technique to the calculation of the topological derivatives of the homogenized tensors, by seeking to obtain expansions of the form (1.135) for $\mathbf{C}^h$, $\mathbf{D}^\sharp$, and $\mathbf{D}^h$.

1.3.4 First-order truncation

1.3.4.1 Tensor $\mathbf{C}^h$

First, let us consider the expansion of the homogenized tensors $\mathbf{C}^h$, because we will need it in Chapter 2. To this end, we exclusively need the estimates from Lemma 1.5. The calculations of the topological derivative of $\mathbf{C}^h$ is well-known, and from [Ams+10; Giu+09a] we have the following result.

Theorem 1.8. *The topological asymptotic expansion of the homogenized elasticity tensor $\mathbf{C}^h$ is given by*

$$(\mathbf{C}^h_\varepsilon - \mathbf{C}^h)_{ijkl} = \frac{\pi\varepsilon^2}{V}\mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot e(u_{kl})(\hat{y}) + o(\varepsilon^2), \tag{1.137}$$

which, setting $g(\varepsilon) = \pi\varepsilon^2/V$, allows to identify the topological derivative of any component of $\mathbf{C}^h$, namely

$$(D_T\mathbf{C}^h)_{ijkl} = \mathbb{P}\sigma(u_{ij}) \cdot e(u_{kl}), \tag{1.138}$$

where u_{ij} is given by (1.60) *and the polarization tensor is defined as*

$$\mathbb{P} = -\frac{1-\gamma}{1+\gamma\beta}\left((1+\beta)\mathbb{I} + \frac{1}{2}(\alpha-\beta)\frac{1-\gamma}{1+\gamma\alpha}\mathrm{I}\otimes\mathrm{I}\right), \tag{1.139}$$

with the parameters α and β given by

$$\alpha = \frac{\lambda+\mu}{\mu} \quad \textit{and} \quad \beta = \frac{\lambda+3\mu}{\lambda+\mu}. \tag{1.140}$$

We refer to [Ams+10] for the proof of this result. We underline that in this calculation of the topological derivative of $\mathbf{C}^h$, the adjoint method was not needed. Indeed we can see that problems (1.128) and (1.133) are the same in this case. We don't write this proof, and directly describe the method for the tensor $\mathbf{D}^\sharp$, for which the introduction of adjoint states is required.

1.3.4.2 Tensor $\mathbf{D}^\sharp$

Theorem 1.9. *The topological asymptotic expansion of tensor $\mathbf{D}^\sharp$ is given by*

$$\begin{aligned}(\mathbf{D}^\sharp_\varepsilon - \mathbf{D}^\sharp)_{ijkpqr} =& -\frac{\pi\varepsilon^2}{V}\mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot e(v^{rk}_{pq})(\hat{y}) - \frac{\pi\varepsilon^2}{V}\mathbb{P}\sigma(u_{pq})(\hat{y}) \cdot e(v^{kr}_{ij})(\hat{y}) \\ & - \frac{\pi\varepsilon^2}{V}(1-\gamma)\mathbf{C}(\hat{y})(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r) + o(\varepsilon^2),\end{aligned} \tag{1.141}$$

where $\mathbb{P}$ *is the polarization tensor defined in* (1.139). *By setting* $g(\varepsilon) = \pi\varepsilon^2/V$, *the topological derivative of any component of tensor* $\mathbf{D}^\sharp$ *can be identified, namely*

$$(D_T\mathbf{D}^\sharp)_{ijkpqr} = -\mathbb{P}\sigma(u_{ij})\cdot e(v_{pq}^{rk}) - \mathbb{P}\sigma(u_{pq})\cdot e(v_{ij}^{kr}) - (1-\gamma)\mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k)\cdot(\tilde{u}_{pq}\otimes_s \mathrm{e}_r), \quad (1.142)$$

where u_{ij} *is given by* (1.60), $\tilde{u}_{ij}$ *are solutions to the set of canonical variational problems* (1.56) *and the adjoint states* v_{ij}^{kr} *are solutions to* (1.147).

Proof: Because the original and perturbed fields $\tilde{u}_{ij}$ and $\tilde{u}_{ij}^\varepsilon$ are living in the same function space $\mathcal{V}$, we can perform a direct calculation. We recall that, from the definition of the tensors $\mathbf{D}^\sharp$ given by (1.66) and $\mathbf{D}_\varepsilon^\sharp$ given by (1.111) for its topologically perturbed counterpart, we have

$$(\mathbf{D}_\varepsilon^\sharp - \mathbf{D}^\sharp)_{ijkpqr} = \frac{1}{V}\int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k)\cdot(\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) - \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k)\cdot(\tilde{u}_{pq}\otimes_s \mathrm{e}_r). \quad (1.143)$$

Thus we can derive the topological asymptotic expansion of the tensor $\mathbf{D}^\sharp$ as follows

$$\begin{aligned}(\mathbf{D}_\varepsilon^\sharp - \mathbf{D}^\sharp)_{ijkpqr} &= \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}((\tilde{u}_{ij}^\varepsilon - \tilde{u}_{ij})\otimes_s \mathrm{e}_k)\cdot(\tilde{u}_{pq}\otimes_s \mathrm{e}_r)\\ &+ \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k)\cdot((\tilde{u}_{pq}^\varepsilon - \tilde{u}_{pq})\otimes_s \mathrm{e}_r)\\ &- \frac{1-\gamma}{V}\int_{B_\varepsilon} \mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k)\cdot(\tilde{u}_{pq}^\varepsilon\otimes_s \mathrm{e}_r) + \mathcal{E}_1(\varepsilon), \end{aligned} \quad (1.144)$$

where the remainder $\mathcal{E}_1(\varepsilon)$ is given by

$$\mathcal{E}_1(\varepsilon) = \frac{1}{V}\int_{\mathcal{Y}} \mathbf{C}((\tilde{u}_{ij}^\varepsilon - \tilde{u}_{ij})\otimes_s \mathrm{e}_k)\cdot((\tilde{u}_{pq}^\varepsilon - \tilde{u}_{pq})\otimes_s \mathrm{e}_r), \quad (1.145)$$

and can be bounded as follows

$$|\mathcal{E}_1(\varepsilon)| \le C\|\tilde{u}_{ij}^\varepsilon - \tilde{u}_{ij}\|_{L^2(\mathcal{Y};\mathbb{R}^2)}\|\tilde{u}_{pq}^\varepsilon - \tilde{u}_{pq}\|_{L^2(\mathcal{Y};\mathbb{R}^2)} = o(\varepsilon^2), \quad (1.146)$$

where we have used Lemma 1.5. The term $\mathcal{E}_1(\varepsilon)$ corresponds to the term $\mathcal{R}(\varepsilon)$ in the expression (1.131), while the first two terms of the right hand side of (1.144) corresponds to $D_1 j_0(\boldsymbol{X}_0^i, \boldsymbol{X}_0^j)(\boldsymbol{X}_\varepsilon^i - \boldsymbol{X}_0^i)$ and $D_2 j_0(\boldsymbol{X}_0^i, \boldsymbol{X}_0^j)(\boldsymbol{X}_\varepsilon^j - \boldsymbol{X}_0^j)$ in (1.131) respectively, and the last term of the right hand side of (1.144) correspond to $(j_\varepsilon - j_0)(\boldsymbol{X}_\varepsilon^i, \boldsymbol{X}_\varepsilon^j)$ in (1.131) respectively. Still evoking Lemma 1.5, we notice that the third term of the right-hand side of expression (1.144) gives rise to a ε^2 order term in the asymptotic expansion of $\mathbf{D}_\varepsilon^\sharp$. But we can not use the same arguments to analyse the first two terms of the right-hand side of (1.144).

To overcome this difficult, we make use of the adjoint method presented in Section 1.3.3 by introducing suitable adjoint state $v_{ij}^{kr} \in \mathcal{V}$ for $i, j, k, r \in \{1, 2\}$, solution of the following set of variational problems:

$$\begin{aligned} v_{ij}^{kr} \in \mathcal{V} \ : \ \int_{\mathcal{Y}} \sigma(v_{ij}^{kr})\cdot e(\eta) &= \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k)\cdot(\eta\otimes_s \mathrm{e}_r)\\ &- \int_{\mathcal{Y}} \langle \mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k)\rangle\cdot(\eta\otimes_s \mathrm{e}_r), \quad \forall \eta \in \mathcal{W}. \end{aligned} \quad (1.147)$$

In comparison to the adjoint method for which the adjoint states are obtained by solving the problem defined with the differential of the shape function, we have added the term depending on $\langle \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)\rangle$ in order to be in the framework of Proposition 1.4. After subtracting (1.56) from (1.107), we obtain

$$\int_{\mathcal{Y}} \sigma(\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \cdot e(\eta) = (1-\gamma) \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{pq}) \cdot e(\eta), \tag{1.148}$$

where $u^{\varepsilon}_{pq} := (\mathrm{e}_p \otimes_s \mathrm{e}_q)y + \tilde{u}^{\varepsilon}_{pq}$. By setting $\eta = \tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}$ as test function in the adjoint problem (1.147) for v^{kr}_{ij}, and noting that $\langle \tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}\rangle = 0$, we obtain

$$\int_{\mathcal{Y}} \sigma(v^{kr}_{ij}) \cdot e(\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) = \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot ((\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \otimes_s \mathrm{e}_r). \tag{1.149}$$

After taking $\eta = v^{kr}_{ij}$ as test function in (1.148), we have

$$\int_{\mathcal{Y}} \sigma(\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \cdot e(v^{kr}_{ij}) = (1-\gamma) \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{pq}) \cdot e(v^{kr}_{ij}), \tag{1.150}$$

From the symmetry of the bilinear forms we conclude with (1.149) that

$$\int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot ((\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \otimes_s \mathrm{e}_r) = (1-\gamma) \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{pq}) \cdot e(v^{kr}_{ij}). \tag{1.151}$$

Similarly we have, after replacing the indexes pq by ij in (1.148) and (1.147), that

$$\int_{\mathcal{Y}} \mathbf{C}((\tilde{u}^{\varepsilon}_{ij} - \tilde{u}_{ij}) \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) = (1-\gamma) \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{ij}) \cdot e(v^{rk}_{pq}). \tag{1.152}$$

From (1.144), these results lead to

$$\begin{aligned}(\mathbf{D}^\sharp_\varepsilon - \mathbf{D}^\sharp)_{ijkpqr} = {} & \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{ij}) \cdot e(v^{rk}_{pq}) + \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{pq}) \cdot e(v^{kr}_{ij}) \\ & - \frac{1-\gamma}{V} \int_{B_\varepsilon} \mathbf{C}(\tilde{u}^{\varepsilon}_{ij} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}^{\varepsilon}_{pq} \otimes_s \mathrm{e}_r) + \mathcal{E}_1(\varepsilon).\end{aligned} \tag{1.153}$$

We start simplifying the term which does not depend on the gradient of the solutions: we develop

$$\begin{aligned}\int_{B_\varepsilon} \mathbf{C}(\tilde{u}^{\varepsilon}_{ij} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}^{\varepsilon}_{pq} \otimes_s \mathrm{e}_r) = {} & \int_{B_\varepsilon} \mathbf{C}((\tilde{u}^{\varepsilon}_{ij} - \tilde{u}_{ij}) \otimes_s \mathrm{e}_k) \cdot ((\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \otimes_s \mathrm{e}_r) \\ & + \int_{B_\varepsilon} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) \\ & + \int_{B_\varepsilon} \mathbf{C}((\tilde{u}^{\varepsilon}_{ij} - \tilde{u}_{ij}) \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) \\ & + \int_{B_\varepsilon} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot ((\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \otimes_s \mathrm{e}_r).\end{aligned} \tag{1.154}$$

We deduce directly from the Cauchy-Schwarz inequality and from Lemma 1.5 that the first term of the right-hand side of (1.154),

$$\int_{B_\varepsilon} \mathbf{C}((\tilde{u}^{\varepsilon}_{ij} - \tilde{u}_{ij}) \otimes_s \mathrm{e}_k) \cdot ((\tilde{u}^{\varepsilon}_{pq} - \tilde{u}_{pq}) \otimes_s \mathrm{e}_r) \tag{1.155}$$

is $o(\varepsilon^2)$. Since we assume that the inclusion B_ε is located neither on the interface nor on the boundary, the solutions of elliptic boundary value problems are smooth in B_ε by the elliptic regularity. Then

$$\|\tilde{u}_{ij}\|_{L^2(B_\varepsilon)} = O(\varepsilon), \quad \text{and} \quad \|\tilde{u}_{pq}\|_{L^2(B_\varepsilon)} = O(\varepsilon), \tag{1.156}$$

so that once again from the Cauchy-Schwarz inequality and from Lemma 1.5 we find that the two last terms in (1.154),

$$\int_{B_\varepsilon} \mathbf{C}((\tilde{u}^\varepsilon_{ij} - \tilde{u}_{ij}) \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) + \int_{B_\varepsilon} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot ((\tilde{u}^\varepsilon_{pq} - \tilde{u}_{pq}) \otimes_s \mathrm{e}_r), \tag{1.157}$$

are also $o(\varepsilon^2)$. Finally, from the Lebesgue differentiation theorem, we can rewrite equation (1.154) as follows

$$\int_{B_\varepsilon} \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) = \pi\varepsilon^2 \mathbf{C}(\hat{y})(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r) + o(\varepsilon^2). \tag{1.158}$$

Now we analyse the terms depending on the gradient of the solutions in (1.153). We will show in Section 1.5 that we can write

$$\tilde{u}^\varepsilon_{kl} = \tilde{u}_{kl} + w^\varepsilon_{kl} + R_\varepsilon, \tag{1.159}$$

where $\|R_\varepsilon\|_{H^1(\mathcal{Y})} = o(\varepsilon^2)$, and w^ε_{kl} is the solution of (1.123) written for $\psi = \sigma(\tilde{u}_{kl})(\hat{y})$. Thus we can calculate by taking into account the Lebesgue differentiation theorem

$$\begin{aligned} \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u_{ij}) \cdot e(u^\varepsilon_{kl}) &= \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u_{ij}) \cdot e(u_{kl} + w^\varepsilon_{kl} + R_\varepsilon) \\ &= \frac{1-\gamma}{V} \left(\pi\varepsilon^2 e(u_{ij})(\hat{y}) \cdot \sigma(u_{kl})(\hat{y}) + e(u_{ij})(\hat{y}) \cdot \int_{B_\varepsilon} \sigma(w^\varepsilon_{kl}) \right) + o(\varepsilon^2), \end{aligned} \tag{1.160}$$

where we remind that for all $0 \le \varepsilon$, $u^\varepsilon_{ij} := (\mathrm{e}_i \otimes_s \mathrm{e}_j)y + \tilde{u}^\varepsilon_{ij}$, in such a way that $u^\varepsilon_{ij} - u_{ij} = \tilde{u}^\varepsilon_{ij} - \tilde{u}_{ij}$, and that in view of the properties satisfied by $\mathbf{C}$ given page 19, we have $\sigma(u_{ij}) \cdot e(u_{kl}) = e(u_{ij}) \cdot \sigma(u_{kl})$. From Eshelby's Theorem 1.7

$$\begin{aligned} \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u_{ij}) \cdot e(u^\varepsilon_{kl}) &= \frac{\pi\varepsilon^2}{V}(1-\gamma) \left(e(u_{ij})(\hat{y}) \cdot \sigma(u_{kl})(\hat{y}) + e(u_{ij})(\hat{y}) \cdot \bar{\mathbb{T}}\sigma(u_{kl})(\hat{y}) \right) + o(\varepsilon^2) \\ &= \frac{\pi\varepsilon^2}{V} e(u_{ij})(\hat{y}) \cdot (1-\gamma)(\mathbb{I} + \bar{\mathbb{T}})\sigma(u_{kl})(\hat{y}) + o(\varepsilon^2) \end{aligned} \tag{1.161}$$

From the definition of tensor $\bar{\mathbb{T}}$ (1.126) we have

$$(1-\gamma)(\mathbb{I} + \bar{\mathbb{T}}) = -\mathbb{P}, \tag{1.162}$$

where $\mathbb{P}$ is the polarization tensor given in (1.139). We recall that $\mathbb{P}$ behaves like $\mathbf{C}$, that is $\mathbb{P}_{ijkl} = \mathbb{P}_{jikl} = \mathbb{P}_{klij}$. Consequently, for all second order tensors A and B, we have $\mathbb{P}\mathbf{C}A \cdot B = A \cdot \mathbb{P}\mathbf{C}B$. Then we can write (1.161)

$$\frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u_{ij}) \cdot e(u^\varepsilon_{kl}) = -\frac{\pi\varepsilon^2}{V} \mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot e(u_{kl})(\hat{y}) + o(\varepsilon^2). \tag{1.163}$$

Finally, we have proved Theorem 1.9. □

1.3.5 Second-order truncation

Now we want to investigate the topological sensitivity of the tensors $\mathbf{E}^h$ and $\mathbf{D}^h$ involved in the macroscopic elastic energy calculated for the second order truncation (1.70), and of the tensor $\mathbf{F}^h$ defined in (1.75). We have the following theorems.

Theorem 1.10. *The topological asymptotic expansion of the tensor* $\mathbf{D}^h$ *is given by*

$$\begin{aligned}(\mathbf{D}^h_\varepsilon - \mathbf{D}^h)_{ijkpqr} = &-\frac{\pi\varepsilon^2}{V}\mathbb{P}\sigma(u_{ij})(\hat{y})\cdot(e(p^k_{pqr})(\hat{y}) + (\tilde{\tilde{u}}_{pqr}(\hat{y})\otimes_s \mathrm{e}_k))\\ &-\frac{\pi\varepsilon^2}{V}\mathbb{P}\sigma(u_{pq})(\hat{y})\cdot(e(p^r_{ijk})(\hat{y}) + (\tilde{\tilde{u}}_{ijk}(\hat{y})\otimes_s \mathrm{e}_r))\\ +\frac{\pi\varepsilon^2}{V}\mathbb{P}\Big(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) &+ \mathbf{C}(\tilde{u}_{ij}(\hat{y})\otimes_s \mathrm{e}_k)\Big)\cdot\Big(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y})\otimes_s \mathrm{e}_r)\Big) + o(\varepsilon^2).\end{aligned} \tag{1.164}$$

where $\mathbb{P}$ *is the polarization tensor defined in* (1.139)*. By setting* $g(\varepsilon) = \pi\varepsilon^2/V$*, we can identify the topological derivative of any component of tensor* $\mathbf{D}^h$*, namely*

$$\begin{aligned}(D_T\mathbf{D}^h)_{ijkpqr} = &-\mathbb{P}\sigma(u_{ij})\cdot(e(p^k_{pqr}) + (\tilde{\tilde{u}}_{pqr}\otimes_s \mathrm{e}_k)) - \mathbb{P}\sigma(u_{pq})\cdot(e(p^r_{ijk}) + (\tilde{\tilde{u}}_{ijk}\otimes_s \mathrm{e}_r))\\ &+\mathbb{P}\Big(\sigma(\tilde{\tilde{u}}_{ijk}) + \mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k)\Big)\cdot\Big(e(\tilde{\tilde{u}}_{pqr}) + (\tilde{u}_{pq}\otimes_s \mathrm{e}_r)\Big),\end{aligned} \tag{1.165}$$

where u_{ij} *is given by* (1.60)*,* $\tilde{u}_{ij}$ *are solutions to the set of canonical variational problems* (1.56)*,* $\tilde{\tilde{u}}_{ijk}$ *are solutions to the set of canonical coupled variational problems* (1.68) *and the adjoint states* p^r_{ijk} *are solutions to* (1.177)*.*

Theorem 1.11. *The topological derivatives of* $\mathbf{E}^h$ *and* $\mathbf{F}^h$ *are respectively given by:*

$$\begin{aligned}(D_T\mathbf{E}^h)_{ijpqr} = &\,2\mathbb{P}\sigma(u_{pq})\cdot e(v^r_{ij}) + 2\mathbb{P}\sigma(u_{ij})\cdot e(v^r_{pq})\\ &- 2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr}) + \mathbf{C}\tilde{u}_{pq}\otimes_s \mathrm{e}_r)\cdot e(u_{ij}),\end{aligned} \tag{1.166}$$

and

$$\begin{aligned}(D_T\mathbf{F}^h)_{ijkpqr} = &\,2\Big[\mathbb{P}\sigma(u_{ij})\cdot(v_{Fpqr}\otimes_s \mathrm{e}_k - e(q_{Fpqr^k}))\Big]^{\mathrm{sym}}\\ &- 2\Big[\mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk}) + \mathbf{C}(\tilde{u}_{ij}\otimes_s \mathrm{e}_k))\cdot e(v_{Fpqr})\Big]^{\mathrm{sym}}\\ &+ \mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr}) + \mathbf{C}(\tilde{u}_{pq}\otimes_s \mathrm{e}_r))\cdot(e(\tilde{\tilde{u}}_{ijk}) + (\tilde{u}_{ij}\otimes_s \mathrm{e}_k)),\end{aligned} \tag{1.167}$$

where for a sixth order tensor $\mathbf{F}$*, we define the tensor* $\mathbf{F}^{\mathrm{sym}}$ *by*

$$\mathbf{F}^{\mathrm{sym}}_{ijkpqr} := \frac{1}{2}(\mathbf{F}_{ijkpqr} + \mathbf{F}_{pqrijk}), \tag{1.168}$$

and where v^r_{ij}*,* v_{Fijk}*, and* q_{Fijk^r} *are solutions to the problems* (B.8)*,* (B.16)*, and* (B.23) *respectively.*

In the following, we give a rigorous proof of Theorem 1.10. The proof of Theorem 1.11 is similar to that of Theorem 1.10, so we write it in the Appendix B.1 for the topological derivative of $\mathbf{E}^h$, and in the Appendix B.2 for the topological derivative of $\mathbf{F}^h$.

Proof of Theorem 1.10: As we did for $\mathbf{D}^\sharp$, we perform a direct calculation. Let f and g be two tensor fields, and f^ε and g^ε their topologically perturbed counterpart. We introduce the following notation $\delta(\cdot)^\varepsilon = (\cdot)^\varepsilon - (\cdot)$, and outline the identity

$$\int_{\mathcal{Y}} \gamma_\varepsilon f^\varepsilon \cdot g^\varepsilon - \int_{\mathcal{Y}} f \cdot g = \int_{\mathcal{Y}} \delta f^\varepsilon \cdot \delta g^\varepsilon + \int_{\mathcal{Y}} \delta f^\varepsilon \cdot g + \int_{\mathcal{Y}} f \cdot \delta g^\varepsilon + (\gamma - 1) \int_{B_\varepsilon} f^\varepsilon \cdot g^\varepsilon. \quad (1.169)$$

From this we directly compute

$$\begin{aligned}
(\mathbf{D}^h_\varepsilon - \mathbf{D}^h)_{ijkpqr} = {} & \frac{1}{V} \int_{\mathcal{Y}} \Big(\mathbf{C}(\delta \tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) + \sigma(\delta \tilde{\tilde{u}}^\varepsilon_{ijk}) \Big) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) - \int_{\mathcal{Y}} \sigma(\delta u^\varepsilon_{pq}) \cdot (\tilde{\tilde{u}}_{ijk} \otimes_s \mathrm{e}_r) \\
& + \frac{1}{V} \int_{\mathcal{Y}} \Big(\mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) + \sigma(\tilde{\tilde{u}}_{ijk}) \Big) \cdot (\delta \tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) - \int_{\mathcal{Y}} \sigma(u_{pq}) \cdot (\delta \tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r) \\
& - \frac{1-\gamma}{V} \int_{B_\varepsilon} \Big(\mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) + \sigma(\tilde{\tilde{u}}^\varepsilon_{ijk}) \Big) \cdot (\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) \\
& + \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u^\varepsilon_{pq}) \cdot (\tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r) + \mathcal{E}_1(\varepsilon),
\end{aligned} \quad (1.170)$$

where the remainder $\mathcal{E}_1(\varepsilon)$ is defined as

$$\mathcal{E}_1(\varepsilon) = \frac{1}{V} \int_{\mathcal{Y}} (\sigma(\delta \tilde{\tilde{u}}^\varepsilon_{ijk}) + \mathbf{C}(\delta \tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k)) \cdot (\delta \tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) - \frac{1}{V} \int_{\mathcal{Y}} \sigma(\delta \tilde{u}^\varepsilon_{pq}) \cdot (\delta \tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r), \quad (1.171)$$

since $u^\varepsilon_{ij} := (\mathrm{e}_i \otimes_s \mathrm{e}_j) y + \tilde{u}^\varepsilon_{ij}$, so that $\delta u^\varepsilon_{ij} = \delta \tilde{u}^\varepsilon_{ij}$. By taking into account Lemmas 1.5 and 1.6, the following estimate for the remainder $\mathcal{E}_1(\varepsilon)$ from (1.171) holds true

$$|\mathcal{E}_1(\varepsilon)| = o(\varepsilon^2). \quad (1.172)$$

Let us simplify some other terms in (1.170). We have that $\mathbf{C}^h(\mathrm{e}_p \otimes_s \mathrm{e}_q)$ is a constant tensor and $\delta \tilde{\tilde{u}}^\varepsilon_{ijk}$ is a zero-mean field, so that we can rewrite

$$\int_{\mathcal{Y}} \sigma(u_{pq}) \cdot (\delta \tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r) = \int_{\mathcal{Y}} \Big(\sigma(u_{pq}) - \mathbf{C}^h(\mathrm{e}_p \otimes_s \mathrm{e}_q) \Big) \cdot (\delta \tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r). \quad (1.173)$$

From this, and in view of the variational formulation of $\tilde{\tilde{u}}_{pqr}$ (1.68) written with $\eta = \delta \tilde{\tilde{u}}^\varepsilon_{ijk}$, we can simplify the second term from line one and the third term of line two in (1.170) as follows

$$\begin{aligned}
& \int_{\mathcal{Y}} \sigma(\delta \tilde{\tilde{u}}^\varepsilon_{ijk}) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) - \int_{\mathcal{Y}} \sigma(u_{pq}) \cdot (\delta \tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r) = \\
& \qquad - \int_{\mathcal{Y}} \Big(\sigma(u_{pq}) - \mathbf{C}^h(\mathrm{e}_p \otimes_s \mathrm{e}_q) \Big) \cdot (\delta \tilde{\tilde{u}}^\varepsilon_{ijk} \otimes_s \mathrm{e}_r) + \int_{\mathcal{Y}} \sigma(\delta \tilde{\tilde{u}}^\varepsilon_{ijk}) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) \\
& \qquad = - \int_{\mathcal{Y}} \sigma(\tilde{\tilde{u}}_{pqr}) \cdot e(\delta \tilde{\tilde{u}}^\varepsilon_{ijk}).
\end{aligned} \quad (1.174)$$

We now calculate for all $\eta \in \mathcal{W}$ the equation satisfied by $\delta \tilde{\tilde{u}}^\varepsilon_{ijk}$, subtracting the variational formulation of $\tilde{\tilde{u}}_{ijk}$ (1.68) from the variational formulation of $\tilde{\tilde{u}}^\varepsilon_{ijk}$ (1.108). This gives

$$\begin{aligned}
\int_{\mathcal{Y}} \sigma(\delta \tilde{\tilde{u}}^\varepsilon_{ijk}) \cdot e(\eta) = {} & \int_{\mathcal{Y}} (\sigma(\delta \tilde{u}^\varepsilon_{ij}) - (\mathbf{C}^h_\varepsilon - \mathbf{C}^h)(\mathrm{e}_i \otimes_s \mathrm{e}_j)) \cdot (\eta \otimes \mathrm{e}_k) - \int_{\mathcal{Y}} \mathbf{C}(\delta \tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) \cdot e(\eta) \\
& + (1-\gamma) \int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}^\varepsilon_{ijk}) + \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k)) \cdot e(\eta) - (1-\gamma) \int_{B_\varepsilon} \sigma(u^\varepsilon_{ij}) \cdot (\eta \otimes \mathrm{e}_k).
\end{aligned} \quad (1.175)$$

We set $\eta = \tilde{\tilde{u}}_{pqr}$ in (1.175), and cancel the null terms due to the zero-mean value of $\tilde{\tilde{u}}_{pqr}$, then we inject the resulting expression in (1.174). This leads to the simplification of the all terms depending on $\delta\tilde{\tilde{u}}^{\varepsilon}_{ijk}$ in (1.170). Reordering the members of the equation in order to gather the terms of the type $\delta\tilde{u}^{\varepsilon}_{ij}$ and $\delta\tilde{u}^{\varepsilon}_{pq}$, we find

$$\begin{aligned} V(\mathbf{D}^h_\varepsilon - \mathbf{D}^h)_{ijkpqr} = & \int_{\mathcal{Y}} \Big(\mathbf{C}(\delta\tilde{u}^{\varepsilon}_{ij} \otimes_s \mathrm{e}_k)\Big) \cdot \Big((\tilde{u}_{pq} \otimes_s \mathrm{e}_r) + e(\tilde{\tilde{u}}_{pqr})\Big) - \int_{\mathcal{Y}} \sigma(\delta\tilde{u}^{\varepsilon}_{ij}) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) \\ & + \int_{\mathcal{Y}} \Big(\mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) + \sigma(\tilde{\tilde{u}}_{ijk})\Big) \cdot (\delta\tilde{u}^{\varepsilon}_{pq} \otimes_s \mathrm{e}_r) - \int_{\mathcal{Y}} \sigma(\delta u^{\varepsilon}_{pq}) \cdot (\tilde{\tilde{u}}_{ijk} \otimes_s \mathrm{e}_r) \\ & + (1-\gamma) \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{ij}) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) + (1-\gamma) \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{pq}) \cdot (\tilde{\tilde{u}}^{\varepsilon}_{ijk} \otimes_s \mathrm{e}_r) \\ & - (1-\gamma) \int_{B_\varepsilon} \Big(\sigma(\tilde{\tilde{u}}^{\varepsilon}_{ijk}) + \mathbf{C}(\tilde{u}^{\varepsilon}_{ij} \otimes_s \mathrm{e}_k)\Big) \cdot \Big(e(\tilde{\tilde{u}}_{pqr}) + (\tilde{u}^{\varepsilon}_{pq} \otimes_s \mathrm{e}_r)\Big) \\ & + \mathcal{E}_1(\varepsilon). \end{aligned} \tag{1.176}$$

In order to simplify further analysis, the introduction of convenient adjoint states $p^r_{ijk} \in \mathcal{V}$ for $i, j, k, r \in \{1, 2\}$ is required, which are solutions of the following set of variational problems:

$$\begin{aligned} p^k_{pqr} \in \mathcal{V} \ : \ \int_{\mathcal{Y}} \sigma(p^k_{pqr}) \cdot e(\eta) = & \int_{\mathcal{Y}} \Big(\sigma(\tilde{\tilde{u}}_{pqr}) + \mathbf{C}(\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\Big) \cdot (\eta \otimes_s \mathrm{e}_k) \\ & - \int_{\mathcal{Y}} \mathbf{C}(\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) \cdot e(\eta) \\ & - \int_{\mathcal{Y}} \Big\langle \sigma(\tilde{\tilde{u}}_{pqr}) + \mathbf{C}(\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\Big\rangle \cdot (\eta \otimes_s \mathrm{e}_k), \quad \forall \eta \in \mathcal{W}. \end{aligned} \tag{1.177}$$

Let us set $\eta = \delta\tilde{u}^{\varepsilon}_{ij}$ and $\eta = \delta\tilde{u}^{\varepsilon}_{pq}$ in the adjoint equation (1.177) for p^k_{pqr} and p^r_{ijk}, respectively. We remark that the last term of (1.177) is equal to zero in this case because $\delta\tilde{u}^{\varepsilon}_{ij}$ and $\delta\tilde{u}^{\varepsilon}_{pq}$ have a zero mean value, while $\langle\sigma(\tilde{\tilde{u}}_{pqr}) + \mathbf{C}(\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\rangle$ is a constant volume average by definition (1.44). Now, we set $\eta = p^r_{ijk}$ in the variational formulation satisfied by $\delta\tilde{u}^{\varepsilon}_{pq}$ (1.148), and $\eta = p^k_{pqr}$ after replacing the indexes ij by pq. By combining these two expressions, we can simplify the two first lines of the right-hand side of (1.176), and we obtain

$$\begin{aligned} (\mathbf{D}^h_\varepsilon - \mathbf{D}^h)_{ijkpqr} = & \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{ij}) \cdot (e(p^k_{pqr}) + (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k)) \\ & + \frac{1-\gamma}{V} \int_{B_\varepsilon} \sigma(u^{\varepsilon}_{pq}) \cdot (e(p^r_{ijk}) + (\tilde{\tilde{u}}_{ijk} \otimes_s \mathrm{e}_r)) \\ & - \frac{1-\gamma}{V} \int_{B_\varepsilon} \Big(\sigma(\tilde{\tilde{u}}^{\varepsilon}_{ijk}) + \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)\Big) \cdot \Big(e(\tilde{\tilde{u}}_{pqr}) + (\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\Big) + o(\varepsilon^2). \end{aligned} \tag{1.178}$$

We start developing the third term of the right-hand side of expression (1.178). Once again, we will show in Section 1.5 that we can write

$$\tilde{\tilde{u}}^{\varepsilon}_{ijk} = \tilde{\tilde{u}}_{ijk} + w^{\varepsilon}_{ijk} + R_\varepsilon, \tag{1.179}$$

where $\|R_\varepsilon\|_{H^1(\mathcal{Y})} = o(\varepsilon^2)$, and w^{ε}_{ijk} is the solution of the following transmission problem in elasticity

$$\left\{ \begin{array}{rcll} \mathrm{div}(\gamma_\varepsilon \sigma(w^\varepsilon)) & = & 0 & \text{in} \quad \mathbb{R}^2, \\ w^\varepsilon & \to & 0 & \text{at} \quad \infty, \\ [\![w^\varepsilon]\!] & = & 0 & \text{on} \quad \partial\omega_\varepsilon, \\ [\![\gamma_\varepsilon \sigma(w^\varepsilon)]\!] n & = & \psi & \text{on} \quad \partial\omega_\varepsilon, \end{array} \right. \tag{1.180}$$

where $\psi = -(1-\gamma)\left(\sigma(\tilde{\tilde{u}})(\hat{y}) + \mathbf{C}(\tilde{u}(\hat{y}) \otimes_s \mathrm{e})\right) n$. We recall that the inclusion B_ε is located neither on the interface nor on the boundary, so that the solutions of elliptic boundary value problems are smooth in B_ε by the elliptic regularity. Using the *Ansatz* (1.179) combined with the Lebesgue differentiation theorem, we derive

$$\begin{aligned}\frac{(1-\gamma)}{V}&\int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}^\varepsilon_{ijk}) + \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)) \cdot \left(e(\tilde{\tilde{u}}_{pqr}) + (\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\right)\\ &= \frac{1-\gamma}{V}\Bigg(\pi\varepsilon^2 \left(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)\right) \cdot \left(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)\right)\\ &\qquad + \left[\int_{B_\varepsilon} \sigma(w^\varepsilon)\right] \cdot \left(e(\tilde{\tilde{u}}_{pqr}) + (\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\right)\Bigg) + o(\varepsilon^2).\end{aligned}$$

From Eshelby's Theorem 1.7, we deduce that

$$\begin{aligned}\frac{(1-\gamma)}{V}&\int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}^\varepsilon_{ijk}) + \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)) \cdot \left(e(\tilde{\tilde{u}}_{pqr}) + (\tilde{u}_{pq} \otimes_s \mathrm{e}_r)\right)\\ &= \frac{1-\gamma}{V}\Bigg(\left(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)\right) \cdot \left(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)\right)\\ &\qquad + \pi\varepsilon^2\bar{\mathbb{T}}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot \left(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)\right)\Bigg) + o(\varepsilon^2),\\ &= \frac{\pi\varepsilon^2}{V}(1-\gamma)(\mathbb{I}+\bar{\mathbb{T}})\left(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)\right) \cdot \left(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)\right) + o(\varepsilon^2)\\ &= -\frac{\pi\varepsilon^2}{V}\mathbb{P}\left(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)\right) \cdot \left(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)\right) + o(\varepsilon^2).\end{aligned} \tag{1.181}$$

For the first two terms of the right-hand side of equation (1.178), the calculations to be led are exactly the same as those from the previous section, needing only the estimation on $\tilde{u}^\varepsilon_{ij}$. Then we deduce together with (1.181) the asymptotic expansion (1.164). The main result of this section is proved. □

Remark 4. *We can cover as well the case of three spatial dimensions which is important in applications. In particular, the method of asymptotic analysis performed in $\mathbb{R}^2$ can be extended to $\mathbb{R}^3$. In three spatial dimensions, the topological expansion of homogenized tensors is obtained by setting $g(\varepsilon) = (4/3)\pi\varepsilon^3/V$ and replacing the polarization tensor by [AK07]*

$$\mathbb{P} = -3\beta\mathbb{I} - (\alpha-\beta)\mathrm{I}\otimes\mathrm{I}, \tag{1.182}$$

with the coefficients α and β redefined as follows

$$\alpha = \frac{(1-\nu)(1-\gamma)}{3(1-\nu)-(1+\nu)(1-\gamma)} \quad \textit{and} \quad \beta = \frac{5(1-\nu)(1-\gamma)}{15(1-\nu)-2(4-5\nu)(1-\gamma)}, \tag{1.183}$$

where ν the Poisson ratio.

Finally, it is important to note that formula (1.165) can be used to evaluate the topological derivative of any differentiable function of $\mathbf{D}^h$ through the direct application of the chain rule for composed functions. That is, any such function $\mathbf{D}^h \mapsto \mathcal{J}(\mathbf{D}^h)$ admits the topological derivative of the form

$$D_T\mathcal{J}(\mathbf{D}^h) = \left\langle D\mathcal{J}(\mathbf{D}^h), D_T\mathbf{D}^h \right\rangle , \tag{1.184}$$

with the brackets $\langle\cdot,\cdot\rangle$ denoting the appropriate product between the derivative of $\mathcal{J}$ with respect to $\mathbf{D}^h$ and the topological derivative $D_T\mathbf{D}^h$ of $\mathbf{D}^h$. In order to fix these ideas, let us consider a pair $\Phi_1, \Phi_2 \in \mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R}^2$ of third order tensors. Then we obtain the following results, which can be used in numerical methods of synthesis and/or topology design of microstructures analogously to [Ams+10]:

Example 5. *We consider a function $\mathcal{J}(\mathbf{D}^h)$ of the form*

$$\mathcal{J}(\mathbf{D}^h) := \mathbf{D}^h\Phi_1 \cdot \Phi_2 \; . \tag{1.185}$$

Therefore, according to (1.184)*, its topological derivative is given by*

$$D_T\mathcal{J}(\mathbf{D}^h) = (D_T\mathbf{D}^h)\Phi_1 \cdot \Phi_2 \; . \tag{1.186}$$

If we set $\Phi_1 = \mathrm{e}_i \otimes \mathrm{e}_j \otimes \mathrm{e}_k$ and $\Phi_2 = \mathrm{e}_l \otimes \mathrm{e}_m \otimes \mathrm{e}_n$, for instance, we get $\mathcal{J}(\mathbf{D}^h) = (\mathbf{D}^h)_{ijklmn}$ and its topological derivative is given by $D_T\mathcal{J}(\mathbf{D}^h) = (D_T\mathbf{D}^h)_{ijklmn}$. It means that $D_T\mathcal{J}(\mathbf{D}^h)$ actually represents the topological derivative of the components $(\mathbf{D}^h)_{ijklmn}$ of the tensor $\mathbf{D}^h$.

1.4 Conclusion and perspectives

In [Ams+10], the topological derivative of the fourth order homogenized elasticity tensor $\mathbf{C}^h$ as been calculated. In [BCG18] the topological derivative of the second-order macroscopic model associated with scalar waves in periodic media has been evaluated.

In this chapter, we have calculated the topological derivative of the second order homogenized elasticity tensor $\mathbf{D}^h$ with respect to the nucleation of circular inclusions of weak material at the microscopic level, by adapting to the periodic case a method of direct computation which is explained in [NS13]. The sensitivity of $\mathbf{D}^h$ to this topological perturbation has been derived in closed form with the help of appropriate adjoint states. We obtain the following formula for the topological derivative of $\mathbf{D}^h$, given in index format by

$$\begin{aligned}
(D_T\mathbf{D}^h)_{ijkpqr}(\hat{y}) = & -\mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot (e(p^k_{pqr})(\hat{y}) + (\tilde{\tilde{u}}_{pqr}(\hat{y}) \otimes_s \mathrm{e}_k)) \\
& - \mathbb{P}\sigma(u_{pq})(\hat{y}) \cdot (e(p^r_{ijk})(\hat{y}) + (\tilde{\tilde{u}}_{ijk}(\hat{y}) \otimes_s \mathrm{e}_r)) \\
& + \mathbb{P}\left(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)\right) \cdot \left(e(\tilde{\tilde{u}}_{pqr})(\hat{y}) + (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)\right) ,
\end{aligned}$$

where $\mathbb{P}$ is the polarization tensor given by (1.139). As expected, the computed topological derivatives lead to tensor fields over the microstructural domain, depending on the center of the perturbation $\hat{y}$, and measuring the sensitivity of the homogenized tensors to these topological microstructural changes, with respect to its center $\hat{y}$.

Therefore, we are going to use this information in Chapter 2, in the context of synthesis and optimal design of metamaterials, for instance, accounting for second order mechanical effects.

The topological derivative of the fifth order tensor $\mathbf{E}^h$ appearing at order τ in the expression (1.70) of the macroscopic energy, and the topological derivative of the sixth-order tensor $\mathbf{F}^h$ defined in (1.75) have also been calculated. The method and the computations being of the same kind as those led in Sections 1.3.4 and 1.3.5, we relegate the topological derivatives of $\mathbf{E}^h$ and $\mathbf{F}^h$ to Appendix B. These extra topological derivatives are written with the purpose of further use and applications.

The limit case associated with the nucleation of a very weak inclusion is interesting. This case corresponds to a material of the same type as that described in Section 1.3.2, for which the contrast γ_0 goes to zero. It allows somehow to describe the behaviour of a material with voids. First, the behaviour of the topological derivative is non trivial in this case. Moreover, the computation of the topological derivative in the case where the weak material is replaced by voids is rather complex. Secondly we will see in Section 2.4 that a vanishing contrast is interesting from a numerical topological optimization point of view, and also from the mathematical point of view, although this is a more difficult issue not analyzed in this thesis.

As we illustrate in Section 2.4 (see Figure 27), it is shown in [DK10] that the displacement solution of a material containing weak inclusions converges in H^1-norm to the displacement solution of a material containing voids inclusions.

As a perspective, we are working on the study of the asymptotic behaviour of the homogenized tensors we have presented in this chapter, by varying the size of the inclusion ε together with the contrast γ_0. This work being not accomplished, it does not take part of this thesis manuscript.

Another study that would be very interesting to carry out, is to also take into account the size parameter of homogenization τ. On the one hand we can directly study the asymptotic expansion of the homogenized tensors with respect to the size ε of a void perturbation, and in the same time we can investigate the convergence of the homogenization scheme. Namely we can investigate how behaves the homogenized energy $\mathscr{E}^h_{\tau,\varepsilon}$ when both τ and ε vanishes. This will probably leads to kinds of behaviours which were identified in [MC82]. Recently, this has been studied in the case of elastic materials with Dirichlet inclusions [Jin21]. On the other hand, we can simplify the analysis of the topological sensitivity by considering weak material characterised by a contrast γ_0 instead of voids. Thus we could analyse the behaviour of the homogenized tensors when τ, ε, and γ_0 vary.

1.5 Appendix: proofs of the estimations

For the convenience of the reader we provide the proofs of the auxiliary lemmas which are used to evaluate of the topological derivatives of homogenized tensors.

1.5.1 Preliminary lemmas

We give in this subsection some useful preliminary results for the proof of Lemmas 1.5 and 1.6. We consider $\mathcal{Y}$ an open bounded subset of $\mathbb{R}^2$, with $\partial\mathcal{Y}$ of class C^1, and $\hat{y}$ a fixed arbitrary point of $\mathcal{Y}$. We denote by B_ε be the small disk of radius ε, centered at $\hat{y}$, and take $\varepsilon_0 > 0$, such that $\overline{B_\varepsilon} \subset \mathcal{Y}$ for all $0 < \varepsilon \leqslant \varepsilon_0$. We have the following results.

Lemma 1.12. *Let $\eta \in H^1(\mathcal{Y})$, $\hat{y} \in \mathcal{Y}$. Then for all $0 < \delta \leq 1$ there exists a constant $c_{(\delta)} > 0$ depending on δ and $\mathcal{Y}$, such that for all $0 < \varepsilon \leq \varepsilon_0$*

$$\left| \int_{B_\varepsilon} \eta(x) dx \right| \leqslant c_{(\delta)} \varepsilon^{2-\delta} \|\eta\|_{H^1(\mathcal{Y})}. \tag{1.187}$$

Proof: This result derives directly from the Sobolev Embedding Theorem, giving that $H^1(\mathcal{Y})$ embeds continuously into $L^p(\mathcal{Y})$ for all $2 \leq p < +\infty$ (see e.g. [Bre11]), and with the use of Hölder inequality for $\eta \in L^p(B_\varepsilon)$, $1 \in L^q(B_\varepsilon)$, with $q^{-1} = 1 - p^{-1} \in [1/2, 1)$, setting $\delta := 2(q-1)/q$. □

Lemma 1.13. *Let $\eta \in H^1(\mathcal{Y}; \mathbb{R}^2)$. Then we have for all $\delta > 0$ a constant $c_{(\delta)} > 0$ depending on δ and $\mathcal{Y}$ such that for all $0 < \varepsilon \leq \varepsilon_0$*

$$\|\eta\|_{L^2(\partial B_\varepsilon; \mathbb{R}^2)} \leq c_{(\delta)} \varepsilon^{1/2-\delta} \|\eta\|_{H^1(\mathcal{Y}; \mathbb{R}^2)}. \tag{1.188}$$

Proof: For simplicity we set $\varepsilon_0 = 1$. Let $0 < \varepsilon \leq 1$ and $\eta \in H^1(\mathcal{Y}; \mathbb{R}^2)$. We introduce $\phi_\varepsilon : B_1 \to B_\varepsilon$ the diffeomorphism defined by $\phi_\varepsilon(x) = \varepsilon x$ for all $x \in B_1$. The restriction $\phi_\varepsilon : \partial B_1 \to \partial B_\varepsilon$ is also a diffeomorphism, allowing us the following change of variable

$$\begin{aligned} \int_{\partial B_\varepsilon} \mid \eta \mid^2 d\Gamma_\varepsilon &= \int_{\partial B_1} \mid \eta \circ \phi_\varepsilon \mid^2 \varepsilon \, d\Gamma_1, \\ &= \varepsilon \|\eta \circ \phi_\varepsilon\|^2_{L^2(\partial B_1; \mathbb{R}^2)}, \\ &\leq c^2_{(1)} \varepsilon \|\eta \circ \phi_\varepsilon\|^2_{H^1(B_1; \mathbb{R}^2)}, \end{aligned} \tag{1.189}$$

where $c_{(1)} > 0$ is the fixed constant given by the Trace theorem applied on $H^1(B_1; \mathbb{R}^2)$. Once again, a change of variable yields

$$\|\eta \circ \phi_\varepsilon\|^2_{L^2(B_1; \mathbb{R}^2)} = \frac{1}{\varepsilon^2} \|\eta\|^2_{L^2(B_\varepsilon; \mathbb{R}^2)}, \tag{1.190}$$

and

$$\|\nabla(\eta \circ \phi_\varepsilon)\|^2_{L^2(B_1; \mathbb{R}^2)} = \int_{B_1} \mid \nabla(\eta \circ \phi_\varepsilon) \mid^2 dx = \int_{B_1} \varepsilon^2 \mid \nabla(\eta) \circ \phi_\varepsilon \mid^2 dx = \|\nabla \eta\|^2_{L^2(B_\varepsilon; \mathbb{R}^2)}.$$

Then we have

$$\|\eta\|^2_{L^2(\partial B_\varepsilon; \mathbb{R}^2)} \leq c^2_{(1)} \left(\varepsilon^{-1} \|\eta\|^2_{L^2(B_\varepsilon; \mathbb{R}^2)} + \varepsilon \|\nabla \eta\|^2_{L^2(\mathcal{Y}; \mathbb{R}^2)} \right). \tag{1.191}$$

The Sobolev Embedding Theorem gives $H^1(\mathcal{Y}; \mathbb{R}^2) \hookrightarrow L^p(\mathcal{Y}; \mathbb{R}^2)$ continuously, for all $2 \leq p < +\infty$. Then from Hölder inequality with $q^{-1} = 1 - (p/2)^{-1}$, $q \in (1, +\infty]$ we have

$$\begin{aligned} \int_{B_\varepsilon} \mid \eta \mid^2 dx &\leq \| \, |\eta|^2 \|_{L^{p/2}(B_\varepsilon; \mathbb{R}^2)} \|1\|_{L^q(B_\varepsilon; \mathbb{R}^2)}, \\ &\leq \|\eta\|^2_{L^p(B_\varepsilon; \mathbb{R}^2)} \|1\|_{L^q(B_\varepsilon; \mathbb{R}^2)}, \\ &\leq K_2 \|\eta\|^2_{L^p(\mathcal{Y}; \mathbb{R}^2)} \varepsilon^{2/q}, \\ &\leq K_2 c_{(p)} \varepsilon^{2/q} \|\eta\|^2_{H^1(\mathcal{Y}; \mathbb{R}^2)}. \end{aligned} \tag{1.192}$$

where $c_{(p)}$ is a constant depending only on p and $\mathcal{Y}$ given by the Sobolev Embedding Theorem. Thus we can carry on the derivation of inequality (1.191)

$$\|\eta\|^2_{L^2(\partial B_\varepsilon; \mathbb{R}^2)} \leq c^2_{(1)} (K_2 c_{(p)} \varepsilon^{2/q-1} + \varepsilon) \|\eta\|^2_{H^1(\mathcal{Y}; \mathbb{R}^2)},$$

$$\leq c_{(\delta)}\varepsilon^{1-2\delta}\|\eta\|^2_{H^1(\mathcal{Y};\mathbb{R}^2)}, \tag{1.193}$$

for $\delta > 0$ as small as we want when q goes to 1. We finally conclude taking the square root of the last inequality. □

Proposition 1.14. *Let $\mathcal{Y}_1$ and $\mathcal{Y}_2$ be two open bounded domains, with boundaries $\partial\mathcal{Y}_1$ and $\partial\mathcal{Y}_2$ of class C^1, such that $\overline{\mathcal{Y}_1} \subset \mathcal{Y}_2$. For all $\psi \in H^1(\mathcal{Y}_2 \setminus \overline{\mathcal{Y}_1})$, such that $\operatorname{div}\sigma(\psi) = 0$, we have a constant $c > 0$ such that*

$$\|\sigma(\psi)n\|_{H^{-1/2}(\partial\mathcal{Y}_2)} \leq c|\psi|_{1,\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1}} := c\left(\int_{\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1}} \sigma(\psi)\cdot e(\psi)\right)^{1/2}, \tag{1.194}$$

where n is the unit normal vector to $\partial\mathcal{Y}_2$.

Proof: Let $\phi \in H^{1/2}(\partial\mathcal{Y}_2)$, we denote by $\tilde{\phi} \in H^1(\mathcal{Y}_2 \setminus \overline{\mathcal{Y}_1}, \mathbb{R}^n)$ the unique solution of

$$\begin{cases} -\operatorname{div}\sigma(\tilde{\phi}) = 0 & \text{in } \mathcal{Y}_2 \setminus \overline{\mathcal{Y}_1}, \\ \tilde{\phi} = \phi & \text{on } \partial\mathcal{Y}_2, \\ \tilde{\phi} = 0 & \text{on } \partial\mathcal{Y}_1. \end{cases} \tag{1.195}$$

This way we can write

$$\int_{\partial\mathcal{Y}_2} \sigma(\psi)n\cdot\phi = \int_{\partial\mathcal{Y}_1\cup\partial\mathcal{Y}_2} \sigma(\psi)n\cdot\tilde{\phi},$$

and apply Green formula, which simplifies by the assumption $\operatorname{div}\sigma(\psi) = 0$, according to Hölder inequality, and in view of elliptic regularity for the solution $\tilde{\phi}$. This gives the existence of a positive constant c coming from a priori estimates of the solution of the Dirichlet problem (1.195) posed on $\mathcal{Y}_2 \setminus \overline{\mathcal{Y}_1}$ such that

$$\int_{\partial\mathcal{Y}_2} \sigma(\psi)n\cdot\phi = \int_{\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1}} \sigma(\psi)\cdot e(\tilde{\phi}) \leq |\psi|_{1,\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1}}|\tilde{\phi}|_{1,\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1}} \leq c|\psi|_{1,\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1}}\|\phi\|_{H^{1/2}(\partial\mathcal{Y}_2)}.$$

□

Proposition 1.15 ([GGM01] Section 4.1)**.** *Let $\mathcal{Y}_1$ and $\mathcal{Y}_2$ be two open bounded domains, with boundaries $\partial\mathcal{Y}_1$ and $\partial\mathcal{Y}_2$ of class C^1, such that $\overline{\mathcal{Y}_1} \subset \mathcal{Y}_2$, and $v \in H^{1/2}(\partial\mathcal{Y}_1)$. The usual norm on $H^{1/2}(\partial\mathcal{Y}_1)$ is equivalent to the following one*

$$\|v\|_{H^{1/2}(\partial\mathcal{Y}_1)} = \inf\left\{\|u\|_{H^1(\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1})};\ u = v \text{ on } \partial\mathcal{Y}_1\right\}$$

In particular, if $v \in H^1(\mathcal{Y}_2)$, we have

$$\|v\|_{H^{1/2}(\partial\mathcal{Y}_1)} \leq \|v\|_{H^1(\mathcal{Y}_2\setminus\overline{\mathcal{Y}_1})}$$

We end this preliminary section presenting convenient notation used to name the norms and seminorms of the needed function spaces. For an open set $\mathcal{Y} \subset \mathbb{R}^2$, bounded, connected and with Lipschitz continuous boundary, $H^1(\mathcal{Y}, \mathbb{R}^2)$ is endowed with a norm equivalent to the usual one, due to Korn's inequality [Neč67], defined by

$$\|\eta\|_{1,\mathcal{Y}}^2 := \int_{\mathcal{Y}} (\sigma(u) \cdot e(u) + u \cdot u). \tag{1.196}$$

We also define in $H^1(\mathcal{Y}, \mathbb{R}^2)$ the seminorm

$$|\eta|_{1,\mathcal{Y}}^2 := \int_{\mathcal{Y}} \sigma(u) \cdot e(u). \tag{1.197}$$

We finally denote the usual norms of $L^2(\mathcal{Y}, \mathbb{R}^2)$, $H^{1/2}(\partial\mathcal{Y}, \mathbb{R}^2)$ and $H^{-1/2}(\partial\mathcal{Y}, \mathbb{R}^2)$, respectively by $\|\eta\|_{0,\mathcal{Y}}$, $\|\eta\|_{1/2,\partial\mathcal{Y}}$, and $\|\eta\|_{-1/2,\partial\mathcal{Y}}$.

1.5.2 Proof of Lemma 1.5

Proof: Let us introduce an *Ansatz* of the form [KMM99]

$$\tilde{u}_{ij}^{\varepsilon}(y) = \tilde{u}_{ij}(y) + w_{ij}^{\varepsilon}(y) + z_{ij}^{\varepsilon}(y), \tag{1.198}$$

where w_{ij}^{ε} is solution to the following transmission problem:

$$\left\{ \begin{array}{rcll} \mathrm{div}(\gamma_\varepsilon \sigma(w_{ij}^{\varepsilon})) & = & 0 & \text{in} \quad \mathbb{R}^2, \\ w_{ij}^{\varepsilon} & \to & 0 & \text{at} \quad \infty, \\ [\![w_{ij}^{\varepsilon}]\!] & = & 0 & \text{on} \quad \partial B_\varepsilon, \\ [\![\gamma_\varepsilon \sigma(w_{ij}^{\varepsilon})]\!] n & = & h & \text{on} \quad \partial B_\varepsilon, \end{array} \right. \tag{1.199}$$

where $h = -(1-\gamma)\sigma(u_{ij})(\hat{y})n$, n being the inward normal vector on ∂B_ε, and $[\![\cdot]\!]$ denotes the jump across the interface of the inclusion:

$$[\![\cdot]\!] = (\cdot)_{\mathcal{Y}\setminus\overline{B_\varepsilon}} - (\cdot)_{B_\varepsilon} \quad \text{on} \quad \partial B_\varepsilon. \tag{1.200}$$

The solution w_{ij}^{ε} of this classical problem is explicitly known [Bar92], and gives rise to the following estimates:

$$\|w_{ij}^{\varepsilon}\|_{0,\mathcal{Y}} = o(\varepsilon), \tag{1.201}$$

$$\|w_{ij}^{\varepsilon}\|_{1,\mathcal{Y}} = O(\varepsilon), \tag{1.202}$$

$$\|w_{ij}^{\varepsilon}\|_{1,\mathcal{Y}_R} = O(\varepsilon^2), \tag{1.203}$$

where $\mathcal{Y}_R$ is defined by (1.116) as

$$\mathcal{Y}_R := \mathcal{Y} \setminus B_R(\hat{y}), \tag{1.204}$$

where $B_R(\hat{y})$ is the ball of radius R and center $\hat{y}$, and R is chosen such that $B_R(\hat{y})$ does not intersect an interface nor the boundary, and contains the inclusion $B_\varepsilon(\hat{y})$ (see Figure 9). We want to estimate z_{ij}^{ε} which compensates the discrepancies introduced by w_{ij}^{ε}. Defined as in (1.198), we don't have $z_{ij}^{\varepsilon} \in H^1_{\mathrm{per}}(\mathcal{Y}; \mathbb{R}^2)$. To overcome this drawback, we slightly modify w_{ij}^{ε} near the boundary $\partial\mathcal{Y}$. We define the ring

$$C := \{y \in \mathcal{Y} \mid \mathrm{dist}(y, \partial\mathcal{Y}) < \epsilon\}, \tag{1.205}$$

$$\partial C^{\mathrm{int}} := \{y \in \mathcal{Y} \mid \mathrm{dist}(y, \partial\mathcal{Y}) = \epsilon\}, \tag{1.206}$$

with $\partial C = \partial \mathcal{Y} \cup \partial C^{\rm int}$, for a fixed $\epsilon > 0$ small enough to have $\overline{B_R(\hat{y})} \subset \mathcal{Y} \setminus \overline{C}$. Then we set

$$w_{ij}^{\varepsilon,\epsilon}(y) := \begin{cases} w_{ij}^{\varepsilon}(y) & \text{if } y \in \mathcal{Y} \setminus \overline{C}, \\ w_{C,ij}^{\varepsilon}(y) & \text{if } y \in C, \end{cases} \tag{1.207}$$

where $w_{C,ij}^{\varepsilon}$ is solution to the following boundary value problem

$$\left\{ \begin{array}{rcll} \operatorname{div}(\sigma(w_{C,ij}^{\varepsilon})) & = & 0 & \text{in } \ C, \\ w_{C,ij}^{\varepsilon} & = & 0 & \text{on } \ \partial\mathcal{Y}, \\ w_{C,ij}^{\varepsilon} & = & w_{ij}^{\varepsilon} & \text{on } \ \partial C^{\rm int}. \end{array} \right. \tag{1.208}$$

Defined this way, we have that $w_{ij}^{\varepsilon,\epsilon}$ belongs to $H^1(\mathcal{Y}, \mathbb{R}^2)$. Let us introduce the new *Ansatz*

$$\tilde{u}_{ij}^{\varepsilon}(y) = \tilde{u}_{ij}(y) + \tilde{w}_{ij}^{\varepsilon}(y) + \tilde{z}_{ij}^{\varepsilon}(y), \tag{1.209}$$

with

$$\tilde{w}_{ij}^{\varepsilon} := w_{ij}^{\varepsilon,\epsilon} - \langle w_{ij}^{\varepsilon,\epsilon} \rangle, \tag{1.210}$$

where $\langle \cdot \rangle$ denotes the mean value over $\mathcal{Y}$ defined as in (1.44), so that $\tilde{w}_{ij}^{\varepsilon} \in \mathcal{V}$, and therefore $\tilde{z}_{ij}^{\varepsilon} \in H^1_{\rm per}(\mathcal{Y}; \mathbb{R}^2)$ with $\langle \tilde{z}_{ij}^{\varepsilon} \rangle = 0$. Thus we can calculate the variational problem satisfied by $\tilde{z}_{ij}^{\varepsilon}$. First we recall that $\tilde{u}_{ij}$ and $\tilde{u}_{ij}^{\varepsilon}$ satisfy the following variational equations

$$\tilde{u}_{ij} \in \mathcal{V} \ : \ \int_{\mathcal{Y}} \sigma(\tilde{u}_{ij}) \cdot e(\eta) + \int_{\mathcal{Y}} \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot e(\eta) = 0 \quad \forall \eta \in \mathcal{V}, \tag{1.211}$$

and

$$\tilde{u}_{ij}^{\varepsilon} \in \mathcal{V} \ : \ \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{u}_{ij}^{\varepsilon}) \cdot e(\eta) + \int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot e(\eta) = 0 \quad \forall \eta \in \mathcal{V}. \tag{1.212}$$

Let us apply the operator $\gamma_\varepsilon \sigma$ to (1.209), multiply the obtained expression by $e(\eta)$ where η is a test function in $H^1_{\rm per}(\mathcal{Y}; \mathbb{R}^2)$, and integrate over $\mathcal{Y}$. From (1.211) and (1.212), we can directly simplify the term

$$\begin{aligned} \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{z}_{ij}^{\varepsilon}) \cdot e(\eta) &= \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{u}_{ij}^{\varepsilon}) \cdot e(\eta) - \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{u}_{ij}) \cdot e(\eta) - \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{w}_{ij}^{\varepsilon}) \cdot e(\eta) \\ &= \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{u}_{ij}^{\varepsilon}) \cdot e(\eta) - \int_{\mathcal{Y}} \sigma(\tilde{u}_{ij}) \cdot e(\eta) + (1-\gamma) \int_{B_\varepsilon} \sigma(\tilde{u}_{ij}) \cdot e(\eta) \\ &\quad - \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{w}_{ij}^{\varepsilon}) \cdot e(\eta) \\ &= (1-\gamma) \int_{B_\varepsilon} \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot e(\eta) + (1-\gamma) \int_{B_\varepsilon} \sigma(\tilde{u}_{ij}) \cdot e(\eta) \\ &\quad - \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{w}_{ij}^{\varepsilon}) \cdot e(\eta) \\ &= (1-\gamma) \int_{B_\varepsilon} \sigma(u_{ij}) \cdot e(\eta) - \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{w}_{ij}^{\varepsilon}) \cdot e(\eta), \end{aligned} \tag{1.213}$$

where the last simplification arises from the definition (1.60) of u_{ij}. Applying the Green formula over $C \cap \mathcal{Y}$, $(\mathcal{Y} \setminus \overline{C \cup B_\varepsilon})$, and B_ε to the integral term depending on $\tilde{w}_{ij}^{\varepsilon}$, we obtain

$$\begin{aligned} \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\tilde{z}_{ij}^{\varepsilon}) \cdot e(\eta) = (1-\gamma) \int_{B_\varepsilon} \sigma(u_{ij}) \cdot e(\eta) \\ + \int_{\mathcal{Y} \cap C} \operatorname{div}(\sigma(w_{C,ij}^{\varepsilon})) \cdot \eta + \int_{B_\varepsilon} \gamma \operatorname{div}(\sigma(w_{ij}^{\varepsilon})) \cdot \eta + \int_{\mathcal{Y} \setminus (B_\varepsilon \cup C)} \operatorname{div}(\sigma(w_{ij}^{\varepsilon})) \cdot \eta \end{aligned}$$

$$
\begin{aligned}
&-\int_{\partial\mathcal{Y}} \sigma(w^{\varepsilon}_{C,ij})n\cdot\eta - \int_{\partial C^{\text{int}}} (\sigma(w^{\varepsilon}_{C,ij}) - \sigma(w^{\varepsilon}_{ij}))n\cdot\eta \\
&-\int_{\partial B_\varepsilon} \sigma(w^{\varepsilon}_{ij}))n\cdot\eta + \int_{\partial B_\varepsilon} \gamma\sigma(w^{\varepsilon}_{ij}))n\cdot\eta,
\end{aligned}
\tag{1.214}
$$

where n is the normal vector systematically pointing outward of $\partial\mathcal{Y}$, inward on ∂B_ε, and outward from C on ∂C^{int}. In view of (1.199) and (1.208), we can cancel the second line of the right-hand side of (1.214), and we can simplify the last line being equal to $-\int_{\partial B_\varepsilon}[\![\gamma_\varepsilon\sigma_y(w^{\varepsilon}_{ij})]\!]n\cdot\eta$, because of the boundary condition satisfied by w^{ε}_{ij} on ∂B_ε in (1.199), namely

$$
-\int_{\partial B_\varepsilon}[\![\gamma_\varepsilon\sigma_y(w^{\varepsilon}_{ij})]\!]n\cdot\eta = -\int_{\partial B_\varepsilon}(-(1-\gamma))\sigma(u_{ij})(\hat{y})n\cdot\eta
\tag{1.215}
$$

We have then

$$
\begin{aligned}
\int_{\mathcal{Y}} \gamma_\varepsilon\sigma(\tilde{z}^{\varepsilon}_{ij})\cdot e(\eta) =&(1-\gamma)\int_{B_\varepsilon}\sigma(u_{ij})\cdot e(\eta) - (1-\gamma)\int_{\partial B_\varepsilon}\sigma(u_{ij})(\hat{y})(-n)\cdot\eta \\
&-\int_{\partial\mathcal{Y}} \sigma(w^{\varepsilon}_{C,ij})n\cdot\eta - \int_{\partial C^{\text{int}}} (\sigma(w^{\varepsilon}_{C,ij}) - \sigma(w^{\varepsilon}_{ij}))n\cdot\eta.
\end{aligned}
\tag{1.216}
$$

Applying again Green's formula to $\int_{\partial B_\varepsilon}\sigma(u_{ij})(\hat{y})(-n)\cdot\eta$, we get

$$
\begin{aligned}
\tilde{z}^{\varepsilon}_{ij}\in\mathcal{W}\ :\ \int_{\mathcal{Y}}\gamma_\varepsilon\sigma(\tilde{z}^{\varepsilon}_{ij})\cdot e(\eta) &= (1-\gamma)\int_{B_\varepsilon}(\sigma(u_{ij}) - \sigma(u_{ij})(\hat{y}))\cdot e(\eta) \\
&-\int_{\partial\mathcal{Y}} \sigma(w^{\varepsilon}_{C,ij})n\cdot\eta - \int_{\partial C^{\text{int}}} (\sigma(w^{\varepsilon}_{C,ij}) - \sigma(w^{\varepsilon}_{ij}))n\cdot\eta, \quad \forall\eta\in\mathcal{W}.
\end{aligned}
\tag{1.217}
$$

The inclusion $B_\varepsilon(\hat{y})$ being located neither on the interface nor on the boundary, the data are C^∞ at the vicinity of the center $\hat{y}$ so that by interior regularity of the solutions to elliptic boundary value problems, u_{ij} is smooth in B_ε for ε small enough. Then we have $\sigma(y) = \sigma(\hat{y}) + \nabla\sigma(\hat{y})\cdot(y-\hat{y}) + o(|y-\hat{y}|^2)$, where $|y-\hat{y}|\le\varepsilon$, and we have the following estimate

$$
\left|\int_{B_\varepsilon}(\sigma(u_{ij}) - \sigma(u_{ij})(\hat{y}))\cdot e(\eta)\right| \le c\,\varepsilon^2\|\eta\|_{1,\mathcal{Y}}.
\tag{1.218}
$$

Now we estimate the following term, from the definition of the dual norm

$$
\left|\int_{\partial\mathcal{Y}}\sigma(w^{\varepsilon}_{C,ij})n\cdot\eta\right| \le \|\sigma(w^{\varepsilon}_{C,ij})n\|_{-1/2,\partial\mathcal{Y}}\|\eta\|_{1/2,\partial\mathcal{Y}}.
\tag{1.219}
$$

We can show that there exists a constant $c>0$ such that for all $\eta\in H^1(C,\mathbb{R}^2)$ satisfying $\operatorname{div}\sigma(\eta)=0$, we have (see Proposition 1.14)

$$
\|\sigma(\eta)n\|_{-1/2,\partial\mathcal{Y}} \le c\,|\eta|_{1,C}\,.
\tag{1.220}
$$

Thus we have

$$
\left|\int_{\partial\mathcal{Y}}\sigma(w^{\varepsilon}_{C,ij})n\cdot\eta\right| \le c|w^{\varepsilon}_{C,ij}|_{1,C}\|\eta\|_{1,\mathcal{Y}},
\tag{1.221}
$$

where we also used the continuity of the Trace operator to estimate $\|\eta\|_{1/2,\partial\mathcal{Y}}\le c\|\eta\|_{1,\mathcal{Y}}$. In view of the elliptic regularity of the problem (1.208), we have

$$
\left|\int_{\partial\mathcal{Y}}\sigma(w^{\varepsilon}_{C,ij})n\cdot\eta\right| \le c\|w^{\varepsilon}_{ij}\|_{1/2,\partial C^{\text{int}}}\|\eta\|_{1,\mathcal{Y}}.
\tag{1.222}
$$

Next we apply Proposition 1.15 to derive

$$\left|\int_{\partial\mathcal{Y}} \sigma(w^\varepsilon_{C,ij})n\cdot\eta\right| \leq c\|w^\varepsilon_{ij}\|_{1,\mathcal{Y}_R\setminus\overline{C}}\|\eta,\|_{1,\mathcal{Y}} \tag{1.223}$$

and finally, the estimate (1.203) allows us to conclude that

$$\left|\int_{\partial\mathcal{Y}} \sigma(w^\varepsilon_{C,ij})n\cdot\eta\right| \leq c\varepsilon^2\|\eta\|_{1,\mathcal{Y}}. \tag{1.224}$$

We can use the same argumentation to show that

$$\begin{aligned}\left|\int_{\partial C^{int}} \sigma_y(w^\varepsilon_{C,ij})n\cdot\eta\right| &\leq \|\sigma_y(w^\varepsilon_{C,ij})n\|_{-1/2,\partial C^{int}}\|\eta\|_{1/2,\partial C^{int}}\\ &\leq c\|\sigma_y(w^\varepsilon_{C,ij})n\|_{-1/2,\partial C^{int}}\|\eta\|_{1,\mathcal{Y}}\\ &\leq c\left|w^\varepsilon_{C,ij}\right|_{1,C}\|\eta\|_{1,\mathcal{Y}}\\ &\leq c\|w^\varepsilon_{ij}\|_{1/2,\partial C^{int}}\|\eta\|_{1,\mathcal{Y}}\\ &\leq c\|w^\varepsilon_{ij}\|_{1,\mathcal{Y}_R\setminus\overline{C}}\|\eta\|_{1,\mathcal{Y}}\\ &\leq c\varepsilon^2\|\eta\|_{1,\mathcal{Y}},\end{aligned} \tag{1.225}$$

where once again the estimate (1.203) has been used. Finally

$$\begin{aligned}\left|\int_{\partial C^{int}} \sigma_y(w^\varepsilon_{ij})n\cdot\eta\right| &\leq c\|\sigma_y(w^\varepsilon_{ij})n\|_{-1/2,\partial C^{int}}\|\eta\|_{1/2,\partial C^{int}} \leq c\|\sigma_y(w^\varepsilon_{ij})n\|_{-1/2,\partial C^{int}}\|\eta\|_{1,\mathcal{Y}}\\ &\leq c\left|w^\varepsilon_{ij}\right|_{1,C}\|\eta\|_{1,\mathcal{Y}} \leq c\left|w^\varepsilon_{ij}\right|_{1,\mathcal{Y}_R}\|\eta\|_{1,\mathcal{Y}}\\ &\leq c\varepsilon^2\|\eta\|_{1,\mathcal{Y}},\end{aligned} \tag{1.226}$$

where c does not depend on ε. Noting that the bilinear form of the problem (1.217) is uniformly coercive on $\mathcal{W}$, and because $\tilde{z}^\varepsilon_{ij}\in\mathcal{V}$, we can conclude, making use of Poincaré-Wirtinger inequality, that

$$|\tilde{z}^\varepsilon_{ij}|_{1,\mathcal{Y}} = O(\varepsilon^2), \tag{1.227}$$

$$\|\tilde{z}^\varepsilon_{ij}\|_{0,\mathcal{Y}} = O(\varepsilon^2). \tag{1.228}$$

We can finally write the following expansion

$$\tilde{u}^\varepsilon_{ij} = \tilde{u}_{ij} + w^\varepsilon_{ij} + \left(\tilde{z}^\varepsilon_{ij} + \tilde{w}^\varepsilon_{ij} - w^\varepsilon_{ij}\right), \tag{1.229}$$

for which it remains to estimate the term $\tilde{w}^\varepsilon_{ij} - w^\varepsilon_{ij}$.

We start calculating its $|\cdot|_{1,\mathcal{Y}}$ norm.

$$\begin{aligned}|\tilde{w}^\varepsilon_{ij} - w^\varepsilon_{ij}|^2_{1,\mathcal{Y}} &= \int_{\mathcal{Y}} \sigma(\tilde{w}^\varepsilon_{ij} - w^\varepsilon_{ij})\cdot e(\tilde{w}^\varepsilon_{ij} - w^\varepsilon_{ij})\\ &= \int_{\mathcal{Y}} \sigma(w^{\varepsilon,\epsilon}_{ij} - w^\varepsilon_{ij})\cdot e(w^{\varepsilon,\epsilon}_{ij} - w^\varepsilon_{ij})\\ &= \int_{C} \sigma(w^\varepsilon_{C,ij} - w^\varepsilon_{ij})\cdot e(w^\varepsilon_{C,ij} - w^\varepsilon_{ij})\\ &= |w^\varepsilon_{C,ij} - w^\varepsilon_{ij}|^2_{1,C},\end{aligned} \tag{1.230}$$

by definition (1.210) of $\tilde{w}^{\varepsilon}_{ij}$ and definition (1.207) of $w^{\varepsilon,\epsilon}_{ij}$. Furthermore we know, from the calculations (1.221), (1.222), and (1.223) led above, that we have

$$|w^{\varepsilon}_{C,ij}|_{1,C} \leq \|w^{\varepsilon}_{ij}\|_{1,\mathcal{Y}_R\setminus\overline{C}}. \tag{1.231}$$

Then we deduce with (1.203) that

$$\begin{aligned}|\tilde{w}^{\varepsilon}_{ij} - w^{\varepsilon}_{ij}|^2_{1,\mathcal{Y}} &\leq |w^{\varepsilon}_{C,ij}|^2_{1,C} + |w^{\varepsilon}_{ij}|^2_{1,C} + 2|w^{\varepsilon}_{C,ij}|_{1,C}|w^{\varepsilon}_{ij}|_{1,C} \\ &\leq O(\varepsilon^4) + O(\varepsilon^4) + O(\varepsilon^4).\end{aligned} \tag{1.232}$$

For the $\|\cdot\|_{0,\mathcal{Y}}$ norm we have

$$\begin{aligned}\|\tilde{w}^{\varepsilon}_{ij} - w^{\varepsilon}_{ij}\|^2_{L^2(\mathcal{Y})} &= \int_{\mathcal{Y}} |\tilde{w}^{\varepsilon}_{ij} - w^{\varepsilon}_{ij}|^2 = \int_{\mathcal{Y}} |w^{\varepsilon,\epsilon}_{ij} - \langle w^{\varepsilon,\epsilon}_{ij}\rangle - w^{\varepsilon}_{ij}|^2 \\ &= \int_C |w^{\varepsilon}_{C,ij} - \langle w^{\varepsilon,\epsilon}_{ij}\rangle - w^{\varepsilon}_{ij}|^2 + \int_{\mathcal{Y}\setminus\overline{C}} |\langle w^{\varepsilon,\epsilon}_{ij}\rangle|^2,\end{aligned} \tag{1.233}$$

where

$$|\langle w^{\varepsilon,\epsilon}_{ij}\rangle| = \left|\frac{1}{V}\int_{\mathcal{Y}} w^{\varepsilon,\epsilon}_{ij}\right| \leq \frac{1}{V}\|w^{\varepsilon,\epsilon}_{ij}\|_{L^2(\mathcal{Y})}\left(\int_{\mathcal{Y}} 1^2\right)^{1/2} \leq \frac{1}{\sqrt{V}}\|w^{\varepsilon,\epsilon}_{ij}\|_{L^2(\mathcal{Y})}. \tag{1.234}$$

From this, by using the estimate (1.201) and $\|w^{\varepsilon}_{ij}\|^2_{1/2,\partial C^{\text{int}}} = O(\varepsilon^4)$ (see calculations (1.221), (1.222), and (1.223)), we have

$$\begin{aligned}\|w^{\varepsilon,\epsilon}_{ij}\|^2_{L^2(\mathcal{Y})} &= \|w^{\varepsilon,\epsilon}_{ij}\|^2_{L^2(\mathcal{Y}\setminus\overline{C}))} + \|w^{\varepsilon,\epsilon}_{ij}\|^2_{L^2(C)} \\ &= \|w^{\varepsilon}_{ij}\|^2_{L^2(\mathcal{Y}\setminus\overline{C}))} + \|w^{\varepsilon,\epsilon}_{ij}\|^2_{L^2(C)} \\ &\leq o(\varepsilon^2) + \|w^{\varepsilon,\epsilon}_{ij}\|^2_{1,C} \\ &\leq o(\varepsilon^2) + \|w^{\varepsilon}_{ij}\|^2_{1/2,\partial C^{\text{int}}} \\ &\leq o(\varepsilon^2) + O(\varepsilon^4)\end{aligned} \tag{1.235}$$

We have shown that

$$|\tilde{w}^{\varepsilon}_{ij} - w^{\varepsilon}_{ij}|_{1,\mathcal{Y}} = O(\varepsilon^2), \tag{1.236}$$

$$\|\tilde{w}^{\varepsilon}_{ij} - w^{\varepsilon}_{ij}\|_{0,\mathcal{Y}} = o(\varepsilon). \tag{1.237}$$

We finally find the estimates (1.117), (1.118) and (1.119), from the expansion (1.229) together with the estimations (1.227), (1.228), (1.236) and (1.237). □

1.5.3 Proof of Lemma 1.6

Proof: We want to introduce the same kind of *Ansatz* for the expansion of $\tilde{\tilde{u}}^{\varepsilon}_{ijk}$ as in Lemma 1.5. For this purpose, let us set the field w^{ε}_{ijk} meant to cancel the first terms of the right hand sides of equations (1.253) and (1.260). So w^ε_{ijk} is defined as the solution to the following transmission problem:

$$\left\{\begin{array}{rcll} \operatorname{div}(\gamma_\varepsilon\sigma(w^\varepsilon_{ijk})) & = & 0 & \text{in} \quad \mathbb{R}^2, \\ w^\varepsilon_{ijk} & \to & 0 & \text{at} \quad \infty, \\ [\![w^\varepsilon_{ijk}]\!] & = & 0 & \text{on} \quad \partial B_\varepsilon, \\ [\![\gamma_\varepsilon\sigma(w^\varepsilon_{ijk})]\!]n & = & h & \text{on} \quad \partial B_\varepsilon, \end{array}\right. \tag{1.238}$$

where $h = -(1-\gamma)(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k))n$. The above boundary value problem admits an explicit solution with the same estimates as in Lemma 1.5 (see e.g., [Bar92]), namely

$$\|w^\varepsilon_{ijk}\|_{0,\mathcal{Y}} = o(\varepsilon), \tag{1.239}$$

$$\|w^\varepsilon_{ijk}\|_{1,\mathcal{Y}} = O(\varepsilon), \tag{1.240}$$

$$\|w^\varepsilon_{ijk}\|_{1,\mathcal{Y}_R} = O(\varepsilon^2). \tag{1.241}$$

Once again let us introduce

$$w^{\varepsilon,\epsilon}_{ijk}(y) := \left\{\begin{array}{ll} w^\varepsilon_{ijk}(y) & \text{if } y \in \mathcal{Y} \setminus \overline{C}, \\ w^\varepsilon_{C,ijk}(y) & \text{if } y \in C, \end{array}\right. \tag{1.242}$$

where C is the ring defined in (1.205), and $w^\varepsilon_{C,ijk}$ is solution to the following problem:

$$\left\{\begin{array}{rcll} \operatorname{div}(\sigma(w^\varepsilon_{C,ijk})) & = & 0 & \text{in} \quad C, \\ w^\varepsilon_{C,ijk} & = & 0 & \text{on} \quad \partial\mathcal{Y}, \\ w^\varepsilon_{C,ijk} & = & w^\varepsilon_{ijk} & \text{on} \quad \partial C^{\text{int}}, \end{array}\right. \tag{1.243}$$

where ∂C^{int} is defined in (1.206). Now we can introduce the new *Ansatz*:

$$\tilde{\tilde{u}}^\varepsilon_{ijk} = \tilde{\tilde{u}}_{ijk} + w^\varepsilon_{ijk} + \left(\tilde{z}^\varepsilon_{ijk} + \tilde{w}^\varepsilon_{ijk} - w^\varepsilon_{ijk}\right), \tag{1.244}$$

where $\tilde{w}^\varepsilon_{ijk} = w^{\varepsilon,\epsilon}_{ijk} - \langle w^{\varepsilon,\epsilon}_{ijk}\rangle$, so that $\tilde{w}^\varepsilon_{ijk} \in \mathcal{V}$. In this way, we effectively have $\tilde{z}^\varepsilon_{ijk} \in H^1_{\text{per}}(\mathcal{Y};\mathbb{R}^2)$, with $\langle \tilde{z}^\varepsilon_{ijk}\rangle = 0$. Our goal is to estimate $\|\tilde{\tilde{u}}^\varepsilon_{ijk} - \tilde{\tilde{u}}_{ijk}\|_{1,\mathcal{Y}}$ by controlling the terms of the equation (1.244), namely

$$\|\tilde{\tilde{u}}^\varepsilon_{ijk} - \tilde{\tilde{u}}_{ijk}\|_{1,\mathcal{Y}} \leq \|w^\varepsilon_{ijk}\|_{1,\mathcal{Y}} + \|\tilde{z}^\varepsilon_{ijk}\|_{1,\mathcal{Y}} + \|\tilde{w}^\varepsilon_{ijk} - w^\varepsilon_{ijk}\|_{1,\mathcal{Y}}. \tag{1.245}$$

We directly have an estimation on the term w^ε_{ijk} given by (1.240). Let us investigate **1)** the behaviour of $\tilde{w}^\varepsilon_{ijk} - w^\varepsilon_{ijk}$, and next **2)** the behaviour of $\tilde{z}^\varepsilon_{ijk}$.

1) The solution w^ε_{ijk} of the classical problem (1.238) is explicitly known (see e.g.,[Bar92]), gives rise to the same estimates as those written equations (1.201). The same developments as those led in the proof of Lemma 1.5 in Section 1.5.2 give

$$\|\tilde{w}^\varepsilon_{ijk} - w^\varepsilon_{ijk}\|_{1,\mathcal{Y}} = O(\varepsilon^2), \tag{1.246}$$

$$\|\tilde{w}^\varepsilon_{ijk} - w^\varepsilon_{ijk}\|_{0,\mathcal{Y}} = o(\varepsilon). \tag{1.247}$$

2) We denote by a_ε the bilinear form on $\mathcal{W} \times \mathcal{W}$ of problem (1.108), that is to say

$$a_\varepsilon(u, v) := \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(u) \cdot e(v), \quad \forall u, v \in \mathcal{W}. \tag{1.248}$$

As in the proof of Lemma 1.5, we write the variational problem satisfied by $\tilde{z}^\varepsilon_{ijk}$, applying the bilinear form a_ε to $\tilde{z}^\varepsilon_{ijk}$ and a test function η. In view of (1.244) and the notations introduced above, the problem is expressed by

$$\tilde{z}^\varepsilon_{ijk} \in \mathcal{W} \ : \ a_\varepsilon(\tilde{z}^\varepsilon_{ijk}, \eta) = a_\varepsilon(\tilde{\tilde{u}}^\varepsilon_{ijk}, \eta) - a_\varepsilon(\tilde{\tilde{u}}_{ijk}, \eta) - a_\varepsilon(\tilde{w}^\varepsilon_{ijk}, \eta), \quad \forall \eta \in \mathcal{W}. \tag{1.249}$$

Let us make some preliminary calculations, for which the results directly derive from Lemma 1.5. We want to estimate, for all $\eta \in \mathcal{W}$, the expression $a_\varepsilon(\tilde{\tilde{u}}^\varepsilon_{ijk}, \eta) - a_\varepsilon(\tilde{\tilde{u}}_{ijk}, \eta)$. According to expressions (1.108) and (1.68), we find

$$\begin{aligned} a_\varepsilon(\tilde{\tilde{u}}^\varepsilon_{ijk}, \eta) - a_\varepsilon(\tilde{\tilde{u}}_{ijk}, \eta) = &- \int_{\mathcal{Y}} (\gamma_\varepsilon \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) - \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)) \cdot e(\eta) \\ &+ \int_{\mathcal{Y}} (\gamma_\varepsilon \sigma(u^\varepsilon_{ij}) - \sigma(u_{ij}) - \int_{\mathcal{Y}} (\mathbf{C}^h_\varepsilon - \mathbf{C}^h)(\mathrm{e}_i \otimes_s \mathrm{e}_j))\mathrm{e}_k \cdot \eta \\ &+ (1-\gamma) \int_{B_\varepsilon} \sigma(\tilde{\tilde{u}}_{ijk}) \cdot e(\eta). \end{aligned} \tag{1.250}$$

Recalling the notation $\delta(\cdot)^\varepsilon = (\cdot)^\varepsilon - (\cdot)$, we start developing the first two terms of the right hand side of this expression.

$$\begin{aligned} &- \int_{\mathcal{Y}} (\gamma_\varepsilon \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) - \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)) \cdot e(\eta) = - \int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\delta \tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) \cdot e(\eta) \\ &+ (1-\gamma)\mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k) \cdot \int_{B_\varepsilon} e(\eta) + (1-\gamma) \int_{B_\varepsilon} \mathbf{C}((\tilde{u}_{ij} - \tilde{u}_{ij}(\hat{y})) \otimes_s \mathrm{e}_k) \cdot e(\eta), \end{aligned} \tag{1.251}$$

and

$$\begin{aligned} \int_{\mathcal{Y}} (\gamma_\varepsilon \sigma(u^\varepsilon_{ij}) - \sigma(u_{ij}))\mathrm{e}_k \cdot \eta = \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\delta \tilde{u}^\varepsilon_{ij})\mathrm{e}_k \cdot \eta - (1-\gamma)\sigma(u_{ij})(\hat{y})\mathrm{e}_k \cdot \int_{B_\varepsilon} \eta \\ - (1-\gamma) \int_{B_\varepsilon} (\sigma(u_{ij}) - \sigma(u_{ij})(\hat{y}))\mathrm{e}_k \cdot \eta. \end{aligned} \tag{1.252}$$

In view of estimates in Lemma 1.5, the regularity of u_{ij}, and the behaviour of $(\mathbf{C}^h_\varepsilon - \mathbf{C}^h)$ given by (1.137), we have for all $\eta \in \mathcal{W}$

$$- \int_{\mathcal{Y}} (\gamma_\varepsilon \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) - \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k)) \cdot e(\eta) = (1-\gamma)\mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k) \cdot \int_{B_\varepsilon} e(\eta) + o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}, \tag{1.253}$$

and

$$\begin{aligned} \int_{\mathcal{Y}} (\gamma_\varepsilon \sigma(u^\varepsilon_{ij}) - \sigma(u_{ij}) - (\mathbf{C}^h_\varepsilon - \mathbf{C}^h)(\mathrm{e}_i \otimes_s \mathrm{e}_j))\mathrm{e}_k \cdot \eta = \int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\delta \tilde{u}^\varepsilon_{ij})\mathrm{e}_k \cdot \eta \\ - (1-\gamma)\sigma(u_{ij})(\hat{y})\mathrm{e}_k \cdot \int_{B_\varepsilon} \eta + o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}. \end{aligned} \tag{1.254}$$

Let us show that the second term of the right hand side of relation (1.250), written in relations (1.253) and (1.254), is actually $o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}$. The estimate from Lemma 1.12 gives, for $\delta > 0$ small enough, a constant $c_{(\delta)} > 0$ such that for all $\eta \in H^1(\mathcal{Y})$

$$\left| \int_{B_\varepsilon} \eta(x) dx \right| \le c_{(\delta)} \varepsilon^{2-\delta} \|\eta\|_{1,\mathcal{Y}}. \tag{1.255}$$

In this manner, the second term of the right-hand side of equation (1.254) behaves as follows

$$-(1-\gamma)\sigma(u_{ij})(\hat{y})\mathrm{e}_k \cdot \int_{B_\varepsilon} \eta = o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}. \tag{1.256}$$

Let us develop the first term of the right-hand side of (1.254), i.e. $\int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\delta\tilde{u}^\varepsilon_{ij})\mathrm{e}_k \cdot \eta$. We apply Green's formula to this integral separated over $\mathcal{Y}_1 \setminus \overline{B_\varepsilon}$, $\mathcal{Y}_\gamma \setminus \overline{B_\varepsilon}$, and B_ε. On each of these subdomains, the tensor $\mathbf{C}$ is constant (see definition (1.104)). We recall that the cell is such that $\mathcal{Y} = \mathcal{Y}_1 \cup \mathcal{Y}_\gamma \cup \Gamma_\gamma$, and the ball $\overline{B_\varepsilon(\hat{y})} \subset \mathcal{Y}$ does not cross the interface Γ_γ (see Figure 9). Denoting by n the inward normal to the boundary ∂B_ε, we obtain

$$\begin{aligned}\int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\delta\tilde{u}^\varepsilon_{ij})\mathrm{e}_k \cdot \eta &= \int_{\mathcal{Y}_1\setminus\overline{B_\varepsilon}} \mathbf{C}e(\delta\tilde{u}^\varepsilon_{ij}) \cdot (\eta \otimes \mathrm{e}_k) + \int_{\mathcal{Y}_\gamma\setminus\overline{B_\varepsilon}} \mathbf{C}e(\delta\tilde{u}^\varepsilon_{ij}) \cdot (\eta \otimes \mathrm{e}_k) \\ &\quad + \gamma \int_{B_\varepsilon} \mathbf{C}e(\delta\tilde{u}^\varepsilon_{ij}) \cdot (\eta \otimes \mathrm{e}_k), \\ &= -\int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}\mathrm{div}((\eta \otimes_s \mathrm{e}_k)) \cdot \delta\tilde{u}^\varepsilon_{ij} + \int_{\partial\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\eta \otimes_s \mathrm{e}_k)n \cdot \delta\tilde{u}^\varepsilon_{ij} \\ &\quad + (1-\gamma)\int_{\Gamma_\gamma} \mathbf{C}(\eta \otimes_s \mathrm{e}_k)n \cdot \delta\tilde{u}^\varepsilon_{ij} + (1-\gamma)\int_{\partial B_\varepsilon} \mathbf{C}(\eta \otimes \mathrm{e}_k)n \cdot \delta\tilde{u}^\varepsilon_{ij}.\end{aligned} \tag{1.257}$$

The first term of the right hand side of equation (1.257) is $o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}$ according to Lemma 1.5 estimate (1.118). The second one is null because $\mathbf{C}$, η and $\delta\tilde{u}^\varepsilon_{ij}$ are $\mathcal{Y}$-periodic. The third term is controlled by $\|\mathbf{C}(\eta\otimes_s \mathrm{e}_k)n\|_{-1/2,\Gamma_\gamma}\|\delta\tilde{u}^\varepsilon_{ij}\|_{1/2,\Gamma_\gamma}$. On one hand we have $\|\mathbf{C}(\eta\otimes_s \mathrm{e}_k)n\|_{-1/2,\Gamma_\gamma} \leq c\|\eta\|_{1,\mathcal{Y}}$, on the other $\|\delta\tilde{u}^\varepsilon_{ij}\|_{1/2,\Gamma_\gamma} \leq c\|\delta\tilde{u}^\varepsilon_{ij}\|_{1,\mathcal{Y}_R}$, so that the third term is $O(\varepsilon^2)\|\eta\|_{1,\mathcal{Y}}$. The fourth term of the right hand side of equation (1.257) is controlled by $\|\eta\|_{L^2(\partial B_\varepsilon;\mathbb{R}^2)}\|\tilde{u}^\varepsilon_{ijk} - \tilde{u}_{ijk}\|_{L^2(\partial B_\varepsilon;\mathbb{R}^2)}$. We know from Lemma 1.13 that for all $\delta > 0$ there exists a constant $c_{(\delta)} > 0$ such that

$$\forall \eta \in H^1(\mathcal{Y};\mathbb{R}^2), \quad \|\eta\|_{L^2(\partial B_\varepsilon;\mathbb{R}^2)} \leq c_{(\delta)}\varepsilon^{1/2-\delta}\|\eta\|_{1,\mathcal{Y}}. \tag{1.258}$$

The fourth term of the right hand side of equation (1.257) is $O(\varepsilon^{1-2\delta})\|\delta\tilde{u}^\varepsilon_{ij}\|_{1,\mathcal{Y}}\|\eta\|_{1,\mathcal{Y}}$, which is, regarding the estimate from Lemma 1.5, $O(\varepsilon^{2-2\delta})\|\eta\|_{1,\mathcal{Y}}$. Thus

$$\int_{\mathcal{Y}} \gamma_\varepsilon \sigma(\delta\tilde{u}^\varepsilon_{ij})\mathrm{e}_k \cdot \eta = o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}. \tag{1.259}$$

Finally, we end the preliminary calculations by rewriting the third term of equation (1.250) in view of the regularity of solutions. We find for all $\eta \in \mathcal{V}$

$$\begin{aligned}(1-\gamma)\int_{B_\varepsilon} \sigma(\tilde{\tilde{u}}_{ijk}) \cdot e(\eta) &= (1-\gamma)\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) \cdot \int_{B_\varepsilon} e(\eta) \\ &\quad + (1-\gamma)\int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}_{ijk}) - \sigma(\tilde{\tilde{u}}_{ijk})(\hat{y})) \cdot e(\eta), \\ &= (1-\gamma)\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) \cdot \int_{B_\varepsilon} e(\eta) + o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}.\end{aligned} \tag{1.260}$$

Now we go back to the computation of $a_\varepsilon(\tilde{z}^\varepsilon_{ijk}, \eta)$ in (1.249). Let us develop this expression thanks to preliminary calculations (1.250), (1.253), (1.254) (1.256), (1.259), and (1.260). We obtain the variational problem

$$\tilde{z}^{\varepsilon}_{ijk} \in \mathcal{W} \ : \ \int_{\mathcal{Y}} \gamma_{\varepsilon} \sigma(\tilde{z}^{\varepsilon}_{ijk}) \cdot e(\eta) = (1-\gamma)\mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k) \cdot \int_{B_{\varepsilon}} e(\eta)$$
$$+ (1-\gamma)\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) \cdot \int_{B_{\varepsilon}} e(\eta) - \int_{\mathcal{Y}} \gamma_{\varepsilon} \sigma(\tilde{w}^{\varepsilon}_{ijk}) \cdot e(\eta) + o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}, \quad \forall \eta \in \mathcal{W}. \quad (1.261)$$

Let us apply the Green formula to $-\int_{\mathcal{Y}} \gamma_{\varepsilon} \sigma(\tilde{w}^{\varepsilon}_{ijk}) \cdot e(\eta)$ on domains $C \cap \mathcal{Y}$, $(\mathcal{Y} \setminus \overline{C \cup B_{\varepsilon}})$, and B_{ε}. In view of the definition of $\tilde{w}^{\varepsilon}_{ijk}$ (1.238), and denoting by n the inward normal to the boundary ∂B_{ε}, we finally obtain that $\tilde{z}^{\varepsilon}_{ijk}$ follows the variational problem:

$$\tilde{z}^{\varepsilon}_{ijk} \in \mathcal{W} \ : \ \int_{\mathcal{Y}} \gamma_{\varepsilon} \sigma(\tilde{z}^{\varepsilon}_{ijk}) \cdot e(\eta) = -\int_{\partial \mathcal{Y}} \sigma(w^{\varepsilon}_{C,ijk}) n \cdot \eta$$
$$-\int_{\partial C^{\mathrm{int}}} (\sigma(w^{\varepsilon}_{C,ijk}) - \sigma(w^{\varepsilon}_{ijk})) n \cdot \eta + o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}, \quad \forall \eta \in \mathcal{W}. \quad (1.262)$$

In the same way as in Lemma 1.5, we find that the two first terms of the right-hand side of equation (1.262) are $o(\varepsilon)\|\eta\|_{1,\mathcal{Y}}$, and the bilinear form of the problem (1.217) being uniformly coercive on $\mathcal{W}$, and $\tilde{z}^{\varepsilon}_{ij} \in \mathcal{V}$, we obtain

$$\|\tilde{z}^{\varepsilon}_{ijk}\|_{1,\mathcal{Y}} = o(\varepsilon). \quad (1.263)$$

Finally, the expansion (1.244) gives rise to the intended estimates (1.120), (1.121) and (1.122). □

Chapter 2

Microstructure synthesis by topological optimization

2.1 Introduction

Numerical shape optimization is a widely studied field, in particular in structural optimization ([Dij+13], [Roz09]). Numerous other applications have to be mentioned, for which we only give a small fragment of the literature, such as imagery ([Lar+09], [Amm+12], [Lau+13]), fluid mechanics ([GI04], [Ams05]), heat conduction problems ([NS16]), acoustic ([FOP04], [AD08], [BBC13], [Isa+14]), electromagnetic ([AK03], [MPS05], [HLN12]), inverse problems ([GB04; GB06]) and piezoelectric ([GMS14], [Leu+10]). Generally speaking, a shape optimization problem can be defined as follows.

$$\inf_{\chi \in \mathcal{U}_{\mathrm{ad}}} \left\{ \mathcal{J}(\chi) := \int_{\mathrm{D}} j(\chi, u_\chi) \right\}, \tag{2.1}$$

where $\chi : \mathrm{D} \to \{0, 1\}$ stands for the design variable and represents the characteristic function of a sub domain of a fixed domain D, also called *hold-all domain*. The functions $\chi \in \mathcal{U}_{\mathrm{ad}}$ belongs to a class of admissible characteristic functions for which we can imagine some constraint to be satisfied, and u_χ is the solution of a boundary value problem defined on D and depending on χ. The function $j(\chi, u_\chi)$ is often a smooth function such as the energy density, or the compliance.

We briefly introduce the main shape and topological optimization techniques for investigating problem (2.1). Far from being exhaustive, the aim is to give an idea of the different existing methods. For more detailed introduction to numerical shape and topology optimization techniques, the reader may refer to [All07], [SM13], [Dij+13], focusing on level-set methods for topological and shape optimization. Even though several other methods exist, such as *evolutionary approaches* (see e.g., [All07]) or *phase-field* approaches (see e.g., [WRA12]), the shape optimization techniques are usually classified into three main families: the *density methods*, the *level-set methods* and the methods using the topological derivative.

We promptly designate by *density methods*, the *homogenization approach* to topological optimization, and also all the methods deriving from the homogenization method. From a theoretical standpoint, the homogenization method was initiated by F. Murat and L. Tartar [Mur85] and in the pioneering works [LC18], [KS86a; KS86b; KS86c] (see Section 1.2). One can also cite [BK88] regarding the study of the homogenization approach, which was then developed in the 90's (see e.g. [All+97b], [All02]). We present the idea of the homogenization method following Section 7 in [All07], considering the optimization of the design of a 2-dimensional membrane made of two materials α ($\{\chi = 0\}$) and β ($\{\chi = 1\}$), with a constant volume ratio of materials ($\int_{\mathrm{D}} \chi(x)\, dx = V$). Let $0 < \alpha < \beta$, going back to problem (2.1) we have that u_χ satisfies

$$\begin{cases} -\operatorname{div}(A^\chi \nabla u_\chi) = f & \text{in D}, \\ u_\chi = 0 & \text{on } \partial\text{D}, \end{cases} \tag{2.2}$$

where $A^\chi := \alpha\chi + \beta(1-\chi)$. The problem (2.1) is then "relaxed", or "homogenized", that is we a priori include as admissible design variables all the possible limits in the sense of homogenization (or H-convergence, see [All07] Chapter 7) of mixtures of material α and β with a proportion V. This relaxation is made possible thanks to compactness results regarding the H-convergence. For a sequence of characteristic functions $(\chi_n)_n$ such that $\int_\text{D} \chi_n(x)\,dx = V$ for all $n \geq 0$, there exists a sub-sequence still denoted by $(\chi_n)_n$, which converges weakly to $\theta \in L^\infty(\text{D})$, and there exists an homogenized tensor A^* belonging to an admissible space G_θ depending on θ, such that for all $f \in L^2(\text{D})$, u_{χ_n} converges in $L^2(\text{D})$ to the solution u^* of the following problem.

$$\begin{cases} -\operatorname{div}(A^* \nabla u^*) = f & \text{in D}, \\ u^* = 0 & \text{on } \partial\text{D}, \end{cases} \tag{2.3}$$

Furthermore, the weak limit θ is such that $0 \leq \theta \leq 1$ and $\int_\text{D} \theta(x)\,dx = V$.

Thus the new design variables are the density fields $0 \leq \theta(x) \leq 1$ such that $\int_\text{D} \theta(x)\,dx = V$, and the homogenized tensors A^* depending on θ. The relaxed problem is written as follows

$$\inf_{\theta, A^* \in G_\theta} \left\{ \mathcal{J}(\theta, A^*) := \int_\text{D} j(u^*) \right\}. \tag{2.4}$$

The advantage is twofold. The relaxed formulation of the problem admits a solution, and we can differentiate the shape functional $\mathcal{J}$ with respect to θ and A^*. Indeed some well-known results such as Lamination formulas or Hashin-Shtrikman bounds allows for identifying the admissible set of A^* and simplifying calculations (see e.g., [All07] Section 7.3.5). Finally a *penalization* procedure is applied in order to get a two phases material back from the density θ. A variant of the homogenization method consists in replacing A^* by θA, where A is fixed. That is the only design variable is θ. The Simplified Isotropic Material with Penalization method (SIMP method [Ben89], [ZR91]) corresponds to the case where A^* is replaced by $\theta^p A$, with $p \geq 1$. But in this case, we do not have a relaxation theorem. Nevertheless, this method allows to obtain interesting results from an engineering point of view, but one must keep in mind that it is not mathematically correct and does not produce exact solutions (see [Gao18]).

Another approach is the *level-set methods*, which were introduced in [OS88] and have known further development to be applied to topological and shape optimization. We can find the beginning of such applications in [SW00] for the optimization of cantilever with an evolutionaty stress criterion, and in [DV00]. The level-set methods kept developing for example in [Set99; Set01], especially with the use of the shape sensitivity such as in [OF01; OF03], [WWG03], [AJT04]. We refer to [Dij+13] for a review of level-set methods. Still taking problem (2.1) as a reference, we consider that $\Omega := \{\chi = 1\}$ stands for a subdomain of D, for which we look for the optimal design regarding the criteria $\mathcal{J}(\Omega) := \mathcal{J}(\chi)$. The level-set method consists in characterizing the domain Ω by the level set of a scalar function ψ with $\Omega := \{\psi < 0\}$, $\text{D} \setminus \overline{\Omega} := \{\psi > 0\}$ and $\partial\Omega := \{\psi = 0\}$.

In general, within an optimization procedure, the level-set plays the role of a design variable, and its evolution is conducted by the Hamilton-Jacobi equation, such as in

[OF01], [WWG03], [AJT04]. We refer for example to [Lau18] Section 5 for further explanation on the method. In Hamilton-Jacobi equation, a speed function acts a direction of evolution for the hole level set ψ. This speed function is defined from the underlying optimization problem, in order to ensure that the updated level-set allows for an improvement of the shape function $\mathcal{J}$. A classical manner to define this speed function is the use of the *shape derivative method* (or *velocity field method*, see e.g. [SZ92], [HP06]). The concept of shape derivative has first emerged in the paper [Had08], and with the pioneering works [Sch46], [GS53]. It experienced a resurgence of interest with the following works [Céa71; CGM73; Céa81], [MS74; MS76], [Sim80; Sim87], [Pir84]. For more details regarding how the shape derivative is used to update the level-set, we refer for example to [Lau18]. Nevertheless, one drawback of this method making use of the shape derivative is that it does not allow to change the topology of the domain. They only perform a smooth transformation of the initial domain.

It is also efficient to couple the level-set method with an *ersatz material* approximation (see e.g. [DK10]). For example in the case of a drilled material, it consists in mimicking voids by filling the void domain with a material of weaker stiffness.

Another kind of approaches, allowing for changes of topology, are the methods based on the *topological derivative* (see Section 1.3.1). First time topological derivative were used in [Sch96], [EKS94] within the so-called *bubble method*. The idea is to perform a classic shape optimization procedure transforming the boundary of the domain, and when a minimum is reached for a fixed topology, small holes are added with respect to the topological derivative of the shape functional. Topological derivative has also been used in level-set approach ([AJT04], [BHR04])

For the investigation we lead regarding the design of microstructures, we use a gradient-type method introduced in [AA06], and that we describe in the next section. It essentially relies on

- the topological derivative of the cost functional,
- a level-set representation of the domain,
- an ersatz material, allowing us to use a single mesh, leading to an efficient optimization numerical scheme.

The idea of the following chapter is to generate new kind of microstructures, by performing a topological optimization of the constitutive *unit cell* of a periodic material, for which we aim to improve the homogenized behaviour. For this, we choose functionals depending on the homogenized tensors as an optimization criterion. In Section 2.2, we introduce the gradient type algorithm from [AA06]. We start by a presentation of the periodic homogenization context, followed by a description of the algorithm, and then we give the details of the implementation in Matlab of the topological optimization procedure. In Section 2.3, we investigate the maximization of some characteristic lengths defined as ratios between coefficients of the first order elasticity tensor $\mathbf{C}^h$ and the second order elasticity tensor $\mathbf{D}^h$. We also analyse the behaviour of the homogenization scheme and the behaviour of the optimization procedure. We pursue this study in Section 2.4, in the case where the material contrast vanishes . Finally, Section 2.5 is devoted to the definition of invariants for the homogenized tensors, and the optimization of a functional based on these invariants.

This work is the result of a close collaboration with Antonio André Novotny (Laboratório Nacional de Computação Científica LNCC/MCT, Petrópolis, RJ, Brazil), with whom I have implemented the higher order homogenization procedure, the higher order homogenized tensors, their topological derivatives, a symbolic procedure allowing to compute automatically any shape functional depending on the coefficients of the homogenized tensors, together with its topological derivative. Furthermore I worked significantly with Baptiste Durand[1] and Arthur Lebée on the optimization of characteristic lengths. Finally I have collaborated with Nicolas Auffray[2] and Jean-françois Ganghoffer on the optimization of invariants.

2.2 Gradient type method for topological optimization

We describe the gradient type method for topological optimization in Section 2.2.2, by directly applying it to our homogenization framework presented below.

2.2.1 General setting: periodic homogenization

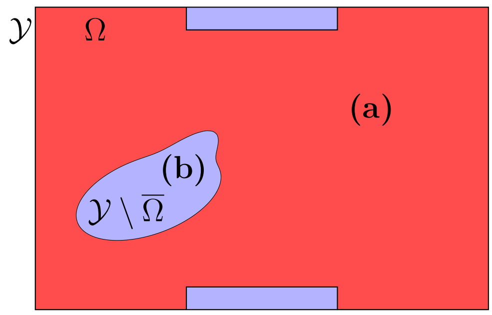

Figure 10: Unit cell $\mathcal{Y}$ composed with two materials **(a)** and **(b)**.

The problem we are concerned with is the shape and topological optimization of "architectured materials". Indeed the microstructural organisation of a material can bring interesting effective properties out. Our framework is the behaviour of periodic materials. We only work on the design of the microscopic scale. The material is constructed with a unique cell whose pattern is repeated periodically, and our goal is to design the shape of the cell for optimizing some resulting homogenized effects. We refer to Section 1.2 for a detailed presentation of the homogenization framework (see also [JS20] for a well-written presentation of the issues). Following the homogenization scheme proposed in [SC00], we are interested in the case where the homogenized material is a second-gradient or strain-gradient material, that is the homogenized elastic energy depends on the second gradient of the displacement or equivalently the gradient of the strain field. We don't meet a great deal of examples for this kind of materials (see e.g., [PS97], [BC07], [ASD03], [AD15], [Bou+17], [del+16], [SAI11], [AS18a], [AS18b], [ASB19]).

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There is a kind of paradox when using such a second gradient model. We homogenize the material in order to ignore variations which occur at the length-scale of the cell, but we finally take into account effects having this length-scale. Indeed we will see in Section 2.3.2 that intrinsic lengths can be defined with the square root of any component of $\tau^2\mathbf{D}^h$ divided by any component of $\mathbf{C}^h$, so that this intrinsic lengths are of order τ.

Nevertheless, when we talk about second gradient homogenization, we make a difference between what we call the “limit” and the “correction” approaches. The first one concerns the process of homogenization dealing with the limit model when the size of the cell goes to zero. In this case we wish to obtain a limit model depending on the second gradient. The second one concerns the case where the limit model is eventually a Cauchy model (that is the macroscopic energy depends only on the macroscopic strain field), but where the size of the microscopic periodic cell is “small but not too small”. In this situation, taking into account higher order corrective terms leads to better approximations and description of the behaviour of the effective medium. Indeed the formulas proposed in [SC00] seems quite efficient for the evaluation of these corrective terms. For a significant Young modulus of order of τ^{-1}, then $\tau^2\mathbf{D}^h$ may become of order one. This effect is studied and well analysed in [Dur+20] for a *pantographic* structure yielding second-gradient effects at the leading order. We will give more details and study this structure in Section 2.3.4.

Problem: we consider the unit cell composing a periodic macroscopic medium in a 2-dimensional framework. The macroscopic medium does not interest us, we only deal with the shape of the unit cell. Let $\{\mathrm{e}_1, \mathrm{e}_2\}$ be the orthonormal canonical base of $\mathbb{R}^2$. The *unit cell*, or *periodicity unit cell*, is defined by

$$\mathcal{Y} = (0, l_1) \times \ (0, l_2), \tag{2.5}$$

being an open rectangle of $\mathbb{R}^2$ written in that base, with $0 < l_1$, $0 < l_2$. This unit cell is made up of two different homogeneous and isotropic elastic materials: the material **(a)** and the material **(b)**. The first one is represented by an open subset Ω of $\mathcal{Y}$, and the second one is represented by $\mathcal{Y} \setminus \overline{\Omega}$ (see Figure 10). These two elastic phases are characterised by the same *Poisson's coefficient* ν, and by *Young's moduli* having a ratio $0 < \gamma_0 < +\infty$, where γ_0 is called the *contrast* between the two materials. That is, denoting by $\mathbf{C}_0$ the stiffness tensor describing the first elastic material filling the domain Ω, we can write the stiffness tensor $\mathbf{C}(\Omega)$ entirely defined by Ω of the unit cell associated to this distribution of material as follows

$$\mathbf{C}(\Omega)(x) := \begin{cases} \mathbf{C}_0, & x \in \Omega, \\ \gamma_0 \mathbf{C}_0, & x \in \mathcal{Y} \setminus \overline{\Omega}, \end{cases} \tag{2.6}$$

where denoting by E the Young's modulus associated to the first material (material **(a)**) we have

$$\mathbf{C}_0 = \frac{E}{1-\nu^2}\left((1-\nu)\mathbb{I} + \nu \mathrm{I} \otimes \mathrm{I}\right), \tag{2.7}$$

where I and $\mathbb{I}$ are defined in (1.102) and (1.103).

As we saw in Section 1.2, such a distribution of material yield the homogenized elastic energy

$$\mathscr{E}^h(\Omega)(\tau) = \frac{1}{2} E \cdot \mathbf{C}^h(\Omega) \cdot E + \frac{1}{2}\tau E \cdot \mathbf{E}^h(\Omega) \cdot K + \frac{1}{2}\tau^2 K \cdot \mathbf{D}^h(\Omega) \cdot K + o(\tau^2), \tag{2.8}$$

and allow to define homogenized tensors: $\mathbf{C}^h(\Omega)$, $\mathbf{E}^h(\Omega)$, and $\mathbf{D}^h(\Omega)$. Here τ is a small parameter representing the ratio of the "microscopic" size of the cell to the "macroscopic" size of the medium, $E = \nabla^s U$ is the macroscopic strain, and $K = \nabla\nabla^s U$ is the macroscopic strain gradient, where U is the macroscopic displacement field. These homogenized tensors encapsulate some information on the effective behaviour of periodic materials built with the cell $\Omega \cup \mathcal{Y} \setminus \overline{\Omega}$. From this, it is interesting to optimize the material distribution within the unit cell in order to improve some criteria based on these tensors.

This question has been widely studied concerning the optimization of the underlying microstructure with the aim of maximizing or minimizing some effective properties from the first order homogenized elasticity tensor (see e.g, [GNS10], [Ams+10]).

But as we said previously, macroscopic models relying on the second gradient or on the strain gradient can be used. Consequently new questions are emerging:

1. What kind of architectured materials with non classical behaviour can arise from optimization problems taking into account higher order effective properties?

2. Can we define interesting cost functional depending on higher order homogenized tensors?

The effective mechanical properties contained in the fourth order tensor $\mathbf{C}(\Omega)$ are known. For example the in-plane average *Poisson ratio* $\mathbf{S}^{hom}_{1122}/\mathbf{S}^{hom}_{1111} + \mathbf{S}^{hom}_{1122}/\mathbf{S}^{hom}_{2222}$ measures the deformation in directions perpendicular to the specific direction of loading, the *shear modulus* $4\mathbf{S}^{hom}_{1212}$ measures the stiffness, and the *bulk modulus* $\mathbf{S}^{hom}_{1111} + 2\mathbf{S}^{hom}_{1122} + \mathbf{S}^{hom}_{2222}$ measures the resistance to compression, where $\mathbf{S}^{hom} := (\mathbf{C}^h)^{-1})$. However it is not trivial to derive from the higher order tensors $\mathbf{E}^h(\Omega)$ and $\mathbf{D}^h(\Omega)$ some coefficients being meaningful from a mechanical point of view. In a first step we investigate quite natural intrinsic length, and then we will look at some invariants of tensors related to symmetries satisfied by the material.

From this point we consider the following minimization problem:

$$\inf_{\Omega \in \mathcal{U}_{\mathrm{ad}}} \mathcal{J}(\Omega), \tag{2.9}$$

where $\mathcal{U}_{\mathrm{ad}}$ is a class of admissible open subsets of $\mathcal{Y}$, and $\mathcal{J}$ is a shape functional defined by

$$\mathcal{J}(\Omega) := j\left(\mathbf{C}^h(\Omega), \mathbf{E}^h(\Omega), \mathbf{D}^h(\Omega)\right), \tag{2.10}$$

where j is a smooth map from $\otimes^4\mathbb{R}^2 \times \otimes^5\mathbb{R}^2 \times \otimes^6\mathbb{R}^2$ to $\mathbb{R}$. Here $\otimes^m\mathbb{R}^n$ denotes the space of m-order tensors on $\mathbb{R}^n$. Now we present the implemented method.

2.2.2 The algorithm

To solve problem (2.9), we make use to a gradient-type method based on the *topological derivative* (see Section 1.3.1). In some sense, this method use the same ideas as the methods based on the linear approximation of the cost functional in classical optimization. We recall that in the case of a circular perturbation of a domain $\Omega := \{\chi = 1\}$ by a ball $B(y,\varepsilon) \subset\subset \Omega$ of radius ε and center y, the topological derivative $D_T\mathcal{J}(\Omega)(y)$ of the functional $\mathcal{J}(\Omega)$ is a scalar field $D_T\mathcal{J}(\Omega)(y)$ defined while assuming that the following expansion holds true

$$\mathcal{J}(\Omega \setminus \overline{B(y,\varepsilon)}) = \mathcal{J}(\Omega) + g(\varepsilon) D_T\mathcal{J}(\Omega)(y) + o(g(\varepsilon)), \tag{2.11}$$

where $g(\varepsilon)$ goes to 0 when ε goes to 0 (see Section 1.3.1 for more details). In [Céa+00], Cea et al. proposed an algorithm of topological optimization in which the topological derivative is used. In [AA06], Amstutz and Andrä have improved this procedure by coupling it with a level-set representation of the domain. Their algorithm is the one we have chosen to use for our numerical study of the higher order homogenized tensors.

2.2.2.1 The level-set procedure

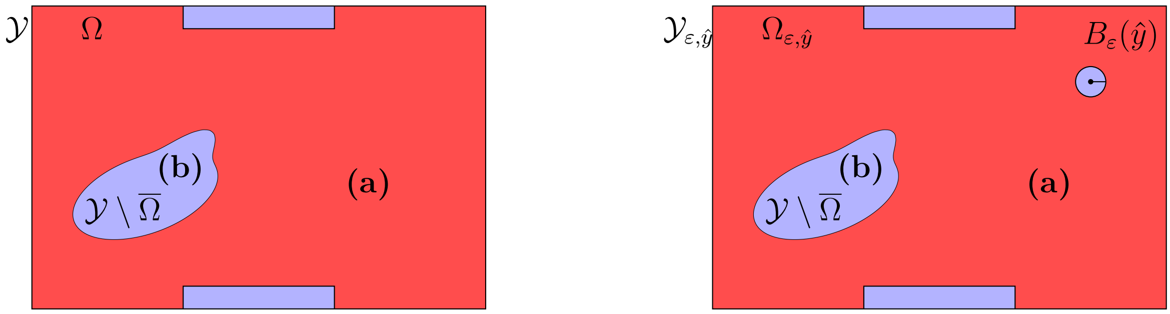


Figure 11: Initial unit cell $\mathcal{Y}$ (left) and perturbed unit cell $\mathcal{Y}_{\varepsilon,\hat{y}}$ (right).

In this section we detail this topology optimization algorithm. The basic idea is to make use of the topological derivative as a steepest-descent direction, analogously to the methods using the gradient of the cost function in classical optimization. The advantage is that the topological derivative represents the exact first order term of the asymptotic expansion of the shape functional with respect to a small parameter measuring the size of a singular domain perturbations. Here we consider the case where the perturbation of the domain is performed by either the inclusion of a small circular set of material **(a)** into the material **(b)**, or the inclusion of a small circular set of material **(b)** into the material **(a)** (see Figure 11). When this circular perturbation is a disk $B(\hat{y}, \varepsilon)$ centered at $\hat{y}$ with a small enough positive radius $0 < \varepsilon$, we define the perturbed domain $\Omega_{\varepsilon,\hat{y}}$ as follows

$$\Omega_{\varepsilon,\hat{y}} := \begin{cases} \Omega \setminus \overline{B(\hat{y}, \varepsilon)} & \text{if } \hat{y} \in \Omega, \\ \Omega \cup B(\hat{y}, \varepsilon) & \text{if } \hat{y} \in \mathcal{Y} \setminus \overline{\Omega}. \end{cases} \tag{2.12}$$

Thus we want to use the following topological asymptotic expansion to implement an optimization procedure:

$$\mathcal{J}(\Omega_{\varepsilon,\hat{y}}) = \mathcal{J}(\Omega) + g(\varepsilon) D_T \mathcal{J}(\Omega)(\hat{y}) + o(g(\varepsilon)), \tag{2.13}$$

where $g(\varepsilon) \to 0$ while $\varepsilon \to 0$. This expansion delivers a necessary local minimality condition for the minimization problem (2.9) under the class of domain perturbations depicted above, which is (see [AA06], [Ams11])

$$D_T \mathcal{J}(\Omega)(\hat{y}) \geq 0, \quad \forall \hat{y} \in \Omega \cup (\mathcal{Y} \setminus \overline{\Omega}). \tag{2.14}$$

To take advantage of the optimality condition (2.14), we start representing the distribution of material composing the cell with a level-set function ψ. Namely we have

$$\Omega = \{x \in \mathcal{Y} \mid \psi(x) < 0\}, \tag{2.15}$$
$$\mathcal{Y} \setminus \overline{\Omega} = \{x \in \mathcal{Y} \mid \psi(x) > 0\}, \tag{2.16}$$

$$\Gamma = \{x \in \mathcal{Y} \mid \psi(x) = 0\}. \tag{2.17}$$

Now the idea is somehow to let the topological derivative $D_T\mathcal{J}(\Omega)$ plays the role of a "target level-set". Indeed, by defining a new signed topological derivative g^T_Ω as follows

$$g^T_\Omega(\hat{y}) = \begin{cases} -D_T\mathcal{J}(\Omega)(\hat{y}) & \text{if } \hat{y} \in \Omega, \\ +D_T\mathcal{J}(\Omega)(\hat{y}) & \text{if } \hat{y} \in \mathcal{Y} \setminus \overline{\Omega}, \end{cases} \tag{2.18}$$

we can rewrite the optimality condition (2.14) as being equivalent to the collinearity between the level-set ψ and the signed topological derivative g^T_Ω. Thus the optimality condition becomes

$$\exists \mathrm{c} > 0, \quad \psi = \mathrm{c} g^T_\Omega. \tag{2.19}$$

The distribution defined by the level-set ψ remains unchanged when we multiply it by a positive scalar. We can therefore normalize in L^2 norm both ψ and g^T_Ω without changing the procedure. From now we consider that $\|\psi\|_{L^2(\mathcal{Y})} = 1$ and $\|g^T_\Omega\|_{L^2(\mathcal{Y})} = 1$. In order to control and drive the collinearity between this two fields, we choose to use θ the non orienting angle between them

$$\theta = \arccos(\langle g^T_\Omega, \psi\rangle_{L^2(\mathcal{Y})}). \tag{2.20}$$

For achieving the optimality condition, we make the level-set evolve "in the direction" of the topological derivative by rotating it of an angle $\kappa\theta$ in the plane $\mathrm{span}\{\psi, g^T_\Omega\}$, where $\kappa \in [0, 1]$ plays the role of a step size. We denote by $C_\kappa(\psi)$ the result of this rotation, namely

$$C_\kappa(\psi) = \cos(\kappa\theta)\psi + \sin(\kappa\theta)\frac{P_{\psi^\perp}(g^T_\Omega)}{\|P_{\psi^\perp}(g^T_\Omega)\|_{L^2(\mathcal{Y})}}, \tag{2.21}$$

where

$$P_{\psi^\perp}(g^T_\Omega) = g^T_\Omega - \cos(\theta)\psi \tag{2.22}$$

is the orthogonal projection of g^T_Ω onto the orthogonal hyperplane $\psi^\perp$ of ψ (see Figure 12). The evolution of the level-set will follow the fixed point procedure $\psi = C_\kappa(\psi)$, where some calculations give (see [AA06])

$$C_\kappa(\psi) = \frac{1}{\sin(\theta)}\left(\sin((1-\kappa)\theta)\psi + \sin(\kappa\theta)g^T_\Omega\right). \tag{2.23}$$

The procedure is summarized in the following steps:

- Choose a initial level-set ψ_0 and an initial step size κ_0
- While the optimality condition (2.19) is not satisfied: iterate on $n \geq 0$
  - calculate the associated topological derivative g^T_n
  - update the level-set function within a line search

    $$\psi_{n+1} = \frac{1}{\sin(\theta_n)}\left(\sin((1-\kappa_n)\theta_n)\psi_n + \sin(\kappa_n\theta)g^T_n\right). \tag{2.24}$$

    The step size κ_n is adapted in order to make sure that the level-set follows a descent direction, that is to make sure that the cost function $\mathcal{J}$ decreases, that is $\mathcal{J}(\Omega_{n+1}) < \mathcal{J}(\Omega_n)$, where $\Omega_{n+1} := \{\psi_{n+1} < 0\}$. We finally decrease the step size if the criterion is not improved.

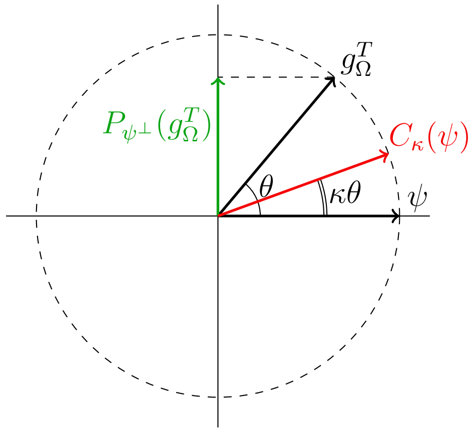


Figure 12: Illustration of the evolution of the level-set from ψ to $C_\kappa(\psi)$, as a function of the signed topological derivative g_Ω^T and of the step size $\kappa \in [0,1]$.

We recall that our topological optimization problem depends on the homogenized tensors. Let us denote by $\boldsymbol{\mathcal{H}}_\Omega$ an arbitrary homogenized tensor depending on Ω. We have demonstrated in Chapter 1, that we have the following rigorous topological asymptotic expansion

$$\boldsymbol{\mathcal{H}}_{\Omega_{\varepsilon,\hat{y}}} = \boldsymbol{\mathcal{H}}_\Omega + g(\varepsilon) D_T \boldsymbol{\mathcal{H}}_\Omega(\hat{y}) + o(g(\varepsilon)),$$

and this expansion is valid for the tensors $\mathbf{C}^h(\Omega)$, $\mathbf{E}^h(\Omega)$, and $\mathbf{D}^h(\Omega)$ we are interested in. From now on we write these tensors more compactly $\mathbf{C}^h_\Omega$, $\mathbf{E}^h_\Omega$, and $\mathbf{D}^h_\Omega$. Moreover we gave explicit formulas for $D_T\boldsymbol{\mathcal{H}}_\Omega$, and we made in the previous section the assumption that j in (2.10) is smooth. Thus we directly have the exact topological derivative of the shape functional $\mathcal{J}$ in (2.10) given by the chain rule

$$D_T\mathcal{J}(\Omega) = \left\langle D_1 j, D_T \mathbf{C}^h_\Omega \right\rangle + \left\langle D_2 j, D_T \mathbf{E}^h_\Omega \right\rangle + \left\langle D_3 j, D_T \mathbf{D}^h_\Omega \right\rangle. \tag{2.25}$$

For the optimization procedure, we will only need to compute the approximated topological derivatives $D_T\boldsymbol{\mathcal{H}}_\Omega$.

2.2.2.2 Numerical computation of the topological derivatives

As we saw in Section 1, in order to, on the one hand calculate the homogenized tensors, and on the other hand calculate the topological derivatives of the homogenized tensors (other than $\mathbf{C}^h_\Omega$), we need to solve auxiliary boundary value problems defined on the cell. Some of them will give us the first and second order correctors $\tilde{u}_{ij}$ and $\tilde{\tilde{u}}_{ijk}$, while others are needed to calculate adjoint-sates. In all cases, the problems to be solved are of the following form:

$$\text{Find } u \in \mathcal{V}: \quad a(u,v) = l(v), \quad \text{for all } v \in \mathcal{W}, \tag{2.26}$$

where we recall that

$$\mathcal{W} := H^1_{\text{per}}(\mathcal{Y};\mathbb{R}^2)/\mathbb{R}, \tag{2.27}$$

$$\mathcal{V} := \left\{ \eta \in H^1_{\text{per}}(\mathcal{Y};\mathbb{R}^2) \,\middle|\, \langle \eta \rangle = 0 \right\}, \tag{2.28}$$

where l is a continuous linear form on $\mathcal{W}$, and a is the bilinear form defined for all $u, v \in \mathcal{V}$

$$a(u,v) = \int_{\mathcal{Y}} \sigma(u) \cdot e(v). \tag{2.29}$$

We solve these problems and implement the optimization procedure in a *Matlab* code, for a computation of the fields by a finite element (FE) discretization. The design variable is the level-set ψ. For the discretization, we select a mesh $\mathcal{M}_h$, and we use P_1 elements for solving (2.26). The numerical level-set ψ is defined by its nodal values. From this we define the field γ characterizing the distribution setting $\gamma = 1$ on the nodes for which the level-set $\psi < 0$, and $\gamma = \gamma_0$ on the nodes where $\psi \geq 0$. At this stage, the contrast field γ is defined by its nodal values. Then by linear interpolation from the nodes to the centers of the triangles, we calculate a contrast field which is constant on each triangle. From this we can construct the stiffness matrix K_ψ and the mass matrix M_ψ once for one iteration of the main optimization loop. Indeed regardless of the corrector or the adjoint state denoted by U we want to calculate, the bilinear form, and then the stiffness matrix remains the same, so that we only adjust the associated linear form L and solve

$$K_\psi U = L. \tag{2.30}$$

We use the *Matlab* function *assema* to assemble the matrix K_ψ, and we wrote a procedure adapted to our problem to calculate L. The periodic boundary conditions imposed for the vector fields is ensured by a procedure described in [Giu+09b], and was implemented by S. Amstutz, and A.A. Novotny (some updates where added by S.M. Giusti, J-M.C. Farias and D.E. Campeão, and myself more recently).

The solutions of approximated auxiliary problems (i.e. correctors and adjoint states) of the form (2.30) are computed. They take their values on the nodes, while their gradients are constant on each triangular element. The homogenized tensors and their topological derivatives depend on the contrast field, and both on the correctors and adjoint states and their gradients. Thus we also interpolate the correctors and adjoint states from the nodes to the center of the triangular elements. With the correctors, we evaluate the approximated constant homogenized tensors by computing the integrals over the unit cell $\mathcal{Y}$ with the constant values of the fields on each triangular element, and hence we evaluate the shape function j. Together with the adjoint states, we compute the approximated topological derivatives fields of the homogenized tensors, which are thus fields given by constant values on each triangular element. Then the application of the chain rule (2.25) allows us to compute directly the approximated signed topological derivative g_Ω^T of j. This scalar field g_Ω^T is also constant within each element of the mesh. Then g_Ω^T is interpolated from the elements to the nodes, in order to be used through expression (2.24) for defining a new level-set function defined on the nodes.

2.2.2.3 The optimization procedure

The optimization produces a sequence of level-set $(\psi_n)_{n\geq 0}$ as follows. For a given initial level-set ψ_0, we compute the homogenized tensors and then evaluate the shape functional. Then we calculate the signed topological derivative of the functional, which is used to update the level-set following (2.24) throughout a line search in which the step size κ is updated ($\kappa = \kappa/2$) until the shape function is improved. If the angle θ between the level-set and the signed topological derivative defined in (2.20) is lower than a predefined threshold $\theta_{\min}$, we consider that the procedure has converged. In the case where the step size is too small ($\kappa < \kappa_{\min}$) – that is the level-set does not progress any more – we try a mesh refinement. The algorithm is summarized Figure 13.

`%Initialisation`
1 ψ_0, j, mesh, $\kappa_0 = \kappa_i$, $n = 0$;
2 **while** $\theta_n > \theta_{\min}$ *or* $\kappa_n > \kappa_{\min}$ **do**
3   `%Homogenization`
4   From the level-set ψ_n ;
5     $\rightarrow$ compute correctors $\tilde{u}_{ij}$, $\tilde{\tilde{u}}_{ijk}$;
6     $\rightarrow$ compute homogenized tensors $\mathbf{C}_n^h$, $\mathbf{E}_n^h$, $\mathbf{D}_n^h$;
7   `%Evaluation of the Shape Functional and the topological derivative`
8     $\rightarrow j_n$, g_n^T ;
9   `%Line-search`
10     $\psi_{old} = \psi_n$, $j_{old} = j_n$, $j_{new} = j_n + 1$;
11   **while** $j_{new} > j_{old}$ *and* $\kappa_n > \kappa_{\min}$ **do**
12   `%Update level-set`
13         $\psi_{new} = C_{\kappa_n}(\psi_n)$;
14   `%Homogenization`
15   From the level-set ψ_{new};
16         $\rightarrow$ compute correctors $(\tilde{u}_{ij})$, $(\tilde{\tilde{u}}_{ijk})$;
17         $\rightarrow$ compute homogenized tensors $\mathbf{C}^h$, $\mathbf{E}^h$, $\mathbf{D}^h$;
18   `%Update Shape Functional and step size`
19         $\rightarrow j_{new}$;
20         $\kappa_n = \kappa_n/2$;
21     $j_{n+1} = j_{new}$, $\kappa_{n+1} = 2\kappa_n$, $n = n + 1$;
22 **if** $\kappa_n > \kappa_{\min}$ **then**
23   Eventually refine the mesh and go back to line 2 ;
24 **else**
    Result: $\psi^\star$

Figure 13: Algorithm: Topological optimization of homogenized tensors

With this algorithm, we investigate in Section 2.3 functionals based on the definition of intrinsic characteristic lengths for a mixture of two materials . We start with a presentation of the setting and of the convergence of the homogenization procedure.

2.3 Results for a mixture of two materials

In this section we consider topological optimization problems of the general form

$$\inf_{\Omega \in \mathcal{U}_{\mathrm{ad}}} \mathcal{J}(\Omega) := j\left(\mathbf{C}_\Omega^h, \mathbf{E}_\Omega^h, \mathbf{D}_\Omega^h\right), \tag{2.31}$$

where Ω is a subdomain of the unit cell $\mathcal{Y}$. The sequence of domains $(\Omega_n)_{n\geq 0}$ produced by the optimization process are defined by $\Omega_n = \{\psi_n < 0\}$ and $\mathcal{Y} \setminus \overline{\Omega_n} = \{\psi_n > 0\}$, where ψ_n is the level-set at the step n (see Section 2.2.2.3), and where the cell is the unit square

$$\mathcal{Y} := (0,1) \times (0,1). \tag{2.32}$$

Both domains are characterized by the same Poisson coefficient

$$\nu := 0.3 \tag{2.33}$$

and by Young's moduli which differ from a contrast $\gamma_0 = 0.01$, that is

$$E_{\{\psi<0\}} = 1, \tag{2.34}$$
$$E_{\{\psi>0\}} = 0.01. \tag{2.35}$$

The initial distribution $\Gamma_0 = \{x \in \mathcal{Y} \mid \psi_0(x) = 0\}$ is a disk (see Figure 14) given by the initial level-set function ψ_0 defined by

$$\psi_0(x, y) = \cos(\pi(x - 0.5))^2 \cos(\pi(y - 0.5))^2 - 0.5. \tag{2.36}$$

Henceforth the homogenized tensors will be written in matrix form, and we simplify the writing by omitting the lower index Ω (indeed we remember that these tensors depend on the distribution of material). This expressions are allowed by the different symmetries satisfied by the tensors, namely $\mathbf{C}^h_{ijkl} = \mathbf{C}^h_{jikl} = \mathbf{C}^h_{klij}$ and $\mathbf{D}^h_{ijkpqr} = \mathbf{D}^h_{jikpqr} = \mathbf{D}^h_{pqrijk}$. Thus we adopt the following convention, also called Voigt notation:

$$\mathbf{C^h} = \begin{pmatrix} \mathbf{C}^h_{1111} & \mathbf{C}^h_{1122} & \sqrt{2}\mathbf{C}^h_{1112} \\ * & \mathbf{C}^h_{2222} & \sqrt{2}\mathbf{C}^h_{2212} \\ * & * & 2\mathbf{C}^h_{1212} \end{pmatrix}, \tag{2.37}$$

and

$$\mathbf{D^h} = \begin{pmatrix} \mathbf{D}^h_{111111} & \mathbf{D}^h_{111221} & \sqrt{2}\mathbf{D}^h_{111121} & \mathbf{D}^h_{111112} & \mathbf{D}^h_{111222} & \sqrt{2}\mathbf{D}^h_{111122} \\ * & \mathbf{D}^h_{221221} & \sqrt{2}\mathbf{D}^h_{221121} & \mathbf{D}^h_{221112} & \mathbf{D}^h_{221222} & \sqrt{2}\mathbf{D}^h_{221122} \\ * & * & 2\mathbf{D}^h_{121121} & \sqrt{2}\mathbf{D}^h_{121112} & \sqrt{2}\mathbf{D}^h_{121222} & 2\mathbf{D}^h_{121122} \\ * & * & * & \mathbf{D}^h_{112112} & \mathbf{D}^h_{112222} & \sqrt{2}\mathbf{D}^h_{112122} \\ * & * & * & * & \mathbf{D}^h_{222222} & \sqrt{2}\mathbf{D}^h_{222122} \\ * & * & * & * & * & 2\mathbf{D}^h_{122122} \end{pmatrix}, \tag{2.38}$$

where $*$ stands for the symmetries of these tensors. This convention is interesting for the following reason. Let $E_{ij}\mathrm{e}_i \otimes \mathrm{e}_j$ be a macroscopic strain tensors. Let Σ be the macroscopic stress tensor defined by $\Sigma_{ij} = \mathbf{C}^h_{ijkl}E_{kl}$. Both are symmetric second order tensors. Thus we can compactly write this tensors by defining two vectors:

$$[\Sigma] = \begin{pmatrix} \Sigma_{11} \\ \Sigma_{22} \\ \sqrt{2}\Sigma_{12} \end{pmatrix}, \quad \text{and} \quad [E] = \begin{pmatrix} E_{11} \\ E_{22} \\ \sqrt{2}E_{12} \end{pmatrix}. \tag{2.39}$$

We can also define the third order tensors $K = \nabla E$ and write it compactly by defining the vector

$$[K] = \begin{pmatrix} K_{111} \\ K_{221} \\ \sqrt{2}K_{121} \\ K_{112} \\ K_{222} \\ \sqrt{2}K_{122} \end{pmatrix}. \tag{2.40}$$

With this definition, we have that the macroscopic energy defined by $(1/2)(\mathbf{C}^h E \cdot E + \mathbf{D}^h K \cdot K) = (1/2)(E_{ij}\mathbf{C}^h_{ijkl}E_{kl} + K_{jik}\mathbf{D}^h_{ijkpqr}K_{pqr})$ can be written with these vectors, and is equal to

$$\frac{1}{2}(\mathbf{C}^h E \cdot E + \mathbf{D}^h K \cdot K) = \frac{1}{2}(\mathbf{C^h}[E] \cdot [E] + \mathbf{D^h}[K] \cdot [K]) = \frac{1}{2}([E]_i \mathbf{C^h}_{ij}[E]_j + [K]_i \mathbf{D^h}_{ij}[K]_j), \tag{2.41}$$

where $\mathbf{C^h}$ is given by (2.37) and $\mathbf{D^h}$ is given by (2.38). Furthermore we have that

$$[\Sigma] = \mathbf{C^h}[E]. \tag{2.42}$$

Apart from the choice of the minimization problem we want to investigate, that is the choice of the functional j, we still have some options to set regarding the initialization. On the one hand we need to defined a mesh, and specify its size. As we said, the vocation of the algorithm procedure we apply is to find local solution to problem (2.31). We have remarked that the procedure can be sensitive to the initialization. It depends both to the size of the mesh and the initial shape Γ_0, and can converge to different local solutions. However we will see in Section 2.3.3 that algorithm encounters a form of stability with respect to the initial data. We start with a rather coarse mesh, so that we can reach rapidly but not precisely a local minimum, and then we refine the mesh. The mesh we choose is made with structured triangles (see Figure 14). We divide the cell $\mathcal{Y}$ with n_i^2 squares crossed by their diagonals, giving $4n_i^2$ triangles elements.

On the other hand we have to determine the initial step size κ_i. In most cases, and when it won't be specified, κ_i will take the value 1. This high value allows the algorithm to initially move quickly through expression (2.24). But in some cases, the first step is too strong and we will choose to start the algorithm with a lower value of κ.

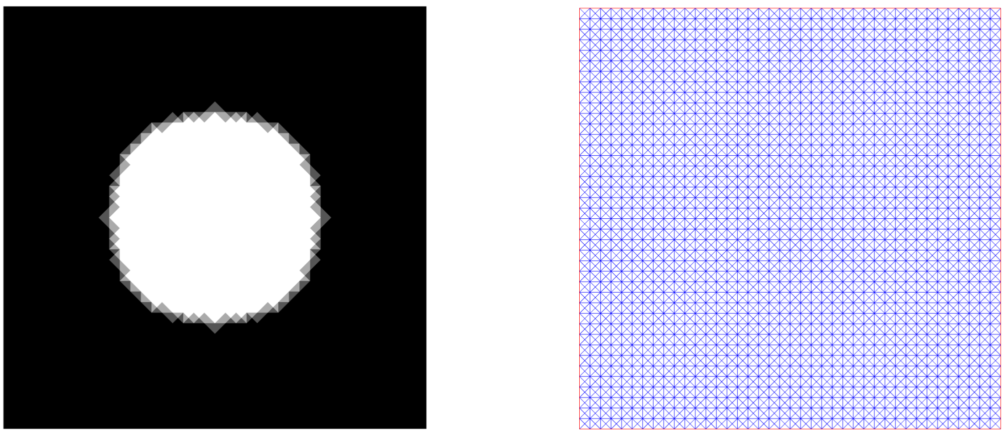


Figure 14: Initial black and white distribution on the left, and initial mesh on the right, both given for a number of squares $n_i = 40$ along one side of $\mathcal{Y}$.

We start in Section 2.3.1 with some properties regarding only the homogenization procedure: that is the computation of the homogenized tensors. Then we study a topological optimization problems of some characteristic lengths and invariants.

2.3.1 Convergence of the homogenization scheme

2.3.1.1 Behaviour with respect to the mesh

We compute the homogenized tensors for the distribution of material given by the initial level-set (2.36), for n_i in the range of 40 to 600, where $4n_i$ represents the number of triangular elements subdividing the square domain $\mathcal{Y} = (0,1) \times (0,1)$. We call $\mathbf{C}^{\mathbf{h}}_{\text{reff}}$, and $\mathbf{D}^{\mathbf{h}}_{\text{reff}}$ the resulting homogenized matrices (2.37) and (2.38) calculated for $n_i = 600$, and we compute the relative differences (see Figure 15)

$$\mathbf{C}^{\mathbf{h}}_{\text{DIFF}}(n_i) = \frac{\|\mathbf{C}^{\mathbf{h}}_{\text{reff}} - \mathbf{C}^{\mathbf{h}}(n_i)\|}{\|\mathbf{C}^{\mathbf{h}}_{\text{reff}}\|}, \quad \mathbf{D}^{\mathbf{h}}_{\text{DIFF}}(n_i) = \frac{\|\mathbf{D}^{\mathbf{h}}_{\text{reff}} - \mathbf{D}^{\mathbf{h}}(n_i)\|}{\|\mathbf{D}^{\mathbf{h}}_{\text{reff}}\|}, \tag{2.43}$$

were for a matrix A, $\|A\|$ is the 2-norm of A, that is to say

$$\|A\| := \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}, \tag{2.44}$$

with $\|x\|_2 = \sqrt{\sum_i x_i^2}$. We can see that for $n_i = 40$ the relative difference made on the matrix $\mathbf{C}^{\mathbf{h}}$ is about 0.6%, and becomes smaller than 0.1% for $n_i \geq 100$. However the relative difference made on $\mathbf{D}^{\mathbf{h}}$ is far greater: 20.6% for $n_i = 40$ and 7.9% for $n_i = 100$. It becomes acceptable from $n_i = 200$, for which the relative difference is 3.1% (see Table 2.1).

n_i	40	60	80	100	200	300	400	500
$\mathbf{C}^{\mathbf{h}}_{\text{DIFF}}(n_i)$ (%)	0.556	0.489	0.163	0.086	0.065	0.012	0.013	0.007
$\mathbf{D}^{\mathbf{h}}_{\text{DIFF}}(n_i)$ (%)	20.643	13.406	10.269	7.298	3.061	1.426	0.724	0.234

Table 2.1

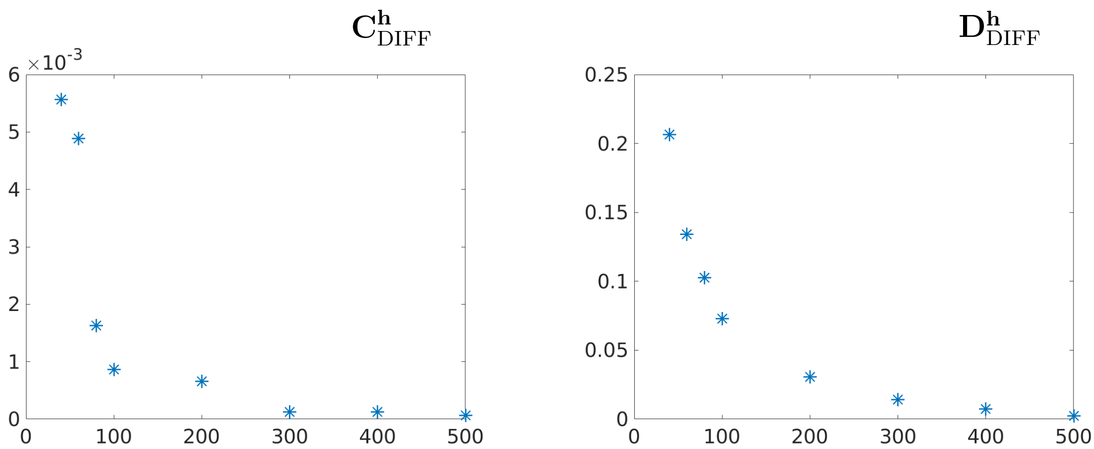


Figure 15: Relative differences in % between $\mathbf{C}^{\mathbf{h}}(n_i)$ and $\mathbf{C}^{\mathbf{h}}_{\text{reff}}$ (left), and between $\mathbf{D}^{\mathbf{h}}(n_i)$ and $\mathbf{D}^{\mathbf{h}}_{\text{reff}}$ (right).

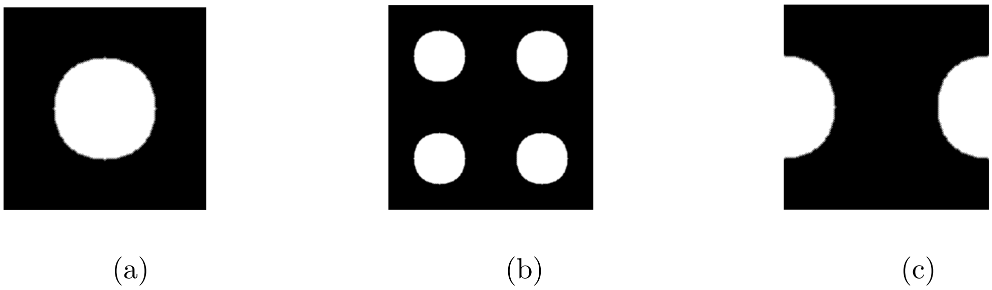


Figure 16: For each figure, the initial level-set is defined by (2.36). From left to right: (a) $ni = 100$, $\mathcal{Y}_a = (0,1) \times (0,1)$. (b) $ni = 200$, $\mathcal{Y}_b = (0,2) \times (0,2)$. (c) $ni = 100$, $\mathcal{Y}_c = (0.5, 1.5) \times (0,1)$.

2.3.1.2 Translation of the unit cell

The definition of the homogenized tensors does depend neither on the size of the unit cell, nor on any translation of it. We want to check numerically this property. To this end we consider for the initial level-set (2.36) the unit cell $\mathcal{Y}_a := \mathcal{Y}$ (case (a)), the translated unit cell $\mathcal{Y}_c := \{(0.5, 0)\} + \mathcal{Y}$ (case (c)), and we can choose another periodicity cell made of four unit cells $\mathcal{Y}_b$ (case (b)) (see Figure 16).

Thus we expect that for each of these configurations, the homogenization procedure provides the same homogenized tensors. That is what we check, paying attention to perform the computations with the same resolution for each cells: that is $n_i = 100$ for (a) and (c), and $n_i = 200$ for (b). Here are the results for matrices $\mathbf{C^h}$ and $\mathbf{D^h}$, calculated for the matrix 2-norm:

$$\frac{\|\mathbf{C^h}(a) - \mathbf{C^h}(b)\|}{\|\mathbf{C^h}(a)\|} = 2.092e - 04, \qquad \frac{\|\mathbf{C^h}(a) - \mathbf{C^h}(c)\|}{\|\mathbf{C^h}(a)\|} = 3.615e - 04 \tag{2.45}$$

$$\frac{\|\mathbf{D^h}(a) - \mathbf{D^h}(b)\|}{\|\mathbf{D^h}(a)\|} = 1.266e - 04, \qquad \frac{\|\mathbf{D^h}(a) - \mathbf{D^h}(c)\|}{\|\mathbf{D^h}(a)\|} = 8.417e - 04. \tag{2.46}$$

This shows that the invariance of homogenized tensors with respect to the unit cell choice is numerically satisfied.

2.3.2 Study based on characteristic lengths

A second-gradient model contains intrinsic lengths. Such model has a macroscopic strain energy depending on the macroscopic strain E and the macroscopic strain-gradient K. Equation (2.8) shows that by picking any coefficients $\mathbf{D}^h_{ijklmn}$ and $\mathbf{C}^h_{ijlm}$, the following ratio without index summation

$$\sqrt{\frac{\mathbf{D}^h_{ijklmn}}{\mathbf{C}^h_{ijlm}}} \tag{2.47}$$

is homogeneous to a length (length dimension is denoted by l). Indeed the strain field E is dimensionless, and the strain-gradient K is of dimension l, while τ is a dimensionless ratio.

These intrinsic lengths can provide us a first naive choice of mechanical quantity to investigate. We could expect that, in some sense, the greater an intrinsic length is, the more significant the second order effects are. We recall that the coefficient $\mathbf{C}^h_{opqr}$ couples the strains E_{op} and E_{qr} in the expression of the macroscopic strain energy, for op (resp.

qr) equal to 11, 22 or 12, and the coefficient $\mathbf{D}^h_{ijklmn}$ couples the strain-gradients K_{ijk} and K_{lmn}, for ijk (resp. lmn) equal to 111, 112, 221, 222, 121 and 122 (recalling that $K_{ijk} = \partial_k E_{ij}$).

A pertinent approach could be the study of lengths related to the eigenvalues $\{E_{\lambda_1}, E_{\lambda_2}, E_{\lambda_3}\}$ of the stiffness matrix $\mathbf{C^h}$, also called *eigenstrains*, defined for all $i = 1,2,3$, $j = 1,2$ by

$$l_{\lambda_i,j} = \sqrt{\frac{(E_{\lambda_i} \otimes \mathrm{e}_j) \cdot \mathbf{D}^h \cdot (E_{\lambda_i} \otimes \mathrm{e}_j)}{E_{\lambda_i} \cdot \mathbf{C}^h \cdot E_{\lambda_i}}}, \tag{2.48}$$

which can be interpreted as a measure of the sensitivity of the material to strain gradients for each eigenstrain of $\mathbf{C}^h$ (see [Dur+20]). We choose a simplified approach in which we look at the unit strains of uniaxial extension E_{11}, and E_{22}, and of pure shear E_{12}. This gives the following definition of the six different arising characteristic lengths:

$$\begin{aligned} l_{111} &= \sqrt{\frac{\mathbf{D}^h_{111111}}{\mathbf{C}^h_{1111}}}, \quad l_{221} = \sqrt{\frac{\mathbf{D}^h_{221221}}{\mathbf{C}^h_{2222}}}, \quad l_{121} = \sqrt{\frac{\mathbf{D}^h_{121121}}{\mathbf{C}^h_{1212}}}, \\ l_{112} &= \sqrt{\frac{\mathbf{D}^h_{112112}}{\mathbf{C}^h_{1111}}}, \quad l_{222} = \sqrt{\frac{\mathbf{D}^h_{222222}}{\mathbf{C}^h_{2222}}}, \quad l_{122} = \sqrt{\frac{\mathbf{D}^h_{122122}}{\mathbf{C}^h_{1212}}}. \end{aligned} \tag{2.49}$$

From this we try first to maximize these lengths. As we said in Section 2.2.1 these characteristic lengths are in fact of order τ. We want to obtain second gradient effects, that means we want to observe a gradient of deformation throughout several cells. For this, we want the unit characteristic lengths (l_Ω not multiplied by τ) to be of order of several cells, or at least one cell. With our definition of the cell in (2.32), we wish to have l_Ω greater than 1.

We start to maximize the characteristic lengths defined in (2.49). In view of the square cell $(0,1) \times (0,1)$, and the isotropic initial shape (see Figure 14), we only consider the maximization of l_{111}, l_{112}, and l_{121}, because we obtain the same results rotated with a $\pi/2$ angle by respectively maximizing l_{222}, l_{221}, and l_{122}. Before numerical investigation, we give the value of the computed homogenized tensors for the initial cell defined by (2.36), and for a mesh $n_i = 100$.

$$\mathbf{C^h} \simeq \begin{pmatrix} 0.6657 & 0.1756 & 0 \\ 0.1756 & 0.6657 & 0 \\ 0 & 0 & 0.3676 \end{pmatrix}, \tag{2.50}$$

$$\mathbf{D^h} \simeq \begin{pmatrix} -0.0889 & -0.0192 & 0 & 0 & 0 & -0.0235 \\ -0.0192 & -0.0057 & 0 & 0 & 0 & -0.0086 \\ 0 & 0 & -0.0032 & -0.0086 & -0.0235 & 0 \\ 0 & 0 & -0.0086 & -0.0057 & -0.0192 & 0 \\ 0 & 0 & -0.0236 & -0.0192 & -0.0889 & 0 \\ -0.0235 & -0.0086 & 0 & 0 & 0 & -0.0032 \end{pmatrix}. \tag{2.51}$$

That is

$$l_{111} \simeq i\,0.3655, \tag{2.52}$$
$$l_{112} \simeq i\,0.0926, \tag{2.53}$$
$$l_{121} \simeq i\,0.0933, \tag{2.54}$$

noting that in each case the lengths are imaginary, because the coefficients $\mathbf{D}^h_{111111}$, $\mathbf{D}^h_{112112}$, and $\mathbf{D}^h_{121121}$ are negative. In the following, we are going to maximize the square of these lengths, and we will observe that for each optimized shape that we obtain, the coefficients of $\mathbf{D}^h$ will be positive, and thus the optimized lengths will be real lengths. Indeed by maximizing these ratios, we force some coefficients of to be small, and even go to zero. In this case we obtain some zero strain energy modes, also called *floppy modes* (see [Dur+20]), corresponding to this apparition of a kernel for $\mathbf{C}^h$, that allows the strain-gradient elastic energy depending on $\mathbf{D}^h$ to be predominant. It is observed in [Dur+20] that in this zero strain energy modes, the corresponding part of $\mathbf{D}^h$ turn to be positive.

2.3.2.1 Length: l_{112}

In this case, we minimize the following functional:

$$j(\mathbf{C}^h, \mathbf{D}^h) := -\frac{\mathbf{D}^h_{112112}}{\mathbf{C}^h_{1111}}. \tag{2.55}$$

The mesh is initialized with $n_i = 100$. After 18 iterations, the level-set reaches almost its final shape, for an angle $\theta \simeq 8.15°$. Then we perform a local refinement of the mesh, and we obtain the final distribution for a total number of iterations of 27, and a final angle $\theta \simeq 5.33°$ (see Figure 17). Here are the values of the component of interest for the final distribution:

$$\mathbf{C}^h_{1111} \simeq 0.0753, \tag{2.56}$$

$$\mathbf{D}^h_{112112} \simeq 0.0034. \tag{2.57}$$

which corresponds to

$$l_{112} \simeq 0.2139. \tag{2.58}$$

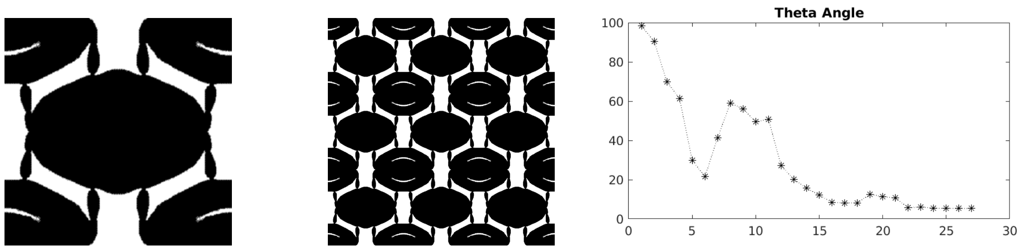


Figure 17: Results for the cost function $j(\mathbf{C}^h, \mathbf{D}^h) = -(\mathbf{D}^h_{112112}/\mathbf{C}^h_{1111})$: maximization of the characteristic length l_{112}. From left to right: optimum unit cell ; periodic microstructure ; convergence history: angle with respect to the number of iterations.

2.3.2.2 Length: l_{121}

In this case, we minimize the following functional:

$$j(\mathbf{C}^h, \mathbf{D}^h) := -\frac{\mathbf{D}^h_{121121}}{\mathbf{C}^h_{1212}}. \tag{2.59}$$

The mesh is initialized with $n_i = 100$. The optimum distribution is reached after 17 iterations for an angle $\theta \simeq 0.01°$ (see Figure 18). Here are the values of the component of interest for the final distribution:

$$\mathbf{C}^h_{1212} \simeq 0.0250, \tag{2.60}$$

$$\mathbf{D}^h_{121121} \simeq 0.0522. \tag{2.61}$$

that is

$$l_{121} \simeq 1.4442. \tag{2.62}$$

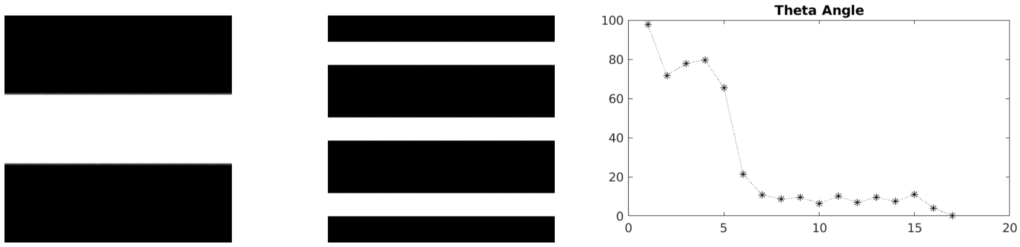


Figure 18: Results for the cost function $j(\mathbf{C}^h, \mathbf{D}^h) = -(\mathbf{D}^h_{121121}/\mathbf{C}^h_{1212})$: maximization of the characteristic length l_{121}. From left to right: optimum unit cell ; periodic microstructure ; convergence history: angle with respect to the number of iterations.

2.3.2.3 Length: l_{111}

In this case, we minimize the functional:

$$j(\mathbf{C}^h, \mathbf{D}^h) = -\frac{\mathbf{D}^h_{111111}}{\mathbf{C}^h_{1111}}. \tag{2.63}$$

The mesh is initialized with $n_i = 100$. We have made two local refinements of the mesh at the iterations 20 and 26, before the level-set finally reached an optimum for a total of 29 iterations, with an angle $\theta \simeq 9.30°$ Surprisingly, in view of the simplicity of the functional involved, we obtain a pantographic like cell (see Figure 19). Here are the value of the component of interest for the final distribution:

$$\mathbf{C}^h_{1111} \simeq 0.1079, \tag{2.64}$$
$$\mathbf{D}^h_{111111} \simeq 0.0183. \tag{2.65}$$

that is

$$l_{111} \simeq 0.4114. \tag{2.66}$$

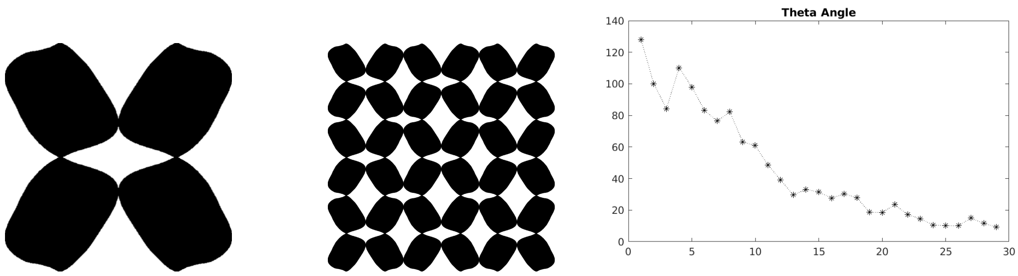


Figure 19: Results for the cost function $j(\mathbf{C}^h, \mathbf{D}^h) = -(\mathbf{D}^h_{111111}/\mathbf{C}^h_{1111})$: maximization of the characteristic length l_{111}. From left to right: optimum unit cell ; periodic microstructure ; convergence history: angle with respect to the number of iterations.

In this section we have obtained some interesting results. Surely we have found some microstructure improving selected characteristic lengths in comparison with the initial distribution (Figure 14). Furthermore, the final coefficient $\mathbf{D}^{\mathbf{h}}_{111111}$ is positive and equal to 0.0183, while it was initially negative: -0.0889 (see (2.51)). But we are quite far from the emergence of *strain gradient* materials. Indeed the characteristic lengths we obtain are quite small. However the optimization scheme has produced an interesting result, especially with the maximization of l_{111} for which we have obtained a *pantographic* material. Thus we are going to investigate with more details this problem in Section 2.3.4. Before this we present some properties concerning the behaviour of the topological optimization algorithm.

2.3.3 Behaviour of the optimization scheme

First we want to investigate the effect of the initial level-set and of the initial mesh on the convergence of the algorithm. For this we consider the problem of minimization of the functional defined in (2.63), for several perturbations of the initial level-set ψ_0 defined in (2.36) as follows. For all i in $\{-4, -3, \cdots, 3, 4\}$ we consider the new initial level-set functions

$$\psi_{0,i} := \psi_0 + i * 0.05. \tag{2.67}$$

In the same time we also consider, for each of these initial level-set functions, different initial meshes. Namely n_i varies in $\{40, 60, 80, 100, 120, 140\}$. The final resulting distributions are gathered in Figure 20 page 78.

As expected, the optimization procedure is sensitive to initial data. We can observe in Figure 20 that both initial level-set and initial mesh influence the final result. We remind that the algorithm produces local optimized topology. We can imagine that even small variations in the data of the problem can lead the procedure to follow different descent directions. Nevertheless, Figure 20 shows some characteristic patterns in the optimized results. In fact we observe that several optimized distributions do look like *pantographic* material (see Figure 19) such as results $(15-18)$, $(21-24)$, $(27, 28)$, (42) in Figure 20. The result (1) has got also a lot of similar results (sometimes translated): $(3-11)$, $(13-14)$, (19), (25), $(29, 30)$, $(33, 34)$, (38), $(40, 41)$, $(45-47)$, and $(52-54)$. This indicates a kind of stability of the topological optimization procedure (at least for the maximization of l_{111}).

Furthermore, even by changing the initial shape of the distribution (but with the same initial topology) the algorithm produces similar results. For example, still within the maximization of l_{111}, we consider an initial rectangular inclusion of material, determined by the following level-set

$$\psi(x, y) = -\max\left(|y-0.5|, 2|x-0.5|\right) + 0.25. \tag{2.68}$$

The final level-set obtained Figure 21 is quite similar to the result (1) from Figure 20.

Now we turn to the effects of the choice of the unit cell on the optimization procedure. In Section 2.3.1.2 we have shown that the homogenization procedure is not affected by the choice of the unit cell. We consider the unit cells (a), (b) and (c) from Figure 16, with meshes defined by $n_i = 50$ for (a) and (c), and $n_i = 100$ for (b). From this we maximize the length l_{111}. For all the cases (a), (b), and (c), we perform a homogeneous refinement of the mesh at iteration 27, and the final topologies are obtained after a total of 37 iterations, for an final angle $\theta \simeq 5.88°$ every time. The results are presented Figure 22, and show that the topological optimization procedure does not depend on the choice of the cell.

Finally we would like to know how behaves the algorithm convergence with respect to the mesh. We have seen in the previous paragraphs that the size of the initial mesh can affects the final result, and leads the algorithm to reach a local optimum rather than

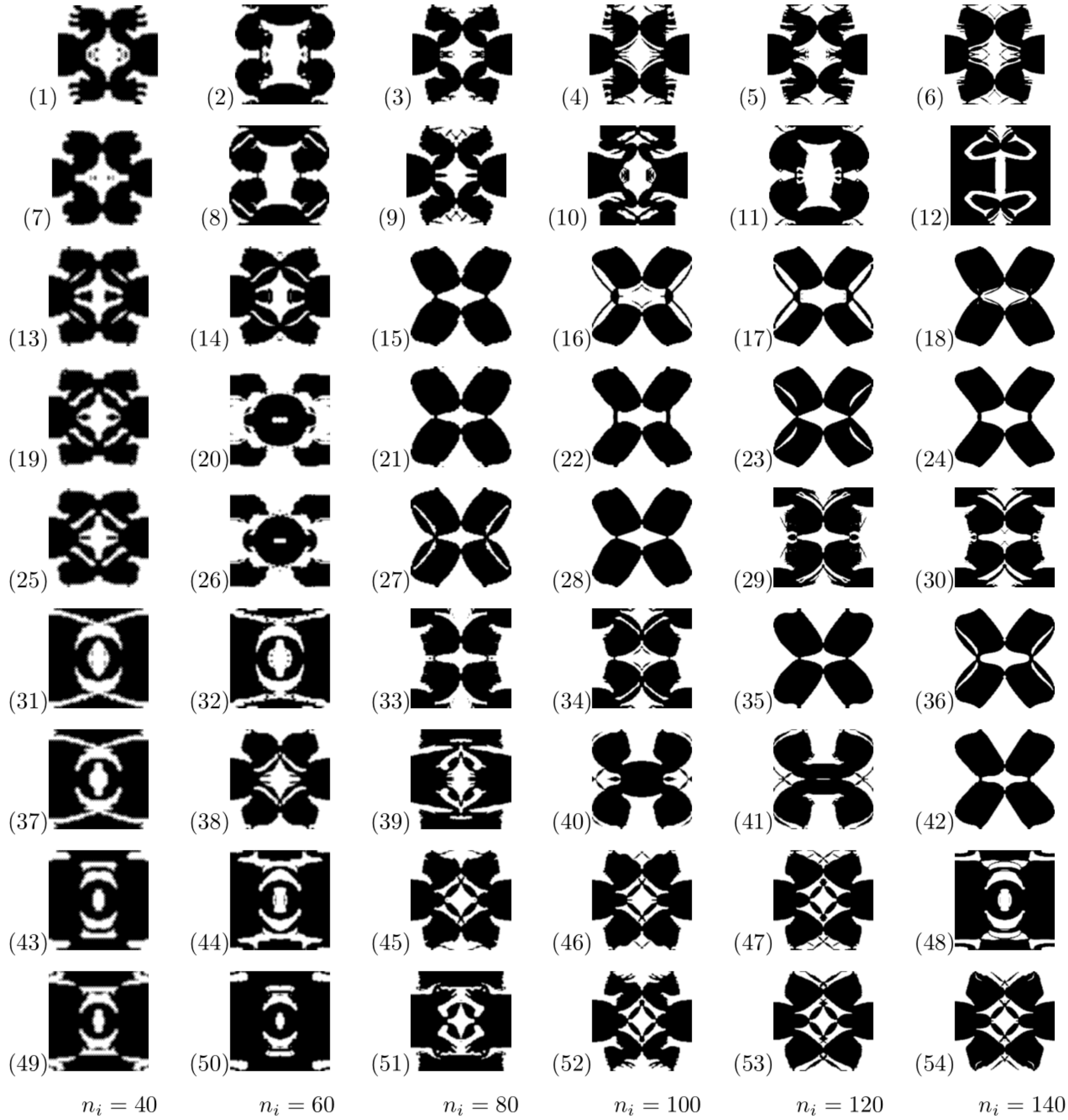


Figure 20: Different final level-sets obtained when the initial level-set and the size of the initial mesh vary. Each line from the top to the bottom is obtained for the level-sets from $\psi_{0,-4}$ to $\psi_{0,4}$ defined in (2.67). Each column corresponds to different mesh sizes.

Figure 21: Maximization of the characteristic length l_{111}. From left to right: initial distribution; optimized distribution.

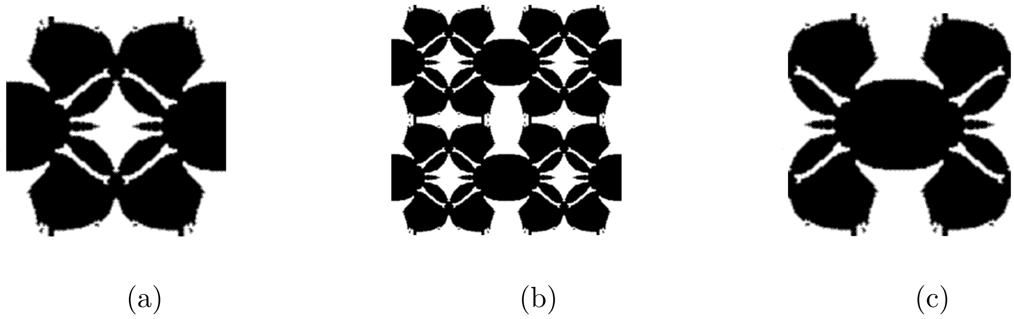


Figure 22: For each figure, the optimized topology obtained by maximization of l_{111}. (a) $ni = 50$, $\mathcal{Y}_a = (0,1) \times (0,1)$. (b) $ni = 100$, $\mathcal{Y}_b = (0,2) \times (0,2)$. (c) $ni = 50$, $\mathcal{Y}_c = (0.5, 1.5) \times (0,1)$.

another. What happens when we get closer to a certain optimum? In order to analyse it, we go back to the maximization of l_{111} for the initial level-set given by (2.36), and for an initial mesh characterized by $n_i = 100$. The algorithm converges to the solution that we display once again (i) Figure 23, for a final angle $\theta \simeq 18.54°$. After the algorithm reached the state (i), we perform a homogeneous refinement of the mesh leading to (ii) Figure 23 for a final angle $\theta \simeq 10.18°$. We repeat the refinements one more time resulting in (iii) for an angle $\theta \simeq 9.08°$.

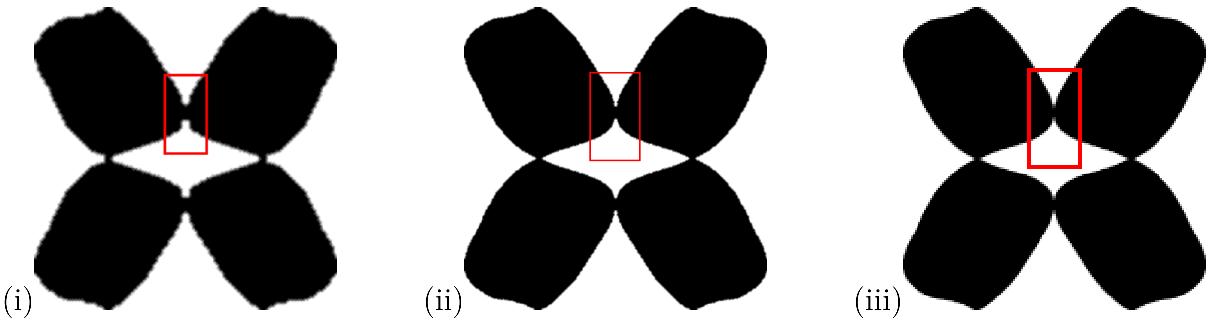
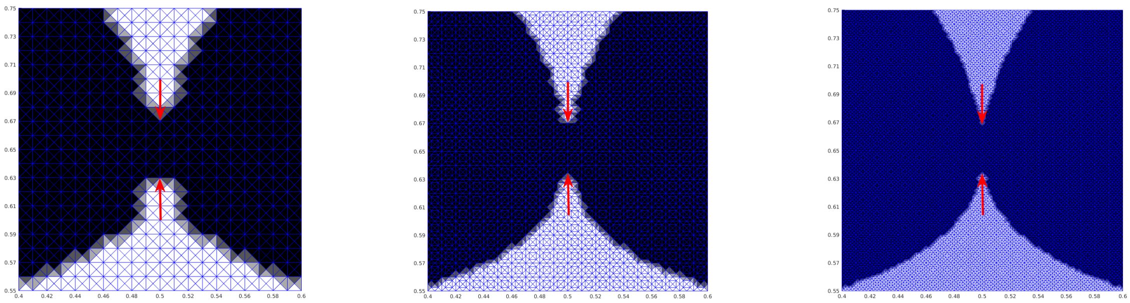


Figure 23: Final optimum topologies for the maximization of l_{111}, initial level-set given by (2.36), $n_i = 100$. (i) no refinement of the mesh. (ii) one refinement of the mesh. (iii) two refinements of the mesh.

We measure the widths of the junction regions surrounded by the red rectangles in Figure 23, which are displayed with a zoom in Figure 24. We find that the width is $\simeq 0.04$ for (i), $\simeq 0.035$ for (ii), and $\simeq 0.0325$ for (iii). It seems that the width of this junction is stable when the mesh goes to zero. The small decrease between (i) and (iii) is specific to the resolution. When we refine the mesh, each element is subdivided into 4 elements, and



(i) (ii) (iii)

Figure 24: Zoom on the junctions surrounded by red rectangles from Figure 23. The new window is $(0.4, 0.6) \times (0.55, 0.75)$.

with the starting mesh, the elements are rectangle triangles of length 0.01 and $0.01\sqrt{2}$, which are of order of the uncertainty on the width of the junction of (i).

2.3.4 Pantographs

The *pantographic continuous material* has been introduced and studied in [Dur+20]. It corresponds to a 2-dimensional periodic material constituted with triangles and lozenges being connected together via fine junctions (see Figure 25). Their layout produces the behaviour of a *pantograph*. This material has got two *floppy modes* in deformation. One in extension E_{11}, and another one in shear E_{12}. When the size of the junctions goes to zero, these floppy modes implies that the first order homogenized matrix $\mathbf{C}^{\mathbf{h}}$ is degenerated, so that a classical macroscopic Cauchy material – whose energy is usually described only by $\mathbf{C}^{\mathbf{h}}$ – is then unsuitable. This is the reason why in [Dur+20] this material has been studied, its macroscopic behaviour is described by a *strain gradient* model, following the formal homogenization scheme proposed in [SC00].

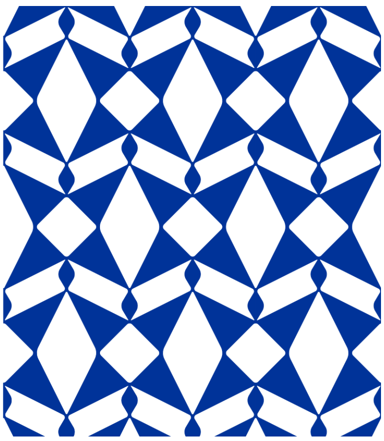


Figure 25: Pantograph (Figure from [Dur+20]).

In Section 2.3.2.3, we have obtained a microstructure being a kind of pantograph, through the maximization of the length l_{111}. This aroused our curiosity, and pushed us to investigate this structure more closely. We start to mimic the framework of the pantograph studied in [Dur+20] (Figure 25). For this we consider the rectangular unit cell

$$\mathcal{Y} = (0, 1) \times (0, 2). \tag{2.69}$$

In their work [Dur+20], Baptiste Durand and Arthur Lebée have evaluated the characteristic lengths of the pantograph for the unit cell $\mathcal{Y}$, and have found $l_{111} \simeq 2.96$ and $l_{112} \simeq 6.16$. We consider the following functional to be minimized

$$j(\mathbf{C}^h, \mathbf{D}^h) = -\frac{\mathbf{D}^h_{111111}}{\mathbf{C}^h_{1111}} - \frac{\mathbf{D}^h_{112112}}{\mathbf{C}^h_{1111}}. \tag{2.70}$$

We choose an initial mesh for which the vertical direction of the rectangle is subdivided into $n_i = 80$ crossed squares, and the horizontal direction is subdivided into $n_i = 40$ crossed squares. The initial step size is $\kappa_i = 0.4$. Finally we choose an initial level-set function defined by

$$\begin{aligned}\psi_0 := &\frac{\cos(3\sqrt{x^2+y^2})^2}{(1+8x^2+10y^2)^2} + \frac{\cos(3\sqrt{x^2+(y-2)^2})^2}{(1+8x^2+10(y-2)^2)^2} + \frac{\cos(3\sqrt{(x-1)^2+y^2})^2}{(1+8(x-1)^2+10y^2)^2} \\ &+ \frac{\cos(3\sqrt{(x-1)^2+(y-2)^2})^2}{(1+8(x-1)^2+10(y-2)^2)^2} + \frac{\cos(3\sqrt{(x-0.5)^2+(y-1)^2})^2}{(1+8(x-0.5)^2+10(y-1)^2)^2} - 0.15\end{aligned} \tag{2.71}$$

resulting in to shifted strips of holes (see Figure 26). After 20 iterations, we perform a homogeneous refinement of the mesh, followed by a local refinement of the mesh after 12 iterations. For a total of 37 iterations, the final angle is $\theta \simeq 7.19°$, and the optimized distribution is shown Figure 26. We finally get

$$l_{111} \simeq 0.2348, \quad l_{112} \simeq 0.4380. \tag{2.72}$$

In comparison with the values $l_{111} \simeq 2.96$ and $l_{112} \simeq 6.16$ obtained by Arthur and Baptiste, the microstructure we have obtained is less efficient. This difference has two possible explanations. First, the computations led by Arthur and Baptiste are made for the case of a cell made up of a material (blue part in Figure 25) and voids (white part). In our case, the white part is a weak material. Secondly, the junction regions of the pantograph in [Dur+20] are built to be small on purpose. We give more details regarding the size of these junction regions in the next section

However, the shape we get in Figure 26 looks pretty much like the pantograph in Figure 25.

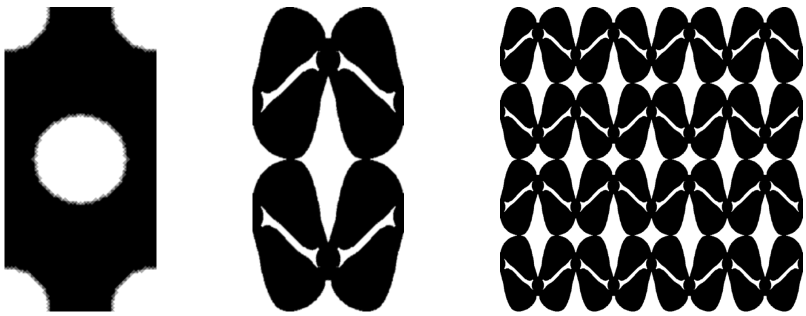


Figure 26: Maximization of the sum $l_{111} + l_{112}$. From left to right: initial distribution; optimized distribution; optimized periodic microstructure

2.4 Behaviour when the contrast vanishes

In the previous section, we have obtained optimal topologies for various functionals, which constitute an interesting result of the proposed topology optimization method.

But the second gradient behaviour, which could be quantified by the characteristic lengths we have introduced, is not very significant. The result we obtained regarding the pantograph is quite new and surprising, but is not competitive with the microstructure studied in [Dur+20]. We can outline two remarks about their home designed pantograph (Figure 25) and the topologically optimized pantograph we obtained (Figure 26). First the solid part of the home designed pantograph (blue part on Figure 25), is surrounded by voids (white part), whereas we compute a microstructure which is a mixture of two materials. Admittedly, the contrast between the stiff and the soft material is important. We recall that the Young's modulus of the stiff material is equal to 1, while the Young's modulus of the soft material is equal to 0.01. The contrast equals to 0.01 is small, but it is non zero. Secondly, we have explained that the second gradient behaviour of the pantograph is exacerbated when the size of the junctions goes to zero, so that these junctions act almost like a ball joint mechanism. With this in mind, the junctions of home designed pantograph [Dur+20] has been set with small junctions whose length is 0.02, when we recall that the length of the unit cell edge is equal to 1. Furthermore in [Dur+20] the authors show that the second gradient model describes perfectly the behaviour of the pantograph for a junction radius of 0.005, while the largest junction in the topological optimized pantograph we compute is of 0.09.

To satisfy in the same time these two restrictions, we found out that we can decrease the contrast γ_0. For this, we need to change slightly the model for the higher order correctors $\tilde{\tilde{u}}_{ijk}$. Indeed we can see on equation (1.51) or (1.68) that we have a volume force depending on $\mathbf{C}^h$ which is applied homogeneously on the unit cell $\mathcal{Y}$. Thus we have a volume force applied to the very weak material **(b)** when the contrast γ_0 goes to zero. We adopt another model for which the weak phase material **(b)** is meant to mimic voids. We describe it below.

In the setting of Section 1.3.2, the topologically perturbed counterpart of the unit cell is given by the characteristic function $\chi^\varepsilon = \chi - \chi_{B_\varepsilon}$, χ_{B_ε} being the characteristic function of the ball B_ε. Let $\varepsilon_0 > 0$, we define a normalized characteristic function for $0 \leq \varepsilon \leq \varepsilon_0$ by

$$\boldsymbol{\varphi}^\varepsilon(y) := \frac{\chi^\varepsilon(y)}{\langle\chi^\varepsilon\rangle} := \frac{V}{\int_\Omega \chi^\varepsilon}\chi^\varepsilon(y) \tag{2.73}$$

Thanks to this normalized characteristic function, we can avoid to apply a volume force on the weak phase. The first auxiliary problem (1.107) remains unchanged, while the second auxiliary problem (1.108) is replaced by

$$\begin{aligned}\tilde{\tilde{u}}^\varepsilon_{ijk} \in \mathcal{V} \ : \ \int_\Omega \gamma_\varepsilon \sigma(\tilde{\tilde{u}}^\varepsilon_{ijk}) \cdot e(\eta) + \int_\Omega \gamma_\varepsilon \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) \cdot e(\eta) = \\ \int_\Omega (\gamma_\varepsilon \sigma(u^\varepsilon_{ij}) - \boldsymbol{\varphi}^\varepsilon \mathbf{C}^h_\varepsilon(\mathrm{e}_i \otimes_s \mathrm{e}_j)) \cdot (\eta \otimes_s \mathrm{e}_k) \quad \forall \eta \in \mathcal{W},\end{aligned} \tag{2.74}$$

with the use of the characteristic function $\boldsymbol{\varphi}^\varepsilon$.

We check the convergence of the model when γ_0 goes to zero. We consider the square unit cell given in (2.32), with the initial level-set (2.36), for a mesh resolution given by $n_i = 200$. With these settings, we compute the relative differences $\mathbf{D}^{\mathbf{h}}_{\mathrm{DIFF}}(\gamma_{0,i})$ of the matrices $\mathbf{D}^{\mathbf{h}}_{\gamma_{0,i}}$ calculated when the contrasts $\gamma_0 = \gamma_{0,i}$ are varying in the set $\{0.0005, 0.001, 0.002, 0.003, 0.004, 0.005, 0.006, 0.007, 0.008, 0.009, 0.01\}$, in comparison to

$\mathbf{D}^{\mathbf{h}}_{\text{reff}}$ calculated for $\gamma_0 = 0.0001$.

$$\mathbf{D}^{\mathbf{h}}_{\text{DIFF}}(\gamma_{0,i}) = \frac{\|\mathbf{D}^{\mathbf{h}}_{\text{reff}} - \mathbf{D}^{\mathbf{h}}_{\gamma_{0,i}}\|}{\|\mathbf{D}^{\mathbf{h}}_{\text{reff}}\|}. \tag{2.75}$$

We can see the results in Figure 27, displaying a linear convergence of the matrix $\mathbf{D}^{\mathbf{h}}$ when the contrast goes to zero.

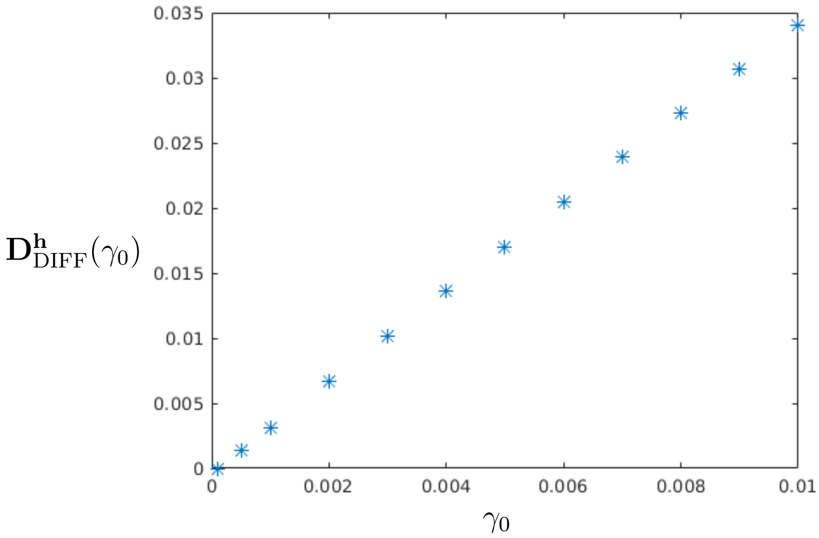


Figure 27: Relative difference of the matrix $\mathbf{D}^{\mathbf{h}}_{\gamma_{0,i}}$ with respect to the contrast $\gamma_{0,i}$, in comparison with $\mathbf{D}^{\mathbf{h}}_{\text{reff}}$ calculated for $\gamma_0 = 0.0001$.

We go back to the problem of the maximization of l_{111} from Section 2.3.2.3, on the square unit cell with an initial circular inclusion of material **(b)**. We found an optimized microstructure with a characteristic length $l_{111} = 0.4114$. We consider the same problem with the above model for which the material **(b)** mimics voids (see Figure 11). The unit cell is given by (2.32), the initial level-set by (2.36).

1. First we start with a initial mesh having a resolution of $n_i = 50$, and a contrast $\gamma_0 = 0.01$. After 47 iterations, we perform a homogeneous refinement of the mesh, and then an local refinement of the mesh at iteration 56, so that the algorithm converges in a total of 62 iterations to the microstructure (I), for an angle $\theta = 7.83°$ (see Figure 28). The final characteristic length is

$$l^{(I)}_{111} = 0.4092, \tag{2.76}$$

and the width of the junction is of 0.035 (see Figure 29).

2. Secondly we follow the same path as the one leading to (I), but this time, together with the local refinement of the mesh at iteration 56, we change the contrast γ_0 from 0.01 to 0.005. We perform another local refinement of the mesh at iteration 64, and then the algorithm converges in a total of 71 iterations to the microstructure (II), for an angle $\theta \simeq 8.42°$ (see Figure 28). The final characteristic length is

$$l^{(II)}_{111} = 0.5849, \tag{2.77}$$

and the width of the junction is of 0.0225 (see Figure 29).

3. Finally we follow the same path as the one leading to (II), but this time, together with the local refinement of the mesh at iteration 64, we change the contrast γ_0 from 0.005 to 0.001. Then we perform a local refinement of the mesh at iteration 73. The algorithm converges in a total of 76 iterations to the microstructure (III), for an angle $\theta \simeq 19.00°$ (see Figure 28). The final characteristic length is

$$l_{111}^{(III)} = 1.2649, \tag{2.78}$$

and the width of the junction is of 0.0125 (see Figure 29).

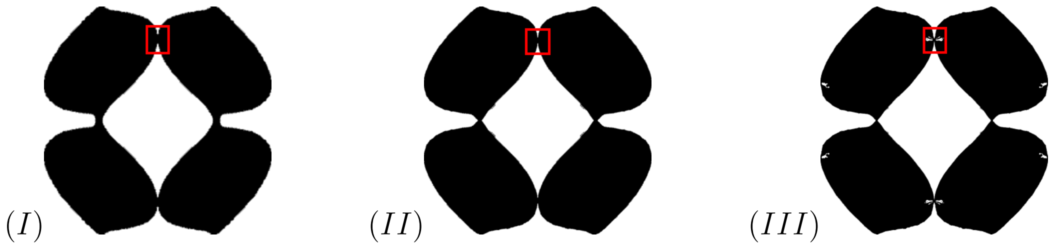


Figure 28: Maximization of the characteristic length l_{111} for different contrasts γ_0. (I) $\gamma_0 = 0.01$. (II) $\gamma_0 = 0.005$. (III) $\gamma_0 = 0.001$.

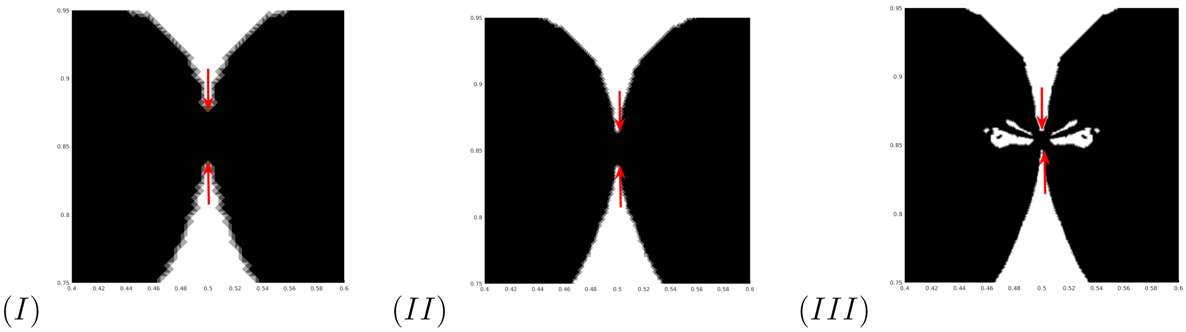


Figure 29: Zoom on the junctions surrounded by red rectangles from Figure 28. The new window is $(0.4, 0.6) \times (0.75, 0.95)$.

In conclusion we have improved the second gradient properties by diminishing the contrast. We find that in this case, the width of the junctions goes to zero. We retrieve this property imposed for the home designed pantograph of [Dur+20] in Figure 25: the small junctions are supposed to act like a ball joint mechanism.

We finally study the problem treated in Section 2.3.4 in the case of vanishing contrast. We recall that the functional to be minimized is

$$j(\mathbf{C}^h, \mathbf{D}^h) = -\frac{\mathbf{D}^h_{111111}}{\mathbf{C}^h_{1111}} - \frac{\mathbf{D}^h_{112112}}{\mathbf{C}^h_{1111}}. \tag{2.79}$$

The initial distribution is given by the level-set defined by (2.71) (see Figure 26) on the rectangular unit cell $\mathcal{Y} = (0,1) \times (0,2)$.

1. First we start with a initial mesh having a resolution of $n_i = 50$, and a contrast $\gamma_0 = 0.01$. After 32 iterations, we perform a homogeneous refinement of the mesh,

and then an local refinement of the mesh at iteration 41, so that the algorithm converges in a total of 48 iterations to the microstructure $(\mathcal{P}_1)$, for an angle $\theta \simeq 9.19°$ (see Figure 30). The final characteristic lengths are

$$l_{111}^{(\mathcal{P}_1)} = 0.3045, \tag{2.80}$$
$$l_{112}^{(\mathcal{P}_1)} = 0.5128. \tag{2.81}$$

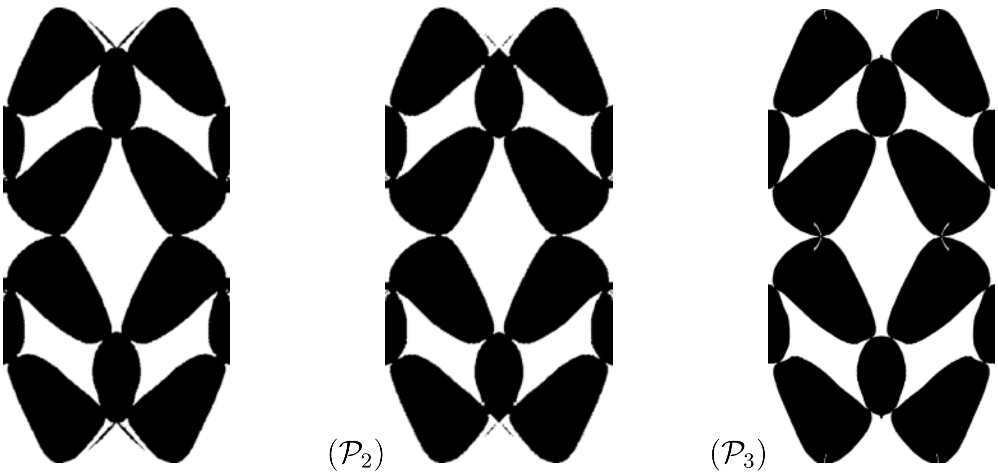
2. Secondly we follow the same path as the one leading to $(\mathcal{P}_1)$, but this time, together with the homogeneous refinement of the mesh at iteration 32, we change the contrast γ_0 from 0.01 to 0.008. We perform another change of the contrast from 0.008 to 0.006 at iteration 39, and from 0.006 to 0.005 plus a local refinement of the mesh one iteration latter. The algorithm converges in a total of 47 iterations to the microstructure $(\mathcal{P}_2)$, for an angle $\theta \simeq 11.76°$ (see Figure 30). The final characteristic lengths are

$$l_{111}^{(\mathcal{P}_2)} = 0.4117, \tag{2.82}$$
$$l_{112}^{(\mathcal{P}_2)} = 0.7476. \tag{2.83}$$

3. Finally we follow the same path as the one leading to $(\mathcal{P}_1)$, but this time, together with the homogeneous refinement of the mesh at iteration 32, we change the contrast γ_0 from 0.01 to 0.005. Then we change the contrast from 0.005 to 0.001 together with a local refinement of the mesh at iteration 40. We perform two additional local refinements of the mesh at iterations 51 and 57. The algorithm converges in a total of 60 iterations to the microstructure $(\mathcal{P}_3)$, for an angle $\theta \simeq 13.80°$ (see Figure 30). The final characteristic lengths are

$$l_{111}^{(\mathcal{P}_3)} = 0.8855, \tag{2.84}$$
$$l_{112}^{(\mathcal{P}_3)} = 1.7838. \tag{2.85}$$

The shapes we get in Figure 30 bear an impressive resemblance to the pantograph in Figure 25.



$(\mathcal{P}_1)$ $(\mathcal{P}_2)$ $(\mathcal{P}_3)$

Figure 30: Maximization of the sum of the characteristic lengths $l_{111} + l_{112}$ for different contrasts γ_0. $(\mathcal{P}_1)$ $\gamma_0 = 0.01$. $(\mathcal{P}_2)$ $\gamma_0 = 0.005$. $(\mathcal{P}_3)$ $\gamma_0 = 0.001$.

2.5 Study based on invariants

In the previous study, we have defined some basic functionals depending on the homogenized tensors, in order to bring out new microstructures. In this first approach we have optimized characteristic lengths expressed in the orthonormal canonical basis $\{\mathrm{e}_1, \mathrm{e}_2\}$ we have fixed. As we said, the mechanical information contained in the second order tensor $\mathbf{D}^h$ is not completely understood. In collaboration with Jean-François Ganghoffer and Nicolas Auffray, we have investigated properties which, even if they are complicated to described from a mechanical point of view, are independent of the spatial orientation of the material. To perform such an optimization problem independently of the spatial orientation of the material, the shape functional needs to be written with respect to some *invariants* of the tensors. For this, we are going to describe concisely how to define these invariants in the framework of the invariant theory, following what has been done in [OKA13], [AR16], [AKO17], [Auf17], [AAD21]. For the sake of simplicity, we confine this short presentation to the case of 4th-order tensors, even though the recent works [AAD21] and [ADA21] allows us to define invariants for tensors of order 5 and 6.

2.5.1 Orientation of a material

The properties of an homogenized elastic material are encapsulated in its homogenized tensors. Let $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ denotes the space of the 4th-order tensors T satisfying the following index symmetries: $T_{ijkl} = T_{jikl}$ and $T_{ijkl} = T_{klij}$. Let $T = T_{ijkl}\mathrm{e}_i \otimes \mathrm{e}_j \otimes \mathrm{e}_k \otimes \mathrm{e}_l$ be an arbitrary tensor belonging to $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$. We also name it the space of fourth order elasticity tensors. We would like to study properties of T whatever the orientation of the material is. Indeed the nature of a material is the same when it is subjected to a rotation or a mirror isometry through a line. Let $O(2)$ be the orthogonal group, that is the group of the 2 dimensional isometric transformations. We consider the action of $O(2)$ on $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ given by

$$\forall Q \in O(2),\ (Q \star T)_{ijkl} = Q_{ip}Q_{jq}Q_{kr}Q_{ls}T_{pqrs}. \tag{2.86}$$

Then with the perspective of a study independent of the orientation, we should not focus on the tensor T, but on its *orbit* Orb_T through the action of $O(2)$, also called $O(2)$-*orbit*, defined by

$$\mathrm{Orb}_T = \{\tilde{T} \in \mathbb{T}_{\underline{(ij)}\ \underline{(kl)}} \mid \exists Q \in O(2),\ \tilde{T} = Q \star T\}. \tag{2.87}$$

In that respect, the idea is to reveal functions depending on the tensor variable T, that will remains constant on these orbits. That is the case for what we call $O(2)$-*invariant polynomial* on $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$.

2.5.2 Definition of polynomial invariants

Let $\mathbb{V}$ be a finite dimensional real vector space on which acts the group $O(2)$. The action is still denoted by $\star$. A polynomial p on $\mathbb{V}$ is said to be an $O(2)$-*invariant polynomial* if

$$\forall x \in \mathbb{V},\ \forall Q \in O(2),\ p(x) = p(Q \star x). \tag{2.88}$$

A classical result of the invariant theory stipulates that for the action of $O(2)$ (the result is valid for compact group in general), there exists a finite set of polynomials $\{p_1, \cdots, p_k\}$ called *integrity basis*, which generates the algebra of the $O(2)$-invariant polynomials (see e.g., [OKA13], [Auf17]). That is any $O(2)$-invariant polynomial on $\mathbb{V}$ is a polynomial in the elements of the integrity basis. Furthermore, such an integrity basis is actually a *functional basis*, that is

$$p_i(x_1) = p_i(x_2),\ \forall i \in \{1, \cdots, k\} \quad \Leftrightarrow \quad \exists Q \in O(2),\ x_1 = Q \star x_2. \tag{2.89}$$

Thus we can characterize the orbits Orb_T with such an integrity basis for the action of $O(2)$ on $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$. But before that, we need to decompose the tensor into elementary tensors irreducible under $O(2)$ action. This is called the *harmonic decomposition*.

2.5.3 Harmonic decomposition

Let $\mathbb{V}$ be a real vector space such that we have an action of $O(2)$ on $\mathbb{V}$. A subspace $\mathbb{U}$ of $\mathbb{V}$ is said to be $O(2)$-irreducible if it is stable under the action of $O(2)$, that is

$$\forall Q \in O(2),\ \forall T \in \mathbb{U}, \quad Q \star T \in \mathbb{U}, \tag{2.90}$$

and if the only stable subspaces of $\mathbb{U}$ are the null space $\{0_{\mathbb{V}}\}$ and $\mathbb{U}$ itself. As a classical result of group theory (valid in general for any action of a compact group on a finite dimensional vector space), we know that $\mathbb{V}$ can be written as a direct sum of $O(2)$-irreducible subspaces. Another result shows that for any finite dimensional $O(2)$-irreducible space $\mathbb{U}$, we have an isomorphism $\phi : \mathbb{U} \to \mathbb{K}^n$, for some n, where $\mathbb{K}^n$ is the space of totally symmetric and traceless n order tensors, and this isomorphism ϕ is $O(2)$-*equivariant*, namely

$$\forall T \in \mathbb{U},\ \forall Q \in O(2), \quad \phi(Q \star T) = Q \star \phi(T). \tag{2.91}$$

Here we consider the natural action of $O(2)$ on $\mathbb{K}^n$ (see [AKO17] or [AAD21]). Finally, this results show that we can find a linear isomorphism $O(2)$-equivariant ϕ between a direct sum of harmonic tensor spaces and $\mathbb{V}$,

$$\phi : \bigoplus_k \alpha_k \mathbb{K}^k \to \mathbb{V}, \quad \text{with } \alpha_k \mathbb{K}^k := \bigoplus_{l=1}^{\alpha_k} \mathbb{K}^k, \tag{2.92}$$

where a finite number of α_k are non zero. This is what we call the *isotypic harmonic decomposition* of $\mathbb{V}$. We can write more compactly

$$\mathbb{V} \simeq \bigoplus_k \alpha_k \mathbb{K}^k. \tag{2.93}$$

Let us apply this harmonic decomposition to $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ following what is done in [AAD21]. We recall that the tensors of $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ appear in the *constitutive law*. The constitutive law in linear elasticity is a linear relation between the Cauchy stress tensor $\sigma \in S^2(\mathbb{R}^2)$, and the strain tensor $e \in S^2(\mathbb{R}^2)$, where $S^2(\mathbb{R}^2)$ is the space of bi-dimensional symmetric second-order tensors, also called *state space*. This law is given for an elasticity tensor $T \in \mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ by

$$\sigma_{ij} = T_{ijkl} e_{kl}. \tag{2.94}$$

That is to say we consider a tensor $T \in \mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ as being a linear map between the stress and the strain state spaces: $T \in \mathcal{L}(S^2(\mathbb{R}^2), S^2(\mathbb{R}^2)) \simeq S^2(\mathbb{R}^2) \otimes S^2(\mathbb{R}^2)$. Thus, rather than directly decompose the space of fourth order elasticity tensors $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$, we decompose in a first time the state space $S^2(\mathbb{R}^2)$. The harmonic structure of $S^2(\mathbb{R}^2)$ is

$$S^2(\mathbb{R}^2) \simeq \mathbb{K}^2 \oplus \mathbb{K}^0. \tag{2.95}$$

In a second step, this decomposition of $S^2(\mathbb{R}^2)$ induces a block decomposition of the space $\mathcal{L}(S^2(\mathbb{R}^2), S^2(\mathbb{R}^2))$, but the blocks of this decomposition are not necessary irreducible. Thus in a third time, the harmonic decomposition of the blocks is performed. We do not present the details of the harmonic decomposition which can be found in [AAD21]. Finally the harmonic structure is of $\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}}$ is the following

$$\mathbb{T}_{\underline{(ij)}\ \underline{(kl)}} \simeq \mathbb{K}^4 \oplus \mathbb{K}^2 \oplus 2\mathbb{K}^0. \tag{2.96}$$

For the case of the 6th order elasticity tensors D, we can consider that D drives the linear constitutive law between the *hyperstress tensor* $\boldsymbol{\tau}$ (defined by this law as follows) and the *strain gradient* tensor $\nabla e = (\partial_k e_{ij})\mathrm{e}_i \otimes \mathrm{e}_j \otimes \mathrm{e}_k$,

$$\boldsymbol{\tau}_{ijk} = D_{ijkpqr}(\nabla e)_{pqr}. \tag{2.97}$$

The state space of the hyperstress and the strain gradient tensors, denoted by $\mathbb{T}_{(ij)k}$, is the space of the third order tensors $\boldsymbol{\tau}$ satisfying the following symmetry relation $\boldsymbol{\tau}_{ijk} = \boldsymbol{\tau}_{jik}$. So that we consider that the space of sixth order elasticity tensors, denoted by $\mathbb{T}_{\underline{(ij)k}\ \underline{(pq)r}}$, is the space of tensors D satisfying $D_{ijkpqr} = D_{jikpqr}$ and $D_{ijkpqr} = D_{pqrijk}$. We have the following harmonic structures ([AAD21])

$$\mathbb{T}_{(ij)k} \simeq \mathbb{K}^3 \oplus 2\mathbb{K}^1, \tag{2.98}$$

$$\mathbb{T}_{\underline{(ij)k}\ \underline{(pq)r}} \simeq \mathbb{K}^6 \oplus 2\mathbb{K}^4 \oplus 5\mathbb{K}^2 \oplus 4\mathbb{K}^0 \oplus \mathbb{K}^{-1}, \tag{2.99}$$

where we recall that $\mathbb{K}^n$ for $n \geq 1$ is the space of totally symmetric and traceless n order tensors, $\mathbb{K}^0$ is the space of scalar tensors, and $\mathbb{K}^{-1}$ is the space of *pseudo-scalar tensors*, which is the space of scalars whose sign changes under a mirror transformation.

2.5.4 A deviatoric/spheric coupling invariant β

As we said in the previous section, before decomposing the tensor space $\mathbb{T}_{\underline{(ij)k}\ \underline{(pq)r}}$, we decompose the state space $\mathbb{T}_{(ij)k}$, in order to obtain a block structure for $\mathbb{T}_{\underline{(ij)k}\ \underline{(pq)r}}$, and finally we decompose these blocks. It is shown in [AAD21] that

$$\mathbb{T}_{(ij)k} \simeq \mathbb{K}^3 \oplus 2\mathbb{K}^1. \tag{2.100}$$

Because of the multiplicity of $\mathbb{K}^1$ in the harmonic structure (2.100), its explicit harmonic decomposition is not uniquely defined. Thus we have a choice to make in its decomposition, and it is preferable make it in such a way that this decomposition is mechanically meaningful. For this, we remember that a tensor in $\mathbb{T}_{(ij)k}$ is the gradient of a tensor in $S^2(\mathbb{R}^2)$, whose harmonic structure is given by (2.95). We decompose a tensor $T \in S^2(\mathbb{R}^2)$ into a deviatoric tensor $T^d \in \mathbb{K}^2$ and into a spheric tensor $T^s \in \mathbb{K}^0$:

$$T = T^d + T^s, \tag{2.101}$$

where $T^s = 1/2\,\mathrm{tr}(T)\mathrm{I}$ and $T^d = T - T^s$. Then we introduce a decomposition of $\mathbb{T}_{(ij)k}$ based on the derivation of the harmonic decomposition (2.101), namely the differentiation of the deviatoric and the spherical parts. This gives for a tensor $K \in \mathbb{T}_{(ij)k}$ the following decomposition

$$K = K^{3d} + K^{1d} + K^{1s}, \tag{2.102}$$

where

$$(K^{3d}, K^{1d}) \in \mathbb{K}^3 \times \mathbb{K}^1 \tag{2.103}$$

stand for the gradient of deviatoric part, and

$$K^{1s} \in \mathbb{K}^1 \tag{2.104}$$

stands for the gradient of the spherical part. This leads to the following per block decomposition for a tensor $D \in \mathbb{T}_{\underline{(ij)k}\ \underline{(pq)r}}$:

$$D = \begin{pmatrix} D^{3d,3d} & D^{3d,1d} & D^{3d,1s} \\ D^{1d,3d} & D^{1d,1d} & D^{1d,1s} \\ D^{1s,3d} & D^{1s,1d} & D^{1s,1s} \end{pmatrix}, \tag{2.105}$$

which corresponds to the harmonic structure (see [AAD21]):

$$\begin{pmatrix} \mathbb{K}^3 \otimes^s \mathbb{K}^3 & \mathbb{K}^3 \otimes \mathbb{K}^1 & \mathbb{K}^3 \otimes \mathbb{K}^1 \\ \mathbb{K}^3 \otimes \mathbb{K}^1 & \mathbb{K}^1 \otimes^s \mathbb{K}^1 & \mathbb{K}^1 \otimes \mathbb{K}^1 \\ \mathbb{K}^3 \otimes \mathbb{K}^1 & \mathbb{K}^1 \otimes \mathbb{K}^1 & \mathbb{K}^1 \otimes^s \mathbb{K}^1 \end{pmatrix}. \tag{2.106}$$

We choose to investigate a particular invariant related to the coupling of the deviatoric part K^{1d} and the spherical part K^{1s}, that is to say an invariant concerning the harmonic block $\mathbb{K}^1 \otimes \mathbb{K}^1$. It is shown in [AAD21] that this harmonic block is decomposed as follows:

$$\mathbb{K}^1 \otimes \mathbb{K}^1 \simeq \mathbb{K}^2 \oplus \mathbb{K}^0 + \mathbb{K}^{-1}. \tag{2.107}$$

For such an harmonic structure, we have two kinds of invariants. The *specific invariants*, concerning a single harmonic component, and the *joint invariants*, concerning more than one harmonic components. We are interesting in the specific invariant β related to the harmonic component $\mathbb{K}^{-1}$. This invariant β is actually invariant under the action of $SO(2)$, which is the subgroup of elements of $O(2)$ which preserve the orientation. We recall that $\mathbb{K}^{-1}$ is the space of *pseudo-scalar tensors*, which is the space of scalars whose sign changes under a mirror transformation (also called reflection). Thus the invariant β changes its sign under a mirror transformation. Let $D \in \mathbb{T}_{\underline{(ij)k}\ \underline{(pq)r}}$, the invariant β_D is defined as follows (see [ADA21]):

$$\beta_D = D_{111112} - \sqrt{2}D_{111121} + \sqrt{2}D_{122112} + \sqrt{2}D_{122222} - \sqrt{2}D_{221121} - D_{221222}. \tag{2.108}$$

We investigate two shape functionals j^+ and j^- depending on the homogenized tensors $\mathbf{C}^h$ and $\mathbf{D}^h$. The purpose regarding $\mathbf{C}^h$ is to maximize the bulk modulus, and regarding $\mathbf{D}^h$ to minimize $+\beta_{\mathbf{D}^h}$ or $-\beta_{\mathbf{D}^h}$. This gives the following problems:

$$\min j^{\pm}(\mathbf{C}^h, \mathbf{D}^h), \tag{2.109}$$

where

$$j^{\pm}(\mathbf{C}^h, \mathbf{D}^h) = \pm\left(\mathbf{D}^h_{111112} - \sqrt{2}\mathbf{D}^h_{111121} + \sqrt{2}\mathbf{D}^h_{122112} + \sqrt{2}\mathbf{D}^h_{122222} - \sqrt{2}\mathbf{D}^h_{221121} - \mathbf{D}^h_{221222}\right) + (\mathbf{S}^{hom}_{1111} + 2\mathbf{S}^{hom}_{1122} + \mathbf{S}^{hom}_{2222}). \quad (2.110)$$

The initial level-set is given by (2.36), and the initial mesh is given by $n_i = 40$.

For both functionals, the algorithm converges in 14 iterations, and the final angle is $\theta \simeq 8.84°$. It is interesting to observe that we obtain two tetrachiral microstructures (see Figure 31), which are the same under a mirror transform, knowing that in one case we minimize $\beta_{\mathbf{D}^h}$, and in the other case we minimize $-\beta_{\mathbf{D}^h}$, where $\beta_{\mathbf{D}^h}$ is a pseudo-scalar, that is where the sign of $\beta_{\mathbf{D}^h}$ changes under a mirror transformation.

It is inspiring to observe that the convergence of the algorithm is uniform, fast when we optimize invariants, and in particular to observe for real some theoretical properties coming from the invariant theory. This gives confidence in a more generalized study of topological optimization problems relying on functionals which depend on the invariants of the homogenized tensors.

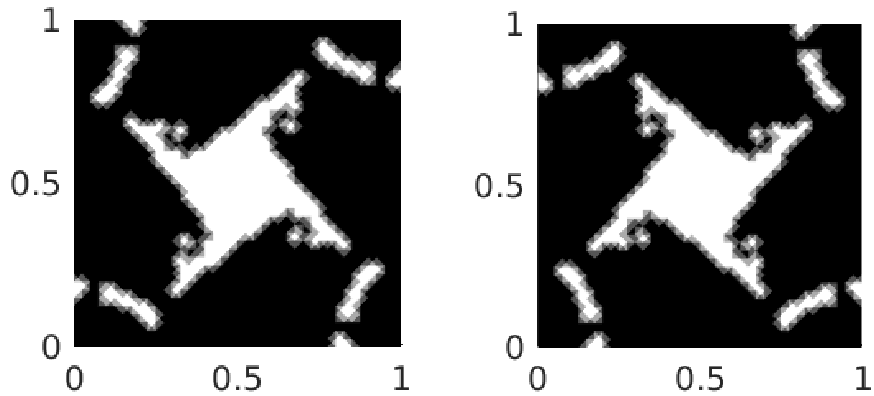


Figure 31: Final shape for the minimization of j^+ (left), and for the minimization of j^- (right).

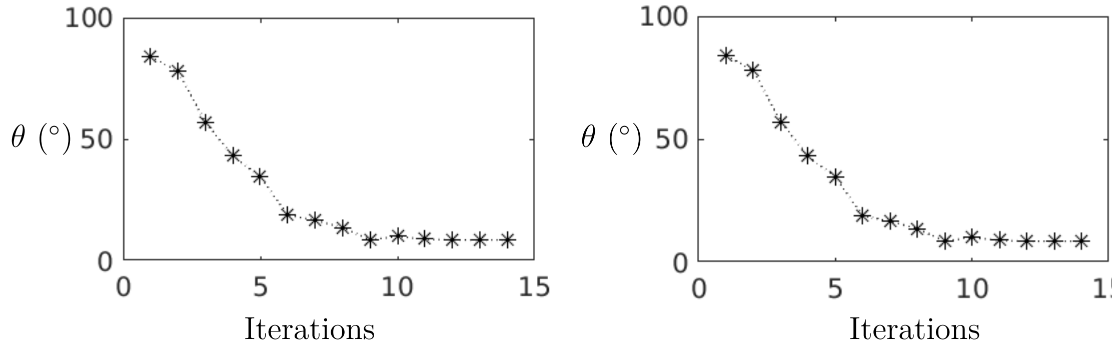


Figure 32: Evolution of θ angle with respect to the number of iterations for the minimization of j^+ (left), and for the minimization of j^- (right).

2.6 Conclusion

In this chapter we have presented a gradient-type method introduced in [AA06]. We have implemented this procedure in order to solve topological optimization problems of a unit cell composing a periodic material. The optimization relies on the distribution of a stiff and a weak material composing this unit cell. The cost functionals we have optimized depend on the first and second order homogenized elasticity tensors we have defined in Chapter 1.

The purpose is to use the topological derivatives (1.138) of the homogenized tensor $\mathbf{C}^h$ calculated in [Ams+10], and the expression (1.165) of the homogenized tensor $\mathbf{D}^h$ calculated in Chapter 1. We have adopted the established topological differentiation method, within the topological derivative procedure, in order to obtained periodic microstructures having significant second gradient effects.

We have obtained non trivial, preliminary, and encouraging microstructures for functionals based on intrinsic characteristic lengths. The latter are defined as a ratio of the coefficients of these two tensors. In particular, we have obtained a pantographic unit cell, similar the one studied in [Dur+20] (see Figure 26).

We have also shown that these characteristic lengths can be improved when we diminish the contrast. Another consequence when we decrease the contrast of moduli between the two materials is the refinement of the junction regions of the optimal unit cells (see Figures 28 and 29).

Finally, we have optimized a functional based on invariants of the homogenized tensors. We have seen that we can control the orientation of the chiral unit cell we have obtained in Figure 31, by changing the sign of the invariant β of tensor $\mathbf{D}^h$.

The topological optimization of the unit cell of a periodic material based on the second order homogenized tensor gave us two kinds of results.

On the one hand, we can improve the second gradient effects in the macroscopic response of the material. This is the case for a pantographic material. Such a material, as the one presented in figure 30, allow an extension in the direction e_1 for almost no first order gradient energy: we call it a floppy mode. Through this extension, the material is subjected to a gradient of deformation: the deformation of the material changes from cell to cell.

On the other hand, we can optimize first gradient effects, while we control properties which are not encapsulated in the first gradient tensor. This is the case for the functional treated in Section 2.5.

There exists a very large number of invariants for sixth order tensors, and their mechanical understanding is still a subject of study. Thus we are still investigating their topological optimization with the procedure presented and tested in this chapter.

We also planed to consider functionals depending of the fifth order tensor $\mathbf{E}^h$ of coupling moduli between first and second gradient effects. Its topological derivative is already computed (see Appendix B) and implemented in the topological procedure. At first we were not interested in this tensor because it cancels in the case of a centro-symmetric unit cell. But we could explore new microstructure by taking it into account.

Chapter 3

Shape optimization of a Fluid-Structure Interaction problem

3.1 Introduction

Fluid structure interaction (FSI) problems are challenging from a mathematical point of view, and also from the point of view of its numerous applications. We can generally define FSI problem as the coupling between a structure which is deformable (although rigid structure studies can be mentioned, such as the motion of a solid body in a fluid) with a surrounding fluid flow, or sometimes an internal fluid flow. We will be interested in particular in problems of interaction of a viscous fluid and an elastic medium. For the several examples of application in engineering one can mention the problem of airfoils [DH01] or engines [SL04]. But we can also mention medical applications such as the study of the blood flow in vessels [GVF05], of the aortic valve [CL20], or studies concerning the human lung system [Tez+08].

As a early study of the FSI problem we can cite [Lio69] in which the existence of weak solutions for the Navier-Stokes equations in a fixed domain coupled with linearized elasticity. We can also refer to [Ser87] investigating the tailspin of a rigid body into a viscous incompressible fluid. But, the first important contributions can be found in [AL93; LA91; LA92] in which the authors study steady flows in nonlinear elastic shells and nonlinear elastic tubes and shells under external flow for which the velocity is prescribed. In the early 2000 mathematicians started to investigate more intensely the interaction of a viscous liquid with elastic bodies in steady and unsteady regime. For the steady-state problems one can cite [Rum98], [Gra98; Gra02], [Bay+04], [Sur07], [GK09], and for the unsteady case, we refer for example to [GM00; GM03], [Des+01], [Bei04], [Cha+05], [CS05; CS06], [BST12; BGT19], [MC13]. One of the difficulty of the study of a steady FSI problem is that the fluid, described in Eulerian coordinates, turn to be defined on a domain depending on the structure displacement which is in contrast described in Lagragian coordinates. For existence result with other type of boundary conditions one can cite [DT19].

We can ask several interesting questions regarding the shape optimization of a Fluid Structure Interaction problem. For example can we have for a well chosen class of domain, the existence of an optimal solution, or even do we have uniqueness of such a solution? We already meet many examples of application for structural optimization problems, as we could see in the introduction of Chapter 2. But there are also numerous works concerning shape and topological optimization problems applied to fluid mechanics only. For example the minimization of the drag in airplane optimization (see e.g., [AP89], [MP01], [GM08], [GMZ09]), the shape minimization of the dissipated energy in a pipe (see e.g., [HP10], [BP13]), the optimization of fluidic flow with or without body forces (see e.g. [DLW13])

These problems are not concerning FSI.

The optimization of FSI problems is more recent. One can cite [Yoo10; Yoo14], [Kre+10], [AS13], [JM15; JM16] where a level-set method is used to characterize the fluid and the structure domains, [PVP15; Pic+20], [Lun+18] in which the FSI problem is relaxed by a density design variable. In [SS18] the shape differentiability of a simplified free-boundary one-dimensional problem is studied, for which it is proved that the shape optimization problem is well-posed. In the recent paper [Fep+19; Fep+20; Fep+21], the shape and topology optimization of a multiphysics thermal-fluid-structure interaction problem is studied with a velocity and adjoint method, for which the structure domain is assumed to be fixed.

We are interested in a FSI problem for which an elastic body in plane strain is immersed in a viscous fluid, and clamped to a rigid support from a part of its boundary. We consider that the system is infinite in the anti-plane dimension. Our goal is to study the shape optimization of this two-dimensional elastic body. For this purpose, we start with a presentation of the Fluid-Structure Interaction problem we work on in Section 3.2. We present in particular what the unknowns of the problem are, how the fluid and the structure problems are coupled, and we finish with the definition of a simplified model for which the elastic structure is incompressible. The Section 3.3 is dedicated to the resolution of the FSI problem, through the resolution of the fluid equations in a first time, followed with the resolution of the structure problem, and completed with a fixed point procedure. Then, after an introduction to the calculus of shape derivatives by the *velocity method*, we apply this method to the FSI problem, we give the boundary value problems satisfied by the *material derivatives* of the solutions of the FSI problem in the Section 3.4.4, and we compute in Section 3.4.5 the shape derivative of an abstract shape functional. After this, we introduce in Section 3.5.1 the *adjoint method* used in order to simplify the expression of the shape derivative computed before. We apply this method to the FSI problem in Sections 3.5.2, 3.5.3, and 3.5.4.

This chapter is the result of a work I carried out with Ilaria Lucardesi[1] and with Jean-François Scheid.

3.2 A two-dimensional Fluid-Structure Interaction model

We are interested in the optimization of a Fluid-Structure Interaction (FSI) problem. We want to investigate some optimality result regarding the shape of a given two-dimensional elastic body (the structure) in plane strain immersed in an incompressible Stokes fluid, and clamped from a part of its boundary, while applying volume forces to both fluid and elastic phases (see Figure 33). We consider that this system is infinite in the anti-plane direction. This results in the deformation of the free boundary of the elastic body, which is the interface where the interaction between the elastic body and the fluid takes place. We start by presenting a Fluid-Structure Interaction model following what is done in [Gra02] and [SS18], then we introduce a simplified model, and finally we present a general shape optimization protocol.

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First we define the geometry for the FSI problem (see Figure 33). Let ω, Ω_0', and D be three simply connected bounded open sets in $\mathbb{R}^2$, such that $\omega \subset\subset \Omega_0' \subset\subset$ D. We denote by Γ_0 and $\partial\omega$ the boundaries of Ω_0' and ω, respectively. The domain

$$\Omega_0 := \Omega_0' \setminus \overline{\omega} \tag{3.1}$$

stands for an elastic body attached to a rigid support ω, namely Ω_0 has an fixed boundary $\partial\omega$ and a deformable one Γ_0. The domain Ω_0 is the configuration at rest of this elastic medium. The domain

$$\Omega_0^c := \mathrm{D} \setminus (\Omega_0 \cup \overline{\omega}) \tag{3.2}$$

is occupied by an incompressible fluid interacting with the elastic body trough the interface Γ_0.

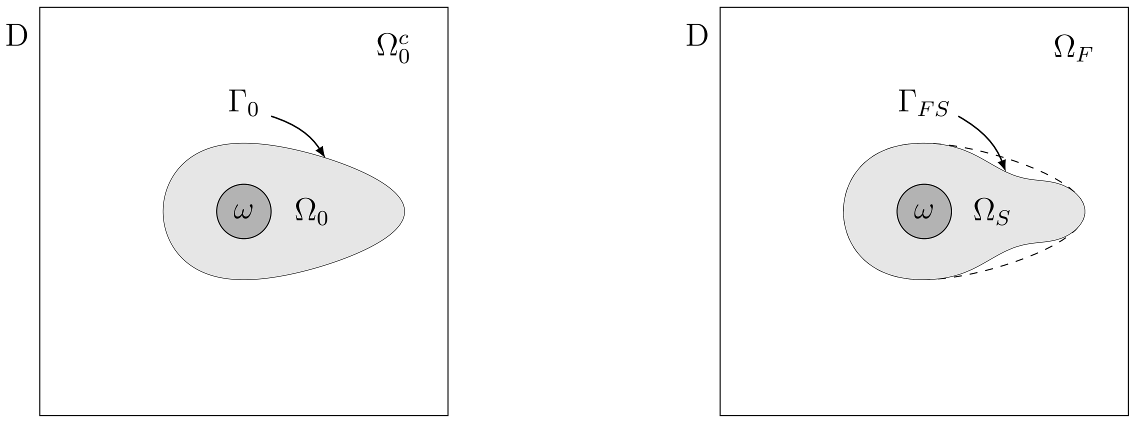

Figure 33: The geometry of the Fluid Structure Interaction system, before (left) and after (right) deformation.

Now we apply *volume forces* f and g to the fluid and the elastic body respectively, and we assume that this interaction through Γ_0 together with the applied forces deform the elastic body and lead to an equilibrium state in the fluid and the structure parts. Each point of the initial elastic body $X \in \Omega_0$ is deformed into a new point $x = T(X)$, where

$$T(X) = (\mathrm{id} + \mathrm{w})(X) \in \Omega_S, \tag{3.3}$$

where $\mathrm{w} : \Omega_S \to \mathbb{R}^2$ is called the *displacement field*, and

$$\Omega_S := T(\Omega_0) = (\mathrm{id} + \mathrm{w})(\Omega_0) \tag{3.4}$$

is the domain representing the deformed elastic body. We also define the deformed fluid-structure interface

$$\Gamma_{FS} := T(\Gamma_0) = (\mathrm{id} + \mathrm{w})(\Gamma_0). \tag{3.5}$$

From this, we describe the elastic body by the Lagrangian coordinate $X \in \Omega_0$. This elastic body is completely determined by the knowledge of the displacement field w. Moreover, the fluid fills the remaining domain

$$\Omega_F := \mathrm{D} \setminus \overline{\Omega_S \cup \omega}, \tag{3.6}$$

and it is described in Eulerian coordinates by a *velocity field* $\mathrm{u} : \Omega_F \to \mathbb{R}^2$, and by a *pressure field* $\mathrm{p} : \Omega_F \to \mathbb{R}$. What remains to be done is to specify what equations govern the two phases of this system, and what is the nature of the interaction. On the one hand, the fluid is considered as being viscous and incompressible. It is described by the Stokes or the Navier-Stokes equations, and a non-slip boundary condition is imposed (i.e., the velocity is set to zero on the boundaries). This gives

$$\left\{\begin{array}{rcll} -\operatorname{div}\varsigma(\mathrm{u},\mathrm{p})+\boldsymbol{\epsilon}(\mathrm{u}\cdot\nabla)\mathrm{u} &=& f & \text{in} \quad \Omega_F, \\ \operatorname{div}\ \mathrm{u} &=& 0 & \text{in} \quad \Omega_F, \\ \mathrm{u} &=& 0 & \text{on} \quad \partial\Omega_F, \end{array}\right. \tag{3.7}$$

where $\boldsymbol{\epsilon}=0$ for Stokes equations and $\boldsymbol{\epsilon}=1$ for Navier-Stokes equations. Denoting by $\nu>0$ the viscosity of the fluid, we define the *Cauchy stress tensor*:

$$\varsigma(\mathrm{u},\mathrm{p}) := 2\nu\nabla^s\mathrm{u}-\mathrm{pI}, \tag{3.8}$$

where I is the identity matrix and

$$\nabla^s\mathrm{u} := \frac{1}{2}\left(\nabla\mathrm{u}+\nabla\mathrm{u}^\top\right). \tag{3.9}$$

The force f in (3.7) is given in D. On the other hand, the elastic body satisfies the equations of equilibrium in the reference configuration for a *St Venant-Kirchhoff* material, that is

$$\operatorname{div}\Sigma(\mathrm{w}) = g \quad \text{in } \Omega_0, \tag{3.10}$$

where $\Sigma(\mathrm{w})$ is the *Piola-Kirchhoff stress tensor* defined by

$$\Sigma(\mathrm{w}) := (\mathrm{I}+\nabla\mathrm{w})\mathbf{C}(E(\mathrm{w})), \tag{3.11}$$

$$\mathbf{C}(E(\mathrm{w})) := 2\mu E(\mathrm{w})+\lambda\operatorname{tr}(E(\mathrm{w}))\mathrm{I}, \tag{3.12}$$

$$E(\mathrm{w}) := \frac{1}{2}\left(\nabla\mathrm{w}+\nabla\mathrm{w}^\top+\nabla\mathrm{w}^\top\nabla\mathrm{w}\right), \tag{3.13}$$

where $\mathbf{C}$ is the stiffness tensor and $\lambda\geq 0$ and $\mu\geq 0$ are the Lamé coefficients. We suppose that the elastic body is attached to the rigid support via the boundary $\partial\omega$, that is we have the following boundary condition

$$\mathrm{w}=0 \quad \text{on } \partial\omega. \tag{3.14}$$

The force g in (3.10) is given in Ω_0. Furthermore we have the equilibrium of the surface forces on the free boundary Γ_0, which reads

$$\int_{\Gamma_0}\Sigma(\mathrm{w})n_0\cdot(v\circ(\mathrm{id}+\mathrm{w}))d\Gamma_0 = \int_{\Gamma_{FS}}\varsigma(\mathrm{u},\mathrm{p})n_{FS}\cdot v\ d\Gamma_{FS}, \tag{3.15}$$

for all function v defined on Ω_F, where $\Gamma_{FS} := (\mathrm{id}+\mathrm{w})(\Gamma_0)$ defined in (3.5) is the boundary between the fluid and the deformed elastic body, and where $d\Gamma_0$ and $d\Gamma_{FS}$ are the length elements of the surfaces Γ_0 and Γ_{FS} respectively, and n_0 and n_{FS} are the outer unit normal vectors to Γ_0 and Γ_{FS} respectively. We have the following identity (see e.g. [Cia88]):

$$n_{FS}d\Gamma_{FS} = [\det(\nabla(T(\mathrm{w})))\nabla T(\mathrm{w})^{-\mathsf{T}}n_0]d\Gamma_0. \tag{3.16}$$

Thus a change of variable in (3.15) with the use of (3.16) gives the following boundary condition

$$\Sigma(\mathrm{w})n_0 = (\varsigma(\mathrm{u},\mathrm{p})\circ T)\operatorname{cof}(\nabla T)n_0 \quad \text{on } \Gamma_0, \tag{3.17}$$

where T is defined in (3.3) and

$$\operatorname{cof}(\nabla T) = \det(\nabla T)(\nabla T)^{-T}, \tag{3.18}$$

is the cofactor matrix of the jacobian matrix of T. Finally we must add a constraint on the displacement field, in order to make the deformation it creates compatible with the incompressibility of fluid. That is we have the following condition

$$|\Omega_S| = |\Omega_0|, \tag{3.19}$$

where $|\cdot|$ denotes the Lebesgue measure. This condition is actually a condition on w:

$$|\Omega_S| = \int_{\Omega_0} \det(\mathrm{I} + \nabla \mathrm{w})\, dx = |\Omega_0|, \tag{3.20}$$

At this stage we have written boundary value problems for each phase, fluid and structure, needing to be completed by a constraint (3.20), and which are strongly coupled in the following way

$$\left\{\begin{array}{rcllr} -\operatorname{div}\varsigma(\mathrm{u},\mathrm{p}) + \boldsymbol{\epsilon}(\mathrm{u}\cdot\nabla)\mathrm{u} &=& f & \text{in} & \Omega_F, \\ \operatorname{div}\ \mathrm{u} &=& 0 & \text{in} & \Omega_F, \\ \mathrm{u} &=& 0 & \text{on} & \partial\Omega_F, \\ \operatorname{div}\Sigma(\mathrm{w}) &=& g & \text{in} & \Omega_0, \\ \mathrm{w} &=& 0 & \text{on} & \partial\omega, \\ \Sigma(\mathrm{w})n_0 &=& (\varsigma(\mathrm{u},\mathrm{p}+c)\circ T)\operatorname{cof}(\nabla T)n_0 & \text{on} & \Gamma_0, \\ \displaystyle\int_{\Omega_0}\det(\mathrm{I}+\nabla\mathrm{w})\,dx &=& |\Omega_0|, & & \end{array}\right. \tag{3.21}$$

where c is a Lagrange multiplier introduced to take into account the non-local area constraint $|\Omega_S| = |\Omega_0|$. We can observe that his coupling is twofold:

- the structure displacement w affects and defines the domain on which the fluid equations are posed and the velocity u and the pressure p are calculated,

- the velocity u and the pressure p of the fluid give rise to a surface force which influences the calculation of the displacement w.

Two difficulties arise in this system of equation. Firstly, we have to deal with a non-local constraint area. Secondly, we have two kinds of variables: Eulerian variables (the fluid velocity u and pressure p, and Lagrangian variables (the displacement w). Moreover, the domain Ω_F on which the fluid equations are written is unknown.

To overcome these difficulties, we first simplify the structure equations in Section 3.2.1, and then we transport the fluid equations into a reference domain in Section 3.2.2.

3.2.1 A simplified model: incompressible material

In seek of simplification, we define a simplified model. First, we consider the case of linear elasticity. That is we define the *linearized stress tensor* or simply *stress tensor*:

$$\sigma(\mathrm{w}) := \mathbf{C}(e(\mathrm{w})), \tag{3.22}$$

$$e(\mathrm{w}) := \nabla^s \mathrm{w}, \tag{3.23}$$

where $e(\mathrm{w})$ stands for the *linearized strain tensor* or simply *strain tensor*, and $\mathbf{C}$ is the elasticity tensor defined in Chapter 1 equation (1.101), which gives, in view of $\mathrm{tr}(e(\mathrm{w})) = \mathrm{div}\,\mathrm{w}$,

$$\sigma(\mathrm{w}) := 2\mu e(\mathrm{w}) + \lambda\,\mathrm{div}(\mathrm{w})\mathrm{I}, \tag{3.24}$$

where λ and μ are the Lamé coefficients.

In this case, we neglect the quadratic terms in (3.11), (3.12), and (3.13). Thus $\sigma(\mathrm{w})$ replaces $\Sigma(\mathrm{w})$ in (3.10) and (3.17), and equation (3.10) turns linear with respect to w. The constraint (3.20) is non linear. We also want to perform a linearization for this constraint. For a matrix A of size 2×2, we recall that

$$\det(\mathrm{I} + A) = 1 + \mathrm{tr}(A) + \det(A). \tag{3.25}$$

Hence, we get

$$\det(\mathrm{I} + \nabla\mathrm{w}) = 1 + \mathrm{div}(\mathrm{w}) + \det(\nabla\mathrm{w}) = 1 + \mathrm{div}(\mathrm{w}) + O\left(\|\nabla\mathrm{w}\|_\infty^2\right). \tag{3.26}$$

If we assume that

$$\mathrm{div}\,\mathrm{w} = 0, \tag{3.27}$$

and if we neglect the second order terms, we obtain that the area constraint (3.20) is verified. A simplified model is then obtained by replacing the (non-local) area constraint (3.20) by the (local) incompressibility condition (3.27). A Lagrange multiplier function s is associated to the incompressibility condition (3.27). The simplified model now deals with the elastic tensor

$$\boldsymbol{\sigma}(\mathrm{w}, \mathrm{s}) := \sigma(\mathrm{w}) - \mathrm{sI}, \tag{3.28}$$

which can be written as follows in view of the incompressibility condition (3.27)

$$\boldsymbol{\sigma} = 2\mu\nabla^s(\mathrm{w}) - \mathrm{sI}, \tag{3.29}$$

and which replaces the Piola-Kirchhoff tensor $\Sigma(\mathrm{w})$ given by (3.11).

The simplified model stands for the couple (w, s) which satisfied:

$$\begin{cases} -2\mu\,\mathrm{div}\,\nabla^s(\mathrm{w}) + \nabla\mathrm{s} = g & \text{in } \Omega_0 \quad (i) \\ \mathrm{div}\,\mathrm{w} = 0 & \text{in } \Omega_0 \quad (ii) \\ \mathrm{w} = 0 & \text{on } \partial\omega \quad (iii) \\ (2\mu\nabla^s(\mathrm{w}) - \mathrm{sI})\, n_0 = (\varsigma(\mathrm{u}, \mathrm{p}) \circ T)\,\mathrm{cof}(\nabla T) n_0 & \text{on } \Gamma_0. \quad (iv) \end{cases} \tag{3.30}$$

The surface forces continuity relation (3.30)(iv) differs from (3.17) by involving the Lagrange multiplier function s.

3.2.2 Fixed domain formulation of the simplified FSI problem

In order to solve the simplified FSI problem, we write the fluid equations onto the fixed domain Ω_0. Until now, we have defined the fluid domain as being the complementary in D of the system composed by the deformed elastic body and the rigid support (see (3.6)). But in order to transport the boundary value problem (3.7) from Ω_F to the initial domain Ω_0^c, we need a bijective map from Ω_0^c to Ω_F which is a C^1-diffeomorphism. We introduce the following map:

$$T(\mathrm{w}) = \mathrm{id} + P(\mathrm{w}), \tag{3.31}$$

where w is a displacement field defined in the initial elastic body domain Ω_0, and P is an extension operator from Ω_0 to D, such that $P(\mathrm{w})$ is defined in D and $T(\mathrm{w})$ is one to one in D. The map T defined above in (3.31) extends the definition of the map we introduced in (3.3). This allows us to define the fluid domain Ω_F in which the velocity and pressure fields are defined:

$$\Omega_F := T(\mathrm{w})(\Omega_0^c), \tag{3.32}$$

where Ω_0^c is defined Figure 33. We will return to this extension procedure later, to give a rigorous definition.

Now we can write the variational formulation of the Navier-Stokes system written on Ω_F, and then we transport it onto the reference domain Ω_0^c, in the same way as in [Gra02]. We recall that $\varsigma(\mathrm{u},\mathrm{p}) := 2\nu\nabla^s\mathrm{u} - \mathrm{p}_t\mathrm{I}$, and because of the incompressibility condition, we have

$$\operatorname{div}(\nabla\mathrm{u}^\top) = \nabla(\operatorname{div}\mathrm{u}) = 0, \tag{3.33}$$

so that

$$\operatorname{div}\varsigma(\mathrm{u},\mathrm{p}) = \operatorname{div}(\nu\nabla\mathrm{u} - \mathrm{pI}). \tag{3.34}$$

Thus the variational formulation of the Navier-Stokes system is written as follows.

$$\begin{cases} \text{Find } (\mathrm{u},\mathrm{p}) \in H_0^1(\Omega_F) \times L^2(\Omega_F), \text{ such that } \forall(\tilde{z},\tilde{\beta}) \in H_0^1(\Omega_F) \times L^2(\Omega_F): \\ \nu\displaystyle\int_{\Omega_F} \nabla\mathrm{u}\cdot\nabla\tilde{z} - \int_{\Omega_F} \mathrm{p}\operatorname{div}(\tilde{z}) + \int_{\Omega_F} \boldsymbol{\epsilon}(\mathrm{u}\cdot\nabla)\mathrm{u}\cdot\tilde{z} = \langle f,\tilde{z}\rangle_{H^{-1},H_0^1}, \\ \displaystyle\int_{\Omega_F} \tilde{\beta}\operatorname{div}(\mathrm{u}) = 0. \end{cases} \tag{3.35}$$

We can define the transported velocity and pressure fields

$$\mathrm{v} = \mathrm{u}\circ T(\mathrm{w}), \tag{3.36}$$
$$\mathrm{q} = \mathrm{p}\circ T(\mathrm{w}), \tag{3.37}$$

and we set $\tilde{z} = z\circ T(\mathrm{w})^{-1}$ and $\tilde{\beta} = \beta\circ T(\mathrm{w})^{-1}$ in equation (3.35), where $z \in H_0^1(\Omega_0^c)$ and $\beta \in L_0^2(\Omega_0^c)$. We obtain with a change of variable $T(\mathrm{w})$ that (v,q) satisfies the following problem:

$$\begin{cases} \text{Find } (\mathrm{v},\mathrm{q}) \in H_0^1(\Omega_0^c)^2 \times L_0^2(\Omega_0^c) \text{ such that for all } (z,\beta) \in H_0^1(\Omega_0^c)^2 \times L_0^2(\Omega_0^c): \\ \nu\displaystyle\int_{\Omega_0} \nabla(\mathrm{v})F(T(\mathrm{w}))\cdot\nabla z - \int_{\Omega_0} \mathrm{q}(G(T(\mathrm{w}))\cdot\nabla z) \\ \qquad\qquad + \displaystyle\int_{\Omega_0} \boldsymbol{\epsilon}(\mathrm{v}\cdot G(T(\mathrm{w}))\nabla)\mathrm{v}\cdot z = \langle J(T(\mathrm{w}))f\circ T(\mathrm{w}), z\rangle_{H^{-1},H_0^1}, \\ \displaystyle\int_{\Omega_0} \beta(G(T(\mathrm{w}))\cdot\nabla\mathrm{v}) = 0, \end{cases} \tag{3.38}$$

where

$$F(T(\mathrm{w})) = (\nabla T(\mathrm{w}))^{-1}\operatorname{cof}(\nabla T(\mathrm{w})), \tag{3.39}$$
$$G(T(\mathrm{w})) = \operatorname{cof}(\nabla T(\mathrm{w})), \tag{3.40}$$
$$J(T(\mathrm{w})) = \det(\nabla T(\mathrm{w})). \tag{3.41}$$

Problem (3.38) is related to the following boundary value problem:

$$\begin{cases} -\nu \operatorname{div}((\nabla \mathrm{v})F(T(\mathrm{w}))) + G(T(\mathrm{w}))\nabla \mathrm{q} + \boldsymbol{\epsilon}(\mathrm{v}_t \cdot G(T(\mathrm{w}))\nabla)\mathrm{v} = (f \circ T(\mathrm{w}))J(T(\mathrm{w})) & \text{in } \Omega_0^c, \\ \operatorname{div}(G(T(\mathrm{w}))^\top \mathrm{v}) = 0 & \text{in } \Omega_0^c, \\ \mathrm{v} = 0 & \text{on } \Gamma_0. \end{cases} \tag{3.42}$$

We recall that the surface force applied on the structure is given in (3.17) by $(\varsigma(\mathrm{u},\mathrm{p}) \circ T)\operatorname{cof}(\nabla T)n_0$. With the definitions of v and q given in (3.36) and (3.37), we can compute the surface force applied on the structure and depending on these new variables. This gives

$$(\varsigma(\mathrm{u},\mathrm{p}) \circ T)\operatorname{cof}(\nabla T)n_0 = (\nu(\nabla \mathrm{v})F(T) - \mathrm{q}_t G(T_t))n_0. \tag{3.43}$$

Thus we can write the complete Fluid Structure Interaction problem, with the fluid equations transported onto the reference domains Ω_0^c.

The fixed domain formulation of the simplified FSI problem reads as

$$\begin{cases} -\nu \operatorname{div}((\nabla \mathrm{v})F(T(\mathrm{w}))) + G(T(\mathrm{w}))\nabla \mathrm{q} & & & & \\ \qquad +\boldsymbol{\epsilon}(\mathrm{v} \cdot G(T(\mathrm{w}))\nabla)\mathrm{v} &=& (f \circ T(\mathrm{w}))J(T(\mathrm{w})) & \text{in} & \Omega_0^c, \\ \operatorname{div}(G(T(\mathrm{w}))^\top \mathrm{v}) &=& 0 & \text{in} & \Omega_0^c, \\ \mathrm{v} &=& 0 & \text{on} & \partial\Omega_0^c, \\ -\operatorname{div}\sigma(\mathrm{w}) + \nabla \mathrm{s} &=& g & \text{in} & \Omega_0, \\ \operatorname{div}\mathrm{w} &=& 0 & \text{in} & \Omega_0, \\ \mathrm{w} &=& 0 & \text{on} & \partial\omega, \\ (\sigma(\mathrm{w}) - \mathrm{sI})n_0 &=& \nu(\nabla \mathrm{v})F(T(\mathrm{w}))n_0 & & \\ & & -\mathrm{q}G(T(\mathrm{w}))n_0 & \text{on} & \Gamma_0, \end{cases} \tag{3.44}$$

where $\boldsymbol{\epsilon} = 0$ or $\boldsymbol{\epsilon} = 1$ for dealing with Stokes or Navier-Stokes equations.

We have to keep in mind that this simplified model is an hybrid model. Indeed we have linearized the equilibrium equation of the structure (that is to say the Pila-Kirchhoff stress tensor) and the area constraint, in order to simplify the mathematical analysis that will follow in this chapter. We will see in Section 3.3 that we obtain an existence and uniqueness result in Theorem 3.9 for our simplified model, while for the three-dimensional Navier-Stokes/St Venant-Kirchhoff FSI problem C. Grandmont obtain an existence result in [Gra02]. For us, the uniqueness is quite important to be able to tackle an optimization problem. But we do not have linearized the fluid equations change of variables, that is to say $J(T(\mathrm{w}))$, $G(T(\mathrm{w}))$, and $F(T(\mathrm{w}))$, because we want to compute shape derivatives in Section 3.4 by keeping as much information as possible, for possible further application and calculation purposes for the complete system. Nevertheless, even by linearizing $J(T(\mathrm{w}))$, $G(T(\mathrm{w}))$, and $F(T(\mathrm{w}))$ in the following, the results we obtain are not trivial, because it keeps a trace of the deformation of the domain.

3.2.3 Objective: optimization of the FSI problem

Our objective is the study of a shape optimization problem of the following form:

$$\min_{\Omega_0 \in \mathcal{U}_{\mathrm{ad}}} \mathcal{J}(\Omega_0), \tag{3.45}$$

where $\mathcal{J}(\Omega_0)$ is an abstract shape functional depending on the initial elastic domain defined by

$$\mathcal{J}(\Omega_0) = \int_{\Omega_0} j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y))\, dY + \int_{\Omega_F} j_F(x, \mathrm{u}(x), \nabla \mathrm{u}(x))\, dx, \tag{3.46}$$

where j_F and j_S are smooth functions depending respectively on $\mathrm{u} = \mathrm{v} \circ T(\mathrm{w})^{-1}$ and w. The fields v and w are the velocity and the displacement solutions of the FSI problem (3.44) posed on Ω_0. The domain $\Omega_0 \in \mathcal{U}_{\mathrm{ad}}$ belongs to a class $\mathcal{U}_{\mathrm{ad}}$ of admissible domains.

To this end, we start in Section 3.3 to present an existence and uniqueness result for the simplified FSI problem (3.44). Then in Section 3.4 we compute shape derivatives of the functional $\mathcal{J}(\Omega_0)$ with the use of the *velocity method*. In Section 3.5 we finally simplify the shape derivative obtained previously by applying an *adjoint method*.

3.3 Existence and uniqueness result for the FSI problem

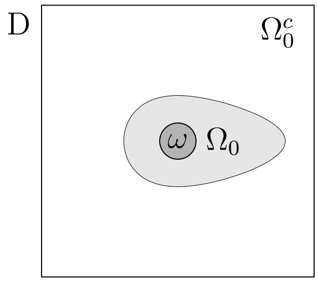

Figure 34: Initial Fluid-Structure configuration.

In this section, we establish an existence and uniqueness result written in Theorem 3.9 for the FSI problem (3.44) with $\boldsymbol{\epsilon} = 0$. In [Gra02], an existence result is obtained for the Navier-Stokes equations coupled with a St Venant-Kirchhoff material (whose stress tensor is given by the Piola-Kirchhoff tensor $\Sigma(\mathrm{w})$ defined in (3.13)) in 3D. For volume forces regular and small enough, C. Grandmont finds a non necessary unique solution to the FSI problem, by applying a fixed point procedure. In our case, we wish to optimize the initial distribution of elastic material, and the uniqueness of the solution seems to be essential. Thus we will obtain an existence and uniqueness result by adapting what is done in [Gra02] to our simplified model.

We start with a sketch of the approach. Let $\mathbf{b}$ be a vector field belonging to $(H^3(\Omega_0))^2$. We define the following extension map:

$$\begin{array}{rccc} T: & (H^3(\Omega_0))^2 & \longrightarrow & (H^3(\Omega_0^c))^2 \\ & \mathbf{b} & \longmapsto & \mathrm{id} + \mathcal{R}(\gamma(\mathbf{b})), \end{array} \tag{3.47}$$

where γ is the trace operator on Γ_0:

$$\gamma : H^3(\Omega_0) \to H^{3-1/2}(\Gamma_0), \tag{3.48}$$

and $\mathcal{R}$ is a lifting operator from Γ_0 to Ω_0^c:

$$\mathcal{R} : H^{3-1/2}(\Gamma_0) \to H^3(\Omega_0^c). \tag{3.49}$$

We introduce two problems.

1. Let $f \in (H^2(\mathrm{D}))^2$, and $(\mathrm{v}(\mathbf{b}), \mathrm{q}(\mathbf{b}))$ be the solution of the first problem

$$\left\{\begin{array}{rcll} -\nu \operatorname{div}((\nabla \mathrm{v}(\mathbf{b}))F(\mathbf{b})) + G(\mathbf{b})\nabla \mathrm{q}(\mathbf{b}) & = & J(\mathbf{b})(f \circ T(\mathbf{b})) & \text{in } \Omega_0^c, \\ \operatorname{div}(G(\mathbf{b})^T \mathrm{v}(\mathbf{b})) & = & 0 & \text{in } \Omega_0^c, \\ \mathrm{v}(\mathbf{b}) & = & 0 & \text{on } \partial\Omega_0^c, \end{array}\right. \tag{3.50}$$

where the maps J, G and F are defined by

$$J(\mathbf{b}) = \det(\nabla T(\mathbf{b})), \tag{3.51}$$

$$G(\mathbf{b}) = \operatorname{cof}(\nabla T(\mathbf{b})), \tag{3.52}$$

$$F(\mathbf{b}) = (\nabla T(\mathbf{b}))^{-1} \operatorname{cof}(\nabla T(\mathbf{b})). \tag{3.53}$$

We will justify the definition of (3.53) in Section 3.3.1.

2. Let $g \in (H^1(\mathrm{D}))^2$, and $(\mathrm{w}(\mathbf{b}), \mathrm{s}(\mathbf{b}))$ be the solution of the second problem

$$\left\{\begin{array}{rcll} -2\mu \operatorname{div}(\nabla \mathrm{w}(\mathbf{b})) + \nabla \mathrm{s}(\mathbf{b}) & = & g & \text{in } \Omega_0, \\ \operatorname{div} \mathrm{w}(\mathbf{b}) & = & 0 & \text{in } \Omega_0, \\ \mathrm{w}(\mathbf{b}) & = & 0 & \text{on } \partial\omega, \\ (2\mu \operatorname{div}(\nabla \mathrm{w}(\mathbf{b})) - \mathrm{s}(\mathbf{b})\mathrm{I})n_0 & = & (\nu \nabla \mathrm{v}(\mathbf{b})F(\mathbf{b}) - \mathrm{q}(\mathbf{b})G(\mathbf{b}))n_0 & \text{on } \Gamma_0. \end{array}\right. \tag{3.54}$$

For a fixed $\mathbf{b}$ small enough, we will show that the problem (3.50) admits a unique solution $(\mathrm{v}(\mathbf{b}), \mathrm{q}(\mathbf{b}))$, and then that the problem (3.54) depending on $(\mathrm{v}(\mathbf{b}), \mathrm{q}(\mathbf{b}))$ admits also a unique solution denoted by $(\mathrm{w}(\mathbf{b}), \mathrm{s}(\mathbf{b}))$:

$$\mathbf{b} \mapsto (\mathrm{v}(\mathbf{b}), \mathrm{q}(\mathbf{b})) \mapsto (\mathrm{w}(\mathbf{b}), \mathrm{s}(\mathbf{b})). \tag{3.55}$$

In particular we will see that $\mathrm{w}(\mathbf{b})$ belongs to $H^3(\Omega_0)$. Thus we will be able to define a map

$$\begin{array}{rccc} \boldsymbol{S} : & (H^3(\Omega_0))^2 & \longrightarrow & (H^3(\Omega_0))^2 \\ & \mathbf{b} & \longmapsto & \mathrm{w}(\mathbf{b}) \end{array}, \tag{3.56}$$

and we will show in Section 3.3.4 that this map is actually a contraction, so that we can apply the Banach Fixed Point Theorem, and deduce that the solution we search for the FSI problem is unique and is given by the fixed point of $\boldsymbol{S}$.

In the following section, with start by presenting useful results for the resolution of problems (3.50) and (3.54), investigated in Sections 3.3.2 and 3.3.3. Then in Section 3.3.4 we show that $\boldsymbol{S}$ is a contraction.

3.3.1 Notations and preliminary results

In a first time we give the notations used in the rest of this chapter. Let $\{\mathrm{e}_1, \cdots, \mathrm{e}_n\}$ be the canonical orthogonal basis of $\mathbb{R}^n$. Let u and v be two vectors of $\mathbb{R}^n$, A and B be two second order tensors of $\mathbb{R}^n$. We write (see also Appendix A)

$$AB = A_{ik}B_{kj}\, \mathrm{e}_i \otimes \mathrm{e}_j, \tag{3.57}$$

$$A \cdot B = A_{ij} B_{ij}, \tag{3.58}$$
$$Au = A_{ij} u_j \, \mathrm{e}_i, \tag{3.59}$$
$$u \cdot v = u_i v_i, \tag{3.60}$$

by using the Einstein summation convention, and where the elements $\mathrm{e}_i \otimes \mathrm{e}_j$ are the element of the canonical basis of the second order tensors on $\mathbb{R}^n$. We define the trace $\mathrm{tr}(A)$ of a matrix A by

$$\mathrm{tr}(A) = \mathrm{I} \cdot A, \tag{3.61}$$

its symmetric part by

$$A^s := \frac{1}{2}\left(A + A^\top\right), \tag{3.62}$$

and its norm $|A|$ by

$$|A| = (A \cdot A)^{1/2}. \tag{3.63}$$

Let Ω be a open subset of $\mathbb{R}^n$. The fields involved in the equations we study belongs to Sobolev Spaces $W^{m,p}(\Omega)$, for $m \geq 0$ a positive integer, and $p > 1$ a real number. With this convention, $W^{0,p}(\Omega)$ stands for the Lebesgue space of $L^p(\Omega)$. Let $u \in W^{m,p}(\Omega)$, we denote by

$$\|u\|_{m,p,\Omega} \tag{3.64}$$

the standard $W^{m,p}$-norm of u. When there is no ambiguity on the open set of definition Ω, we simply write this norm

$$\|u\|_{m,p.} \tag{3.65}$$

In a second step, we give premilinary results that we are going to use to solve problems (3.50) and (3.54).

Problem (3.50) is a slightly perturbed incompressible Stokes problem with non-slip boundary condition, giving rise to a velocity and a pressure weak solutions $(\mathrm{v}, \mathrm{q}) \in H_0^1(\Omega_0^c) \times L_0^2(\Omega_0^c)$ (see e.g., [BF13]), with the space

$$L_0^2(\Omega_0^c) = \left\{ q \in L^2(\Omega_0^c) \;\middle|\; \int_{\Omega_0^c} q \, dx = 0 \right\}. \tag{3.66}$$

In general, for $1 \leq p \leq +\infty$, we denote by $L_0^p(\Omega_0^c)$ the following space

$$L_0^p(\Omega_0^c) = \left\{ q \in L^p(\Omega_0^c) \;\middle|\; \int_{\Omega_0^c} q \, dx = 0 \right\}. \tag{3.67}$$

Furthermore we recall a useful result called the *Piola identity* (see e.g., [Cia88]). Let $n < p$, and $\Psi \in (W^{2,p})^n$, we have

$$\mathrm{div}\,(\mathrm{cof}\,\nabla\Psi) = 0. \tag{3.68}$$

Problem (3.54), even though it describes the behaviour of an incompressible elastic material, can be identified with an incompressible Stokes problem with mixed Dirichlet and Stress boundary conditions, for which we also obtain weak solution $(\mathrm{w}, \mathrm{s}) \in (H^1(\Omega_0))^2 \times L^2(\Omega_0)$In view of the shape optimization related problem, we need higher regularity results for the solutions of problems (3.50) and (3.54). Indeed

- we need the transformation map $T(\mathrm{w})$ to be a C^1-diffeomorphism, which requires some regularity results on the displacement field w (see Lemma 3.2),
- the change of variable in the Stokes problem for the fluid shows up some terms such as $(\nabla \mathrm{v})F(T(\mathrm{w})))$ or $G(T(\mathrm{w}))\nabla \mathrm{q}$. If we want them to be well-defined and integrable, we still need higher regularity for w, and we need an algebra structure allowing products of functions (see Lemma 3.2).

As in [Gra02], we give a Lemma offering an algebra structure for Sobolev spaces. A proof can be found in [AF03] (Theorem 4.39, p. 106).

Lemma 3.1. *Let $n \geq 2$, $1 < p < \infty$, and let Ω be a bounded domain of $\mathbb{R}^n$ Let $m \geq 1$ be an integer. If $mp > n$, then there exists a constant $C_a > 0$ such that for all $u \in W^{m,p}(\Omega)$, and for all $v \in W^{m,p}(\Omega)$, we have the product $uv \in W^{m,p}(\Omega)$, and*

$$\|uv\|_{W^{m,p}(\Omega)} \leq C_a \|u\|_{W^{m,p}(\Omega)} \|v\|_{W^{m,p}(\Omega)} . \tag{3.69}$$

Thus $W^{m,p}(\Omega)$ endowed with the norm $C_a\|\cdot\|_{W^{m,p}(\Omega)}$ is a commutative Banach algebra.

Now we exhibit a threshold below which, for a function $\mathbf{b} \in (H^3(\Omega_0))^2$, the map $T(\mathbf{b})$ defined in (3.47) can be used for a change of variable. A proof can be found in [Gra02].

Lemma 3.2. *There exists a constant $0 < \mathcal{M}$ such that for all $\mathbf{b} \in (H^3(\Omega_0))^2$ satisfying*

$$\|\mathbf{b}\|_{H^3(\Omega_0)} \leq \mathcal{M}, \tag{3.70}$$

Then we have

(i) $\nabla(\mathrm{id} + \mathcal{R}(\gamma(\mathbf{b}))) = \mathrm{I} + \nabla\mathcal{R}(\gamma(\mathbf{b}))$ *is an invertible matrix in* $(H^2(\Omega_0^c))^{2\times 2}$*,*

(ii) $T(\mathbf{b}) = \mathrm{id} + \mathcal{R}(\gamma(\mathbf{b}))$ *is one to one on* $\overline{\Omega_0^c}$*,*

(iii) $T(\mathbf{b})$ *is a C^1-diffeomorphism from Ω_0^c onto $T(\mathbf{b})(\Omega_0^c)$.*

Actually, the constant $\mathcal{M}$ depends only on C_a, $C_{\mathcal{R}}$, C_γ, and C_Ω, where C_a is the constant from Lemma 3.1, $C_{\mathcal{R}}$ is the continuity constant of the Lifting operator from (3.49), C_γ is the continuity constant of the Trace operator from (3.48), and C_Ω is a constant such that

$$\forall \theta \in C^1(\overline{\Omega}) \quad \|\nabla\theta\|_{C^0(\overline{\Omega})} < C_\Omega \Longrightarrow \begin{cases} \det(\mathrm{I} + \nabla\theta)(x) > 0, \ \forall x \in \Omega, \\ \qquad \mathrm{id} + \theta \text{ is injective on } \overline{\Omega}, \end{cases} \tag{3.71}$$

(see e.g. [Cia88], Theorem 5.5.1).

From the two preceding Lemmas, we define the set

$$B_p := \{\mathbf{b} \in (H^3(\Omega_0))^2 \mid \|\mathbf{b}\|_{2,p} \leq \mathcal{M}_1\}, \tag{3.72}$$

and the maps $J : (H^3(\Omega_0))^2 \to H^2(\Omega_0^c)$ defined by

$$J(\mathbf{b}) = \det(\nabla T(\mathbf{b})), \tag{3.73}$$

$G : (H^3(\Omega_0))^2 \to (H^2(\Omega_0^c))^{2\times 2}$ defined by

$$G(\mathbf{b}) = \mathrm{cof}(\nabla T(\mathbf{b})), \tag{3.74}$$

and $F : B_p \to (H^2(\Omega_0^c))^{2\times 2}$ defined by

$$F(\mathbf{b}) = (\nabla T(\mathbf{b}))^{-1} \,\mathrm{cof}(\nabla T(\mathbf{b})). \tag{3.75}$$

In addition we have (see [Gra02])

Lemma 3.3. *The mappings G and J are of class C^∞. The mapping F is infinitely differentiable everywhere in B_p defined in* (3.72). *Moreover, F satisfies a condition of "uniform ellipticity" over B_p, i.e. there exists a constant $\beta > 0$ such that:*

$$\beta|x|^2 \leq F(\mathbf{b})x \cdot x, \quad \forall \mathbf{b} \in B_p, \quad \forall x \in \mathbb{R}^2. \tag{3.76}$$

3.3.2 Resolution of the fluid problem

In this subsection we give an existence and uniqueness result for the fluid problem (3.50). This extends the standard Stokes well known existence result.

To begin with, we recall the standard result of existence, uniqueness and L^q-estimates for the solution of Stokes problem in Proposition 3.4. The regularity result is a consequence of what is established in [ADN59] and [ADN64] (see [BF13]). For a complete proof of existence and regularity, we may refer to [Cat61] for the 3-dimensional case, and to [Tem84] (Proposition 2.3 p. 35) for the 2-dimensional case. A complete development on these questions is carried out in [Gal11].

Proposition 3.4. *Let Ω be a bounded domain of $\mathbb{R}^n$, $n \geq 2$. Suppose Ω of class $C^{\max\{2,m+2\}}$, $m \geq -1$. Then for any*

$$f \in (W^{m,q}(\Omega))^n, \quad h_F \in W^{m+1,q}(\Omega), \quad v_b \in (W^{m+2-1/q,q}(\partial\Omega))^n, \quad 1 < q < +\infty, \tag{3.77}$$

with the compatibility condition

$$\int_\Omega h_F \, dx = \int_{\partial\Omega} v_b \cdot n \, ds, \tag{3.78}$$

where n is the outer unit normal to $\partial\Omega$, there exists a unique pair $(v,p) \in (W^{m+2,q}(\Omega))^n \times W^{m+1,q}(\Omega) \cap L^q_0(\Omega)$ solution of the Stokes system

$$\begin{cases} -\nu\Delta v + \nabla p = f & \text{in } \Omega, \\ \mathrm{div}\, v = h_F & \text{in } \Omega, \\ v = v_b & \text{on } \partial\Omega, \end{cases} \tag{3.79}$$

and which satisfies the following estimate

$$\|v\|_{m+2,q,\Omega} + \|p\|_{m+1,q,\Omega} \leq C_{L_q}(\|f\|_{m,q,\Omega} + \|h_F\|_{m+1,q,\Omega} + \|v_b\|_{m+2-1/q,q,\partial\Omega}). \tag{3.80}$$

where $C_{L_q} = C_{L_q}(n,m,q,\Omega)$.

We notice that problem (3.50) differs from problem (3.79) due to the presence of matrices G and F. Then we follow below what is done in [Gra02] to be able to apply Proposition 3.4.

Theorem 3.5. *Let Ω be a bounded domain of $\mathbb{R}^n$, $n \geq 2$, having a C^{m+2} boundary $\partial\Omega$, $m \geq 0$. Let $1 < q < +\infty$ such that $(m+1)q > n$, $f \in (W^{m,q}(\Omega))^n$, $h_F \in W^{m+1,q}(\Omega)$ such that*

$$\int_\Omega h_F \, dx = 0, \tag{3.81}$$

and $\mathbf{A}, \mathbf{B} \in (W^{m+1,q}(\Omega))^{n\times n}$ two matrices. We assume that $\mathbf{B}$ is invertible in $W^{m+1,q}(\Omega)^{n\times n}$, and there exists $\psi \in (W^{m+2,q}(\Omega))^n$ such that

$$\mathbf{B} = \operatorname{cof} \nabla\psi. \tag{3.82}$$

There exists a positive constant $0 < C_{\text{pert}}$, such that if

$$\|\mathrm{I} - \mathbf{A}\|_{(W^{m+1,q}(\Omega))^{n\times n}} \leq C_{\text{pert}}, \quad \text{and} \quad \|\mathrm{I} - \mathbf{B}\|_{(W^{m+1,q}(\Omega))^{n\times n}} \leq C_{\text{pert}}, \tag{3.83}$$

then there exists a unique solution $(v, p) \in (W^{m+2,q}(\Omega))^n \times W^{m+1,q}(\Omega) \cap L^q_0(\Omega)$ of the perturbed Stokes system:

$$\begin{cases} -\nu \operatorname{div}((\nabla v)\mathbf{A}) + \mathbf{B}\nabla p = f & \text{in } \Omega, \\ \operatorname{div}(\mathbf{B}^\top v) = h_F & \text{in } \Omega, \\ v = 0 & \text{on } \partial\Omega, \end{cases} \tag{3.84}$$

and there exists a positive constant $C_{L_{q,2}} > 0$ such that

$$\|v\|_{m+2,q,\Omega} + \|p\|_{m+1,q,\Omega} \leq C_{L_{q,2}}(\|f\|_{m,q,\Omega} + \|h_F\|_{m+1,q,\Omega}). \tag{3.85}$$

We could have just refered to [Gra02] where the proof of the following result is entirely given, but we rewrite the second step to highlight the behaviour of the constant arising in estimate (3.85), in view of a shape optimization investigation.

Proof: Let $(v_0, p_0) \in (W^{m+2,q}(\Omega))^n \times W^{m+1,q}(\Omega)$ be the unique solution of

$$\begin{cases} -\nu\Delta v_0 + \nabla p_0 = f & \text{in } \Omega, \\ \operatorname{div} v_0 = h_F & \text{in } \Omega, \\ v_0 = 0 & \text{on } \partial\Omega, \end{cases} \tag{3.86}$$

obtained applying Proposition 3.4. We define by induction for all $N \geq 0$ the following problem for (v_{N+1}, p_{N+1})

$$\begin{cases} -\nu \operatorname{div}((\nabla v_{N+1})) + \nabla p_{N+1} = f - \nu \operatorname{div}((\nabla v_N)(\mathrm{I} - \mathbf{A})) + (\mathrm{I} - \mathbf{B})\nabla p_N & \text{in } \Omega, \\ \operatorname{div}(v_{N+1}) = h_F + \operatorname{div}((\mathrm{I} - \mathbf{B}^\top)v_N) & \text{in } \Omega, \\ v_{N+1} = 0 & \text{on } \partial\Omega. \end{cases} \tag{3.87}$$

This problem is well-posed for (v_{N+1}, p_{N+1}) with $(v_N, p_N) \in W^{m+2,q}(\Omega)^n \times W^{m+1,q}(\Omega)$. Indeed, from Lemma 3.1 and in view of the regularity of v_N and p_N, we have that $\operatorname{div}((\nabla v_N)(\mathrm{I} - \mathbf{A})) \in (W^{m,q}(\Omega))^n$ and $\operatorname{div}(p_N(\mathrm{I} - \mathbf{B})) \in W^{m,q}(\Omega)$. Yet we can write

$$(\mathrm{I} - \mathbf{B})\nabla p_N = \operatorname{div}(p_N(\mathrm{I} - \mathbf{B})) \tag{3.88}$$

using the Piola identity (3.68), so that $(\mathrm{I} - \mathbf{B})\nabla p_N \in W^{m,q}(\Omega)$, and then also $\mathbf{B}\nabla p_N \in (W^{m,q}(\Omega))^n$. Still using the Piola identity (3.68) we have

$$\operatorname{div}((\mathrm{I} - \mathbf{B}^\top)v_N) = (\mathrm{I} - \mathbf{B}) \cdot \nabla v_N = (\mathrm{I} - \mathbf{B})_{ij}(\nabla v_N)_{ij}, \tag{3.89}$$

and consequently $\mathrm{div}((\mathrm{I}-\mathbf{B}^\top)v_N) \in (W^{m,q}(\Omega))^n$. Finally the compatibility condition (3.78) is satisfied because $v_N = 0$ on $\partial\Omega$, and

$$\int_\Omega \mathrm{div}((\mathrm{I}-\mathbf{B}^\top)v_N)\,dx = \int_{\partial\Omega} (\mathrm{I}-\mathbf{B}^\top)v_N \cdot n\,ds = 0. \tag{3.90}$$

By subtracting problem (3.87) written for (v_{N+1}, p_{N+1}) by problem (3.87) written for (v_N, p_N), we find

$$\begin{cases} -\nu\,\mathrm{div}(\nabla(v_{N+1}-v_N)) + \nabla(p_{N+1}-p_N) = -\nu\,\mathrm{div}(\nabla(v_N - v_{N-1})(\mathrm{I}-\mathbf{A})) & \\ \qquad\qquad + (\mathrm{I}-\mathbf{B})\nabla(p_N - p_{N-1}) & \text{in } \Omega, \\ \mathrm{div}(v_{N+1}-v_N) = \mathrm{div}((\mathrm{I}-\mathbf{B}^\top)(v_N - v_{N-1})) & \text{in } \Omega, \\ v_{N+1}-v_N = 0 & \text{on } \partial\Omega. \end{cases} \tag{3.91}$$

According to Lemma 3.1, we have the following estimates for any $(v,p) \in (W^{m+2,q}(\Omega))^n \times W^{m+1,q}(\Omega)$, $v = 0$ on $\partial\Omega$:

$$\begin{aligned} \|\mathrm{div}((\mathrm{I}-\mathbf{B}^\top)v)\|_{W^{m+1,q}(\Omega)} &= \|(\mathrm{I}-\mathbf{B})\cdot\nabla v\|_{W^{m+1,q}(\Omega)} \\ &\leq n^2 C_a \|(\mathrm{I}-\mathbf{B})\|_{(W^{m+1,q}(\Omega))^{n\times n}} \|v\|_{(W^{2,q}(\Omega))^n}, \end{aligned} \tag{3.92}$$

$$\|\mathrm{div}((\nabla v)(\mathrm{I}-\mathbf{A}))\|_{(W^{m,q}(\Omega))^n} \leq nC_a \|(\mathrm{I}-\mathbf{A})\|_{(W^{m+1,q}(\Omega))^{n\times n}} \|v\|_{(W^{m+2,q}(\Omega))^n} \tag{3.93}$$

where C_a is the constant appearing in Lemma 3.1, and

$$\begin{aligned} \|\mathrm{div}(p(\mathrm{I}-\mathbf{B}))\|_{(W^{m,q}(\Omega))^n} &= \|(\mathrm{I}-\mathbf{B})\nabla p\|_{(W^{m,q}(\Omega))^n} \\ &\leq nC_a \|(\mathrm{I}-\mathbf{B})\|_{(W^{m+1,q}(\Omega))^{n\times n}} \|p\|_{(W^{m+1,q}(\Omega))^n}, \end{aligned} \tag{3.94}$$

where we used Piola identity (3.68) Thus by applying Theorem 3.4, there exists a unique solution $(v_{N+1}, p_{N+1}) \in W^{m+2,q}(\Omega) \times W^{m+1,q}(\Omega)$ to problem (3.91). Moreover in view of assumption (3.83) we find that

$$\begin{aligned} \|v_{N+1}-v_N\|_{m+2,q} + \|p_{N+1}-p_N\|_{m+1,q} &\leq C(n,\nu) C_{L_q} C_a C_{\mathrm{pert}} (\|v_N - v_{N-1}\|_{m+2,q} \\ &\qquad + \|p_N - p_{N-1}\|_{m+1,q}), \\ &\leq (C(n,\nu) C_{L_q} C_a C_{\mathrm{pert}})^N (\|v_0\|_{m+2,q} + \|p_0\|_{m+1,q}), \end{aligned} \tag{3.95}$$

where $C(n,\nu)$ is a constant depending only on n and ν, where C_a is the constant appearing in Lemma 3.1, C_{L_q} is the constant appearing in estimation (3.80), and C_{pert} the constant appearing in assumption (3.83). For a constant C_{pert} small enough such that

$$\gamma = C(n,\nu) C_{L_q} C_a C_{\mathrm{pert}} < 1 \tag{3.96}$$

the sequence $(v_N, p_N)_{N\geq 0}$ converges strongly in $(W^{m+2,q}(\Omega))^n \times W^{m+1,q}(\Omega)$. We call $(v,p) \in W^{m+2,q}(\Omega) \times W^{m+1,q}(\Omega)$ its strong limit. We pass to the limit in the system (3.87), which is possible thanks to the strong convergence. Hence we find that (v,p) is actually a solution of problem (3.84). Finally, by applying Proposition 3.4 to the system (3.87), we obtain the following estimation

$$\begin{aligned} \|v_{N+1}\|_{m+2,q} + \|p_{N+1}\|_{m+1,q} &\leq (C(n,\nu) C_{L_q} C_a C_{\mathrm{pert}})(\|v_N\|_{m+2,q} + \|p_N\|_{m+1,q}) \\ &\qquad + C_{L_q}(\|f\|_{m,q} + \|h_F\|_{m+1,q}). \end{aligned} \tag{3.97}$$

which yields to

$$\begin{aligned}\|v_{N+1}\|_{m+2,q}+\|p_{N+1}\|_{m+1,q} &\leq \gamma^{N+1}(\|v_0\|_{m+2,q}+\|p_0\|_{m+1,q})\\ &\quad+(\gamma^N+\cdots+1)C_{L_q}(\|f\|_{m,q}+\|h_F\|_{m+1,q}),\\ &\leq(\gamma^{N+1}+\gamma^N+\cdots+1)C_{L_q}(\|f\|_{m,q}+\|h_F\|_{m+1,q}). \quad (3.98)\end{aligned}$$

Passing to the limit in estimation (3.98) yields to the following inequality

$$\|v\|_{m+2,q}+\|p\|_{m+1,q}\leq\frac{C_{L_q}}{1-\gamma}(\|f\|_{m,q,\Omega}+\|h_F\|_{m+1,q,\Omega}). \quad (3.99)$$

The uniqueness of the solution is straightforward due to the estimate (3.99) and the linearity of problem (3.84). We have obtained a unique solution $(v,p)\in(W^{m+2,q}(\Omega))^n\times W^{m+1,q}(\Omega)\cap L_0^q(\Omega)$ for the problem (3.84), satisfying the estimation (3.85). □

3.3.3 Resolution of the structure problem

Now we solve the structure problem (3.54). It is actually a Stokes like problem. The field w stands for the structure displacement. The structure being clamped at $\partial\omega$, we have at this boundary a homogeneous Dirichlet condition. But for the boundary Γ_0, the equilibrium of the surface forces leads to a *stress boundary condition*.

Usually, the Dirichlet condition for the Stokes problem implies that we have a solution for which the pressure field is defined up to a constant (which is often chosen such that the pressure has a zero mean), whereas pure Neumann or pure stress condition brings to a solution for which the velocity field is defined up to a constant. In the case of mixed boundary condition, i.e with Dirichlet condition on a part of the boundary and stress condition on the rest of the boundary, we will note that the velocity together with the pressure are completely determined, and no zero mean value has to be imposed.

We first recall a classical result, that we are going to use to show the existence of the "pressure" field for the structure problem. We refer for example to [BF13] for a proof.

Proposition 3.6 (de Rham's Theorem). *Let Ω be a connected, bounded, Lipschitz domain of $\mathbb{R}^n$, $n\geq 2$. Let f be an element in $(H^{-1}(\Omega))^n$, such that for any function $\varphi\in(\mathcal{D}(\Omega))^n$ satisfying* $\operatorname{div}\varphi=0$*, we have $\langle f,\varphi\rangle_{H^{-1},H_0^1}=0$. Then, there exists a unique function p in $L_0^2(\Omega)$ such that $f=\nabla p$.*

Let $\mathcal{O}$ be a bounded domain of $\mathbb{R}^2$, we denote by Γ its boundary. Let ω be a subset of $\mathcal{O}$ such that $\omega\subset\subset\mathcal{O}$. Thus we define the domain Ω by

$$\Omega:=\mathcal{O}\setminus\overline{\omega}, \quad (3.100)$$

so that the boundary of Ω is

$$\partial\Omega=\Gamma\cup\partial\omega. \quad (3.101)$$

Let us introduce the space

$$H^1_{0,\partial\omega}(\Omega):=\{u\in H^1(\Omega)\mid u=0\text{ on }\partial\omega\}. \quad (3.102)$$

We state the main result of this section, providing the existence, the uniqueness and the regularity of solutions to the structure problem when the stress boundary conditions on Γ are given.

Theorem 3.7. *Let $(g, h_S, f_b) \in (L^2(\Omega))^2 \times H^1(\Omega) \times (H^{1/2}(\partial\Omega))^2$. There exists a unique pair (w, s) in $(H^1_{0,\partial\omega}(\Omega))^2 \times L^2(\Omega)$ solution of the problem:*

$$\begin{cases} -\operatorname{div}\sigma(w) + \nabla s = g & \text{in } \Omega \\ \operatorname{div} w = h_S & \text{in } \Omega \\ w = 0 & \text{on } \partial\omega \\ (\sigma(w) - s\mathrm{I})n = f_b & \text{on } \Gamma, \end{cases} \tag{3.103}$$

where n is the outward normal vector to Γ, and $\sigma(\mathrm{w}) = 2\mu\nabla^s(\mathrm{w})$.

Moreover, if the domain Ω is of class $C^{k+2,1}$ for $k \geq 0$, and if (g, h_S, f_b) belongs to $(H^k(\Omega))^2 \times H^{k+1}(\Omega) \times (H^{k+1/2}(\partial\Omega))^2$, then the pair (w, s) belongs to $(H^{k+2}(\Omega))^2 \times H^{k+1}(\Omega)$ and there exists a constant $0 < C_\mathrm{s}$ depending only on Ω such that

$$\|w\|_{H^{k+2}} + \|s\|_{H^{k+1}} \leq C_\mathrm{s}(\|g\|_{H^k} + \|h_S\|_{H^{k+1}} + \|f_b\|_{H^{k+1/2}}). \tag{3.104}$$

Since problem (3.103) involves non standard boundary conditions of different types, we give a proof of the first part of Theorem 3.7 for the existence of a unique weak solution. The regularity result can be obtained following [BF13]. We follow the approach presented in [BF13] in the case where the stress boundary condition lies on the whole boundary $\partial\Omega$. First we show the following useful Lemma, enabling us to deal with free-divergence field.

Lemma 3.8. *Let Ω be a regular open bounded subset of $\mathbb{R}^2$. There exists a right inverse for the divergence operator, that is there exists a continuous linear operator π from $L^2(\Omega)$ to $(H^1_{0,\partial\omega}(\Omega))^2$, such that for any q in $L^2(\Omega)$:*

$$\operatorname{div}(\pi q) = q. \tag{3.105}$$

<u>*Proof:*</u> Let q be in $L^2(\Omega)$. Because Ω is of class $C^{1,1}$, we have a unique solution ψ in $H^2(\Omega)$ solution of ([Eva10])

$$\begin{cases} -\Delta\psi = q & \text{in } \Omega \\ \psi = 0 & \text{on } \Gamma \\ \partial_n\psi = 0 & \text{on } \partial\omega, \end{cases} \tag{3.106}$$

where ∂_n stands for the normal derivative along $\partial\omega$, and ψ satisfies

$$\|\psi\|_{H^2(\Omega)} \leq C\|q\|_{L^2(\Omega)}. \tag{3.107}$$

We set

$$v = -\nabla\psi, \tag{3.108}$$

such that v belongs to $(H^1(\Omega))^2$, $v \cdot n = 0$ on $\partial\omega$, and $\operatorname{div} v = q$. We would like to have also $v \cdot \tau = 0$, where τ is a tangent vector that we can define by $\tau = (n_2, -n_1)^\top$, where the normal vector is written in a canonical base of $\mathbb{R}^2$: $n = (n_1, n_2)^\top$. So we have $v \cdot \tau$. Let

$$g = v \cdot \tau, \tag{3.109}$$

and let φ be the $(H^2(\Omega))^2$ lifting of $(0, g) \in H^{3/2}(\partial\omega) \times H^{1/2}(\partial\omega)$ ([BF13]), satisfying

$$\varphi = 0 \text{ on } \partial\omega, \tag{3.110}$$

$$\partial_n\varphi = g \text{ on } \partial\omega, \tag{3.111}$$

and

$$\|\varphi\|_{H^2} \leq C\|q\|_{L^2}. \tag{3.112}$$

Thus we have $\nabla\varphi \cdot \tau = 0$. We set

$$w = \operatorname{rot}\varphi = \left(-\frac{\partial\varphi}{\partial x_2}, \frac{\partial\varphi}{\partial x_1}\right)^\top, \tag{3.113}$$

in such a way that

$$\begin{aligned}
&w \cdot n = \nabla\varphi \cdot \tau = 0 && \text{on } \partial\omega,\\
&w \cdot \tau = -\nabla\varphi \cdot n = -g && \text{on } \partial\omega,\\
&\operatorname{div} w = 0 && \text{in } \Omega.
\end{aligned}$$

We conclude by defining

$$\pi q = v + w, \tag{3.114}$$

and easily check that $\pi q \in (H^1_{0,\partial\omega}(\Omega))^2$ satisfies $\operatorname{div} \pi q = q$. □

Proof of Theorem 3.7: First, we can only consider the case where $h_S = 0$ in (3.103). Indeed, from Lemma 3.8 there exists a linear operator

$$\pi : L^2(\Omega) \to (H^1_{0,\partial\omega}(\Omega))^2 \tag{3.115}$$

such that for all q in $L^2(\Omega)$

$$\operatorname{div}(\pi q) = q \text{ in } \Omega. \tag{3.116}$$

We introduce $\tilde{w} := w - \pi h_S$. From (3.103), $\tilde{w}$ satisfies

$$\begin{cases}
-\operatorname{div}\sigma(\tilde{w}) + \nabla s = g + \operatorname{div}\sigma(\pi h_S) & \text{in } \Omega\\
\operatorname{div}\tilde{w} = 0 & \text{in } \Omega\\
\tilde{w} = 0 & \text{on } \partial\omega\\
(\sigma(\tilde{w}) - s\mathrm{I})n = f_b - \sigma(\pi h_S)n & \text{on } \Gamma,
\end{cases} \tag{3.117}$$

which corresponds to the homogeneous data $h_S = 0$ in problem (3.103). Thus we are now only interested in the problem of the following form:

$$\begin{cases}
-\operatorname{div}\sigma(w) + \nabla s = g & \text{in } \Omega\\
\operatorname{div} w = 0 & \text{in } \Omega\\
w = 0 & \text{on } \partial\omega\\
(\sigma(w) - s\mathrm{I})n = f_b & \text{on } \Gamma.
\end{cases} \tag{3.118}$$

We define the Hilbert space

$$W := \{v \in (H^1(\Omega))^2 \mid v = 0 \text{ on } \partial\omega,\ \operatorname{div} v = 0\}, \tag{3.119}$$

and the bilinear form

$$a(u, v) = \int_\Omega \sigma(u) \cdot e(v) \tag{3.120}$$

is obviously continuous on W. Furthermore, a is coercive on W because of the homogeneous Dirichlet condition on $\partial\omega$ allowing the validity of a Poincaré type inequality and of

Korn inequality (see [OSY92] Theorem 2.5). Namely there exists a constant C such that for all $u \in W$, $\|u\|_{H^1} \leq Ca(u,u)^{1/2}$. Thus, by applying Lax-Milgram theorem, we obtain that there exists a unique w in W such that for any z in W

$$a(w,z) = \int_\Omega g \cdot z + \langle f_b, z\rangle_{-1/2,1/2,\Gamma}. \tag{3.121}$$

Thus for all $z \in (\mathcal{D}(\Omega))^2$, we have that

$$\langle -\operatorname{div}\sigma(w) - g, z\rangle_{\mathcal{D}',\mathcal{D}} = 0, \tag{3.122}$$

where we recall that $\mathcal{D}(\Omega)$ is the space of $C^\infty(\Omega)$ functions having a compact support, and $\mathcal{D}'$ is the space of the distributions on Ω. In particular (3.122) holds for all z in $(\mathcal{D}(\Omega))^2$ satisfying $\operatorname{div} z = 0$. We deduce from de Rham's theorem 3.6 that there exists a unique s in $L^2_0(\Omega)$ such that

$$-\operatorname{div}\sigma(w) + \nabla s = g \tag{3.123}$$

in $(H^{-1}(\Omega))^n$. From the regularity of g, we have then $-\operatorname{div}(\sigma(w) - s\mathrm{I}) = g \in L^2(\Omega)$. Hence, Stokes formula leads to

$$\int_\Omega (\sigma(w) - s\mathrm{I}) \cdot \nabla\varphi - \langle(\sigma(w) - s\mathrm{I})n, \varphi\rangle_{-1/2,1/2,\Gamma} = \int_\Omega g \cdot \varphi, \quad \forall \varphi \in (H^1(\Omega))^2. \tag{3.124}$$

Now choosing $\varphi \in (H^1(\Omega))^2$ such that $\operatorname{div}\varphi = 0$, that is to say $\varphi \in W$, we have that

$$s\mathrm{I} \cdot \nabla\varphi = s \operatorname{div}\varphi = 0. \tag{3.125}$$

Then by comparing (3.121) and (3.124), we obtain

$$\langle(\sigma(w) - s\mathrm{I})n, \varphi\rangle_{-1/2,1/2,\Gamma} = \langle f_b, \varphi\rangle_{-1/2,1/2,\Gamma}, \quad \forall \varphi \in W. \tag{3.126}$$

We want that (3.126) holds for all $\varphi \in (H^1(\Omega))^2$. Let φ be in $(H^{1/2}(\Gamma))^2$, we choose a free divergence extension of φ to $(H^1(\Omega))^2$, for example by taking the solution $\tilde\varphi \in (H^1_{0,\partial\omega}(\Omega))^2$ to the problem

$$\begin{cases} -\Delta\tilde\varphi + \nabla r = 0 & \text{in } \Omega \\ \operatorname{div}\tilde\varphi = 0 & \text{in } \Omega \\ \tilde\varphi = 0 & \text{on } \partial\omega \\ \tilde\varphi = \varphi & \text{on } \Gamma, \end{cases} \tag{3.127}$$

where r is a pressure field in $L^2_0(\Omega)$. This solution $\tilde\varphi$ exists as long as the additional condition holds (see e.g. [BF13] Theorem IV.5.2)

$$\int_\Gamma \varphi \cdot n \, ds = 0. \tag{3.128}$$

Thus we have shown in view of (3.126) that for all $\varphi \in (H^{1/2}(\Gamma))^2$ satisfying (3.128),

$$\langle(\sigma(w) - s\mathrm{I})n - f_b, \varphi\rangle_{-1/2,1/2,\Gamma} = \langle(\sigma(w) - s\mathrm{I})n - f_b, \tilde\varphi\rangle_{-1/2,1/2,\Gamma} = 0, \tag{3.129}$$

since $\tilde\varphi \in W$. Let ψ in $H^{1/2}(\Gamma)$, we write

$$\psi = \psi - \left(\frac{1}{|\Gamma|}\int_\Gamma \psi \cdot n\right) n + \left(\frac{1}{|\Gamma|}\int_\Gamma \psi \cdot n\right) n,$$

$$= \psi_1 + \left(\frac{1}{|\Gamma|} \int_\Gamma \psi \cdot n \right) n, \tag{3.130}$$

where by definition $\int_\Gamma \psi_1 \cdot n = 0$. Thus we can write for all ψ in $H^{1/2}(\Gamma)$:

$$\langle (\sigma(w) - s\mathrm{I})n - f_b, \psi \rangle_{-1/2,1/2,\Gamma} = \langle c_0 n, \psi \rangle_{-1/2,1/2,\Gamma}, \tag{3.131}$$

where c_0 is the constant defined by

$$c_0 = \frac{1}{|\Gamma|} \langle (\sigma(w) - s\mathrm{I})n - f_b, n \rangle_{-1/2,1/2,\Gamma} \, . \tag{3.132}$$

We can conclude that

$$(\sigma(w) - (s + c_0)\mathrm{I})n = f_b \quad \text{in } (H^{-1/2}(\Gamma))^2. \tag{3.133}$$

Hence $(w, s + c_0) \in (H^1(\Omega))^2 \times L^2(\Omega)$ is a weak solution of (3.118). □

3.3.4 A fixed point procedure

In this section, we show the main result of Section 3.3: an existence and uniqueness result for the Fluid Structure Interaction problem.

Theorem 3.9. *Let $f \in (H^2(\mathrm{D}))^2$, and $g \in (H^1(\mathrm{D}))^2$. Let $\boldsymbol{S} : (H^3(\Omega_0))^2 \to (H^3(\Omega_0))^2$ be the map defined in* (3.56) *by consecutively solving problem* (3.50) *posed for f and problem* (3.54) *posed for g.*

There exists a constant $C_{\boldsymbol{S}}$ such that if $\|f\|_{2,2} \leq C_{\boldsymbol{S}}$ and $\|g\|_{1,2} \leq C_{\boldsymbol{S}}$, then there exists a unique solution $(\mathrm{v}, \mathrm{q}) \in (H^3(\Omega_0^c))^2 \times H^2(\Omega_0^c) \cap L_0^2(\Omega_0^c)$, $(\mathrm{w}, \mathrm{s}) \in (H^3(\Omega_0))^2 \times H^2(\Omega_0)$ to the Fluid Structure Interaction problem (3.44)*. Furthermore, there exists a constant C_{FS} such that*

$$\|\mathrm{v}\|_{3,2,\Omega_0^c} + \|\mathrm{q}\|_{2,2,\Omega_0^c} + \|\mathrm{w}\|_{3,2,\Omega_0} + \|\mathrm{s}\|_{2,2,\Omega_0} \leq C_{FS}(\|f\|_{2,2,\mathrm{D}} + \|g\|_{1,2,\mathrm{D}}). \tag{3.134}$$

<u>*Proof:*</u> **In a first step** we look at the continuity of the fluid problem. Let $(\mathrm{v}(\mathbf{b}_1), \mathrm{q}(\mathbf{b}_1)$ and $(\mathrm{v}(\mathbf{b}_2), \mathrm{q}(\mathbf{b}_2)$ be the solutions of problem (3.50) for respectively $\mathbf{b}_1$ and $\mathbf{b}_2$ in B_p, where

$$B_p := \{\mathbf{b} \in (H^3(\Omega_0))^2 \mid \|\mathbf{b}\|_{3,2} \leq \mathcal{M}\}, \tag{3.135}$$

for $\mathcal{M}$ a given constant. We set $\boldsymbol{\delta}\mathrm{v} := \mathrm{v}(\mathbf{b}_1) - \mathrm{v}(\mathbf{b}_2)$ and $\boldsymbol{\delta}\mathrm{q} := \mathrm{q}(\mathbf{b}_1) - \mathrm{v}(\mathbf{b}_2)$. In view of (3.50) we can write

$$\begin{cases} -\operatorname{div}(\nabla(\boldsymbol{\delta}\mathrm{v})F(\mathbf{b}_1)) + G(\mathbf{b}_1)\nabla\boldsymbol{\delta}\mathrm{q} = J(\mathbf{b}_1)f \circ T(\mathbf{b}_1) - J(\mathbf{b}_2)f \circ T(\mathbf{b}_2) & \\ \qquad + \operatorname{div}(\nabla(\mathrm{v}(\mathbf{b}_2))(F(\mathbf{b}_1) - F(\mathbf{b}_2))) & \\ \qquad - (G(\mathbf{b}_1) - G(\mathbf{b}_2))\nabla\mathrm{q}(\mathbf{b}_2) & \text{in } \Omega_0^c, \\ \operatorname{div}(G(\mathbf{b}_1)^\top\boldsymbol{\delta}\mathrm{v}) = -\operatorname{div}((G(\mathbf{b}_1) - G(\mathbf{b}_2))^\top\mathrm{v}(\mathbf{b}_2)) & \text{in } \Omega_0^c, \\ \boldsymbol{\delta}\mathrm{v} = 0 & \text{on } \partial\Omega_0^c. \end{cases} \tag{3.136}$$

The compatibility condition (3.81) is valid because of the homogeneous Dirichlet condition satisfied by $\mathrm{v}(\mathbf{b}_2)$. In view of the regularity of $\mathrm{v}(\mathbf{b}_2)$ and $\mathrm{q}(\mathbf{b}_2)$, we can apply Theorem 3.5

for $m = 1$ and $q = 2$, giving that for all $\mathbf{b}_1$, $\mathbf{b}_2$ in B_p, if $\mathcal{M}$ is small enough, the solution $(\boldsymbol{\delta}\mathrm{v}, \boldsymbol{\delta}\mathrm{q})$ of (3.136) belongs to $(H^3(\Omega_0^c))^2 \times H^2(\Omega_0^c) \cap L_0^2(\Omega_0^c)$, and satisfies

$$\|\boldsymbol{\delta}\mathrm{v}\|_{3,2,\Omega_0^c} + \|\boldsymbol{\delta}\mathrm{q}\|_{2,2,\Omega_0^c} \leq C_{L_p}(\|f_F\|_{1,2,\Omega_0^c} + \|h_F\|_{2,2,\Omega_0^c}), \tag{3.137}$$

where f_F and h_F are defined by

$$\begin{aligned} f_F &= J(\mathbf{b}_1) f \circ T(\mathbf{b}_1) - J(\mathbf{b}_2) f \circ T(\mathbf{b}_2) + \operatorname{div}(\nabla(\mathrm{v}(\mathbf{b}_2))(F(\mathbf{b}_1) - F(\mathbf{b}_2))) \\ &\quad - (G(\mathbf{b}_1) - G(\mathbf{b}_2))\nabla \mathrm{q}(\mathbf{b}_2), \end{aligned} \tag{3.138}$$

$$h_F = -\operatorname{div}((G(\mathbf{b}_1) - G(\mathbf{b}_2))^\top \mathrm{v}(\mathbf{b}_2)). \tag{3.139}$$

We first estimate the term f_F, and then we estimate h_F.

From Lemmas 3.1 and 3.3 we have that J defined from B_p into $H^2(\Omega_0^c)$ and G and F defined from B_p into $(H^2(\Omega_0^c))^{2\times 2}$ are of class C^∞, and the norms of their derivatives are bounded on B_p. We set

$$\|DJ\|_{\mathcal{M}} := \sup_{\mathbf{b}\in B_p} \|DJ(\mathbf{b})\|_{\mathcal{L}(H^3(\Omega_0), H^2(\Omega_0^c))}, \tag{3.140}$$

$$\|DG\|_{\mathcal{M}} := \sup_{\mathbf{b}\in B_p} \|DG(\mathbf{b})\|_{\mathcal{L}(H^3(\Omega_0), (H^2(\Omega_0^c))^{2\times 2})}, \tag{3.141}$$

$$\|DF\|_{\mathcal{M}} := \sup_{\mathbf{b}\in B_p} \|DF(\mathbf{b})\|_{\mathcal{L}(H^3(\Omega_0), (H^2(\Omega_0^c))^{2\times 2})}. \tag{3.142}$$

From Theorem 3.5 for $m = 1$ and $q = 2$ applied to problem (3.50) written for $\mathbf{b}_2$, we have the estimation

$$\|\nabla \mathrm{v}(\mathbf{b}_2)\|_{3,2,\Omega_0^c,} \leq C_{L_{p,2}} \|J(\mathbf{b}_2)(f \circ T(\mathbf{b}_2))\|_{1,2,\Omega_0^c}. \tag{3.143}$$

In view of Lemma 3.2, $T(\mathbf{b}_2)$ is a C^1-diffeomorphism, and from the definition of the map J in (3.73), a change of variable gives

$$\|J(\mathbf{b}_2)(f \circ T(\mathbf{b}_2))\|_{1,2,\Omega_0^c} = \|f\|_{1,2,T(\mathbf{b}_2)(\Omega_0^c)} \leq \|f\|_{1,2,\mathrm{D}}. \tag{3.144}$$

From Lemma 3.1, we deduce:

$$\begin{aligned} \|\nabla \mathrm{v}(\mathbf{b}_2)(F(\mathbf{b}_1) - F(\mathbf{b}_2))\|_{2,2,\Omega_0^c} &\leq C_a \|\nabla \mathrm{v}(\mathbf{b}_2)\|_{2,2,\Omega_0^c} \|(F(\mathbf{b}_1) - F(\mathbf{b}_2))\|_{1,p,\Omega_0^c} \\ &\leq C_a C_{L_{p,2}} \|f\|_{1,2,\mathrm{D}} \|DF\|_{\mathcal{M}} \|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0}. \end{aligned} \tag{3.145}$$

Similarly we find

$$\|(G(\mathbf{b}_1) - G(\mathbf{b}_2))\nabla \mathrm{q}(\mathbf{b}_2)\|_{1,2,\Omega_0^c} \leq C_a C_{L_{p,2}} \|f\|_{1,2,\mathrm{D}} \|DG\|_{\mathcal{M}} \|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0}. \tag{3.146}$$

Now we want to estimate

$$\begin{aligned} \|J(\mathbf{b}_1) f \circ T(\mathbf{b}_1) - J(\mathbf{b}_2) f \circ T(\mathbf{b}_2)\|_{1,2,\Omega_0^c} &\leq \|(J(\mathbf{b}_1) - J(\mathbf{b}_2)) f \circ T(\mathbf{b}_1)\|_{1,2,\Omega_0^c} \\ &\quad + \|J(\mathbf{b}_2)(f \circ T(\mathbf{b}_1) - f \circ T(\mathbf{b}_2)\|_{1,2,\Omega_0^c}. \end{aligned} \tag{3.147}$$

We have that $H^2(\Omega_0^c)$ is embeded continuously into $L^\infty(\Omega_0^c)$. Thus $J(\mathbf{b}_2)$ belongs to $L^\infty(\Omega_0^c)$, and there exists a constant $C_\infty > 0$ such that

$$\|J(\mathbf{b}_2)\|_{\infty,p,\Omega_0^c} \leq C_\infty \|J(\mathbf{b}_2)\|_{2,2,\Omega_0^c}. \tag{3.148}$$

We can write point-wise

$$J(\mathbf{b})(x) = \det T(\mathbf{b})(x) = 1 + \mathrm{tr}(\nabla\mathcal{R}(\gamma(\mathbf{b}))(x)) + o(|\nabla\mathcal{R}(\gamma(\mathbf{b}))(x)|), \quad \text{for a.e. } x \in \Omega_0^c, \tag{3.149}$$

and by taking $\mathcal{M}$ small enough, we can obtain both

$$1/2 \leq \|J(\mathbf{b})\|_{0,\infty}, \|J(\mathbf{b})^{-1}\|_{0,\infty} \leq 2 \tag{3.150}$$

for all $\mathbf{b} \in B_p$. With these elements we calculate:

$$\|(J(\mathbf{b}_1) - J(\mathbf{b}_2))f \circ T(\mathbf{b}_1)\|_{1,2,\Omega_0^c} \leq 2\|f\|_{1,2,\mathrm{D}}\|DJ\|_{\mathcal{M}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0}. \tag{3.151}$$

From [HP06] Lemma 5.3.3, we consider $\eta \in W^{1,p}(\mathbb{R}^2)$ for $1 \leq p < +\infty$, and the map

$$\mathbf{b} \in (W^{1,\infty}(\mathbb{R}^2))^2 \mapsto \eta \circ T(\mathbf{b}) \in L^p(\mathbb{R}^2) \tag{3.152}$$

is of class C^1 in the vicinity of 0. Thus for $f \in (H^2(\mathrm{D}))^2$ we have

$$\|f \circ T(\mathbf{b}_1) - f \circ T(\mathbf{b}_2)\|_{1,2} \leq \|D(f \circ T(\mathbf{b}_2))\|_{1,2}\|\mathbf{b}_1 - \mathbf{b}_2\|_{2,\infty} + o(\|\mathbf{b}_1 - \mathbf{b}_2\|_{2,\infty}). \tag{3.153}$$

Once again we have

$$\|\mathbf{b}_1 - \mathbf{b}_2\|_{2,\infty} \leq C_\infty\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2}. \tag{3.154}$$

Moreover, Lemma 5.3.3 in [HP06] gives the following expression for the derivative

$$\|D(f \circ T(\mathbf{b}_2))\|_{1,2} = \|\nabla f \circ T(\mathbf{b}_2)\|_{1,2} \leq 2\|f\|_{2,2,\mathrm{D}}, \tag{3.155}$$

where we have obtained the inequality with a change a variable and in view of the uniform bound we have for $J(\mathbf{b})$ over B_p.

We recall that f_F is given by (3.138). We have completely estimated $\|f_F\|_{1,2}$ by combining (3.145), (3.146), (3.146), (3.146), (3.146), and (3.146). We obtain

$$\begin{aligned}\|f_F\|_{1,2,\Omega_0^c} \leq{}& \|f\|_{1,2,\mathrm{D}}\left(C_a C_{L_{p,2}}(\|DF\|_{\mathcal{M}} + \|DG\|_{\mathcal{M}}) + 2\|DJ\|_{\mathcal{M}}\right)\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0} \\ &+ 2\|f\|_{2,2,\mathrm{D}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0},\end{aligned} \tag{3.156}$$

and finally

$$\|f_F\|_{1,2,\Omega_0^c} \leq \|f\|_{2,2,\mathrm{D}}\left(2 + C_a C_{L_{p,2}}(\|DF\|_{\mathcal{M}} + \|DG\|_{\mathcal{M}}) + 2\|DJ\|_{\mathcal{M}}\right)\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0}. \tag{3.157}$$

For the estimation of $\|h_F\|_{2,2}$, we recall that we can write

$$h_F = -\operatorname{div}((G(\mathbf{b}_1) - G(\mathbf{b}_2))^\top \mathrm{v}(\mathbf{b}_2)) = -(G(\mathbf{b}_1) - G(\mathbf{b}_2)) \cdot \nabla \mathrm{v}(\mathbf{b}_2), \tag{3.158}$$

so that

$$\begin{aligned}\|h_F\|_{2,2,\Omega_0^c} &\leq n^2 C_a\|G(\mathbf{b}_1) - G(\mathbf{b}_2)\|_{2,2,\Omega_0^c}\|\nabla \mathrm{v}(\mathbf{b}_2)\|_{2,2,\Omega_0^c} \\ &\leq n^2 C_a C_{L_{p,2}}\|f\|_{1,2,\mathrm{D}}\|DG\|_{\mathcal{M}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0}.\end{aligned} \tag{3.159}$$

Finally from (3.137) we get

$$\|\boldsymbol{\delta}\mathrm{v}\|_{3,2,\Omega_0^c} + \|\boldsymbol{\delta}\mathrm{q}\|_{2,2,\Omega_0^c} \leq \boldsymbol{C}(\mathcal{M}, C_a, C_{\mathcal{R}\gamma}, C_{L_{p,2}})\|f\|_{2,2,\mathrm{D}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2,\Omega_0}. \tag{3.160}$$

In a second step we look at the continuity of the structure problem. Let $(\mathrm{w}(\mathbf{b}_1), \mathrm{s}(\mathbf{b}_1))$ and $(\mathrm{w}(\mathbf{b}_2), \mathrm{s}(\mathbf{b}_2))$ be the solutions of problem (3.54) for respectively $\mathbf{b}_1$ and $\mathbf{b}_2$ in B_p. We set $\boldsymbol{\delta}\mathrm{w} := \mathrm{w}(\mathbf{b}_1) - \mathrm{w}(\mathbf{b}_2)$ and $\boldsymbol{\delta}\mathrm{s} := \mathrm{s}(\mathbf{b}_1) - \mathrm{s}(\mathbf{b}_2)$. In view of (3.54) we can write

$$\left\{\begin{array}{rcll} 2\mu\,\mathrm{div}(\nabla\boldsymbol{\delta}\mathrm{w}) + \nabla\boldsymbol{\delta}\mathrm{s} & = & 0 & \text{in } \Omega_0, \\ \mathrm{div}\,\boldsymbol{\delta}\mathrm{w} & = & 0 & \text{in } \Omega_0, \\ \boldsymbol{\delta}\mathrm{w} & = & 0 & \text{on } \partial\omega, \\ (2\mu\,\mathrm{div}(\nabla\boldsymbol{\delta}\mathrm{w}) - \boldsymbol{\delta}\mathrm{s}\mathrm{I})n_0 & = & (\nabla\mathrm{v}(\mathbf{b}_1))F(\mathbf{b}_1) - (\nabla\mathrm{v}(\mathbf{b}_2))F(\mathbf{b}_2))n_0 & \\ & & -(q(\mathbf{b}_1)G(\mathbf{b}_1) - q(\mathbf{b}_2)G(\mathbf{b}_2))n_0 & \text{on } \Gamma_0. \end{array}\right. \tag{3.161}$$

Let us denote by f_b the surface force

$$f_b = (\nabla\mathrm{v}(\mathbf{b}_1))F(\mathbf{b}_1) - (\nabla\mathrm{v}(\mathbf{b}_2))F(\mathbf{b}_2))n_0 - (q(\mathbf{b}_1)G(\mathbf{b}_1) - q(\mathbf{b}_2)G(\mathbf{b}_2))n_0. \tag{3.162}$$

In order to apply Theorem 3.7 for $k = 1$, we need that f_b belongs to $(H^{3/2}(\Gamma_0))^2$. In view of the regularity of the fields involved in the expression (3.162), and from Lemma 3.1, we have that

$$(\nabla\mathrm{v}(\mathbf{b}_1))F(\mathbf{b}_1) - (\nabla\mathrm{v}(\mathbf{b}_2))F(\mathbf{b}_2)) \in H^2(\Omega_0^c), \tag{3.163}$$

$$(q(\mathbf{b}_1)G(\mathbf{b}_1) - q(\mathbf{b}_2)G(\mathbf{b}_2)) \in H^2(\Omega_0^c). \tag{3.164}$$

Thus f_b belongs to $(H^{3/2}(\Gamma_0))^2$. We first estimate:

$$\begin{aligned} \|(\nabla\mathrm{v}(\mathbf{b}_1))F(\mathbf{b}_1) - (\nabla\mathrm{v}(\mathbf{b}_2))F(\mathbf{b}_2))n\|_{3/2,2,\Gamma_0} \leq{}& \|(\nabla\mathrm{v}(\mathbf{b}_1) - \nabla\mathrm{v}(\mathbf{b}_2))F(\mathbf{b}_1)\|_{2,2,\Omega_0^c} \\ &+ \|(\nabla\mathrm{v}(\mathbf{b}_2)(F(\mathbf{b}_1) - F(\mathbf{b}_2))\|_{2,2,\Omega_0^c} \end{aligned} \tag{3.165}$$

Thus from (3.145) and (3.160) we have a constant $C > 0$ such that

$$\|(\nabla\mathrm{v}(\mathbf{b}_1))F(\mathbf{b}_1) - (\nabla\mathrm{v}(\mathbf{b}_2))F(\mathbf{b}_2))n\|_{3/2,2,\Gamma_0} \leq C\|f\|_{2,2,\mathrm{D}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2}. \tag{3.166}$$

In a same manner we have a constant $C' > 0$ such that

$$\|(q(\mathbf{b}_1)G(\mathbf{b}_1) - q(\mathbf{b}_2)G(\mathbf{b}_2))n\|_{3/2,2,\Gamma_0} \leq C'\|f\|_{2,2,\mathrm{D}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2}. \tag{3.167}$$

Finally we have obtained by applying Theorem 3.7 for f_b defined as in (3.162), we obtain a constant $C_{\mathcal{M}} = C_{\mathcal{M}}(\mathcal{M}, C_a, C_{\mathcal{R}\gamma}, C_{L_{p,2}}) > 0$ such that:

$$\|\mathrm{w}(\mathbf{b}_1) - \mathrm{w}(\mathbf{b}_2)\|_{3,2} + \|\mathrm{s}(\mathbf{b}_1) - \mathrm{s}(\mathbf{b}_2)\|_{2,2} \leq C_{\mathrm{s}}C_{\mathcal{M}}\|f\|_{2,2,\mathrm{D}}\|\mathbf{b}_1 - \mathbf{b}_2\|_{3,2}. \tag{3.168}$$

In a third step, we show that the map $\boldsymbol{S} : \mathbf{b} \mapsto \mathrm{w}(\mathbf{b})$ defined in (3.56) is a contraction. For a fixed $\mathcal{M}$, we have from (3.168) that there exists a constant C_1 such that if $\|f\|_{2,2,\mathrm{D}} < C_1$, then $\boldsymbol{S}$ is a contraction.

By applying Theorem (3.7) to the problem (3.54) satisfied by $\mathrm{w}(\mathbf{b})$, for a $\mathbf{b} \in B_p$, we obtain that

$$\|\mathrm{w}(\mathbf{b})\|_{3,2} + \|\mathrm{s}(\mathbf{b})\|_{2,2} \leq C_{\mathrm{s}}(C_{\mathcal{M}}\|f\|_{1,p,\mathrm{D}} + \|g\|_{1,2,\Omega_0}). \tag{3.169}$$

Hence, there exists a constant C_2 such that if $\|f\|_{2,2,\mathrm{D}} < C_2$ and $\|g\|_{1,2,\Omega_0} < C_2$, then

$$\|\mathrm{w}(\mathbf{b})\|_{3,2} + \|\mathrm{s}(\mathbf{b})\|_{2,2} \leq \mathcal{M}. \tag{3.170}$$

By defining

$$C_{\boldsymbol{S}} = \min(C_1, C_2), \tag{3.171}$$

we have that if $\|f\|_{2,2,\mathrm{D}} < C_{\boldsymbol{S}}$ and $\|g\|_{1,2,\Omega_0} < C_{\boldsymbol{S}}$, then the map $\boldsymbol{S}$ is a contraction which maps B_p onto B_p. Thus, form the Banach fixed-point theorem, S admits a unique fixed point in B_p denoted by w. It results that the solution $(\mathrm{v(w)}, \mathrm{q(w)}, \mathrm{w}, \mathrm{s(w)})$ is the unique solution to the Fluid Structure Interaction problem (3.44).

□

3.4 Shape derivatives by the velocity method

In this section, we start by a introduction to the velocity method for the computation of shape derivatives. In Section 3.4.2, we present how we apply this method to the FSI problem. Then in Section 3.4.5 we calculate the shape derivative of an abstract shape functional expressed with the material derivatives of the solutions of the FSI problem. We give finally the boundary value problems satisfied by this material derivatives in Section 3.4.4.

3.4.1 General introduction

We are interested in the study of the variations of a shape functional $\mathcal{J}(\Omega)$ with respect to the variation of the domain Ω. In classical optimization, the information offered by the derivative of the cost function is helpful. It gives information on optimality conditions, and can be used for numerical optimization, and it allows us under certain conditions to find its extrema. But in the case of shape optimization, the variable is a geometrical domain, and thus does not belong to a vector space. We therefore need to give an adequate definition of the *derivative* of a shape functional As we mentioned it in the introduction of Chapter 2, the concept of *shape derivative* was introduced in the pioneering paper [Had08]. For further references, the reader may consult for example [SZ92] Chapter 2, [HP06] Section 5.1 or [All07] Chapter 6. We introduce below the concept of shape derivative following what is done in [SZ92], [HP06], and [All07].

We recall that the shape functional we study is defined on a collection of open subset of $\mathbb{R}^n$. Let Ω be such a set. In some sense, we want to explore how behaves the functional $\mathcal{J}$ around the value $\mathcal{J}(\Omega)$, when we slightly "perturb" Ω. For this, we first have to make a choice on the definition of what a perturbation is for Ω, in order to then define a derivative related to this perturbation. To define a perturbation allowing us to calculate derivatives, we generally choose a normed vector space of parameter Θ, and a continuous map Φ from Θ to an affine space $\mathbf{E}$ of map from $\mathbb{R}^n$ into itself (we can say that $\mathbf{E}$ is a set of transformation of $\mathbb{R}^n$), such that $\Phi(0) = \mathrm{id}_{\mathbb{R}^n}$ and Φ is differentiable at 0 (see e.g.,

[MS76]). Thus we can say that $\mathcal{J}$ is *shape differentiable* at Ω (keeping in mind that this definition of shape differentiability depends on Θ, $\mathbf{E}$, and Φ), if we have a neighbourhood V of 0, and a continuous linear map denoted by $D\mathcal{J}(\Omega)$ (or $\mathcal{J}'(\Omega)$) called the "shape derivative" of $\mathcal{J}$ at Ω, such that for all $\theta \in V$:

$$\mathcal{J}(\Phi(\theta)(\Omega)) = \mathcal{J}(\Omega) + D\mathcal{J}(\Omega)(\theta) + o(\|\theta\|_\Theta). \tag{3.172}$$

There exists different ways to define such maps driving to the deformation of the domain. To go further than the fuzzy definition we gave above, we are going to present a classical framework for differentiation with respect to domains (see e.g., [SZ92], [HP06]). First we give the rigorous definition of an appropriate space of transformation of $\mathbb{R}^n$.

Definition 3.10. *We denote by $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ the set of bounded, Lipschitz continuous map from $\mathbb{R}^n$ into itself, endowed with the norm defined for all $\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ by*

$$\|\theta\|_{1,\infty} = \sup_{x,y\in\mathbb{R}^n, x\neq y} \left\{ |\theta(x)| + \frac{|\theta(x) - \theta(y)|}{|x-y|} \right\}. \tag{3.173}$$

The space $W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$ can be identified with the space of $(L^\infty(\mathbb{R}^n))^n$ functions having their gradient in $(L^\infty(\mathbb{R}^n))^{n\times n}$. It will be simply denoted by $W^{1,\infty}$ when there is no ambiguity.

In a general manner, the transformation map is defined as a perturbation of the identity

$$\Phi(\theta) := \mathrm{id}_{\mathbb{R}^n} + \theta, \tag{3.174}$$

for all $\theta \in W^{1,\infty}(\mathbb{R}^n, \mathbb{R}^n)$, such that

$$\|\theta\|_{1,\infty} < 1. \tag{3.175}$$

Such a transformation is then bijective (it is even a Lipschitz homeomorphism from $\mathbb{R}^n$ into itself, with Lipschitz inverse), so that we can define a perturbed domain

$$\Omega_\theta := \Phi(\theta)(\Omega). \tag{3.176}$$

Definition 3.11. *A shape function $\mathcal{J}$ is said to be* shape differentiable *at Ω if the map defined by $\theta \in W^{1,\infty} \mapsto \mathcal{J}(\Omega_\theta)$, where Ω_θ is given by* (3.176)*, is Fréchet differentiable at* 0*. In this case we denote by $D\mathcal{J}(\Omega)$ (or simply $\mathcal{J}'(\Omega)$) the differential of $\mathcal{J}$ at Ω, and we have:*

$$\mathcal{J}(\Omega_\theta) = \mathcal{J}(\Omega) + D\mathcal{J}(\Omega)(\theta) + o(\theta). \tag{3.177}$$

In this manner we have defined a sensitivity of the domain with respect to a vector variable. In practice, it is more simple to make calculation with a real variable. In view of this, for a fixed $\theta \in W^{1,\infty}$, we can define a family of transformations $\Phi(t)$ for $t \in [0, T)$ small enough as follows[2]

$$\Phi(t) = \mathrm{id}_{\mathbb{R}^n} + t\theta. \tag{3.178}$$

For a study of the above transformations we refer to, [MS76], or [Pir84]. An equivalent approach consists in defining Φ as the flux associated to a vector field $V \in C([0, T); W^{1,\infty})$, being the solution of the Cauchy problem $\partial_t \Phi(t) = V(t)$ for all $t \in [0, T)$, $\Phi(0) = \mathrm{id}_{\mathbb{R}^n}$. For

[2] Or more generally we can give a map $\Phi : t \in [0, T[\mapsto \Phi(t) \in \mathrm{id}_{\mathbb{R}^n} + W^{1,\infty}$, differentiable at 0 and such that $\Phi(0) = \mathrm{id}_{\mathbb{R}^n}$.

more details on the general definitions, one can follow the construction given in chapters 8 to 11 of [SZ92]. In definition (3.178), we can call θ the *velocity field*, giving its name to the procedure used to define suitable shape derivative: the *speed method* (also called *velocity method*, or *method of Hadamard*). In some sense, θ plays here the same role as a vector v in the Gateaux differential of a classical vector function $f : \mathbb{R}^d \longrightarrow \mathbb{R}$ given by:

$$\frac{\partial f}{\partial v}(x) = \lim_{t\to 0} \frac{f(x+tv) - f(x)}{t}\,. \tag{3.179}$$

By applying such transformations $\Phi(\theta)$ to our Fluid-Structure interaction problem, we can not ensure that the perturbation $\Phi(\theta)(\Omega_0)$ of Ω_0 will either remain contained in the hold-all domain D, or remain attached to the rigid support ω. We recall that D is a bounded connected open subset of $\mathbb{R}^n$, and ω is an open subset of D such that $\omega \subset\subset \mathrm{D}$ (see Figure 34). Hence we need to restrict the velocity fields θ to a limited class of admissible velocity fields in $W^{1,\infty}$. Let us define the domain

$$\mathrm{D}_\omega = \mathrm{D} \setminus \overline{\omega}, \tag{3.180}$$

such that $\partial\mathrm{D}_\omega = \partial\mathrm{D} \cup \partial\omega$ is piecewise C^k, $k \geq 1$, and we denote by Ξ the set of the singular points of $\partial\mathrm{D}_\omega$. We define a set of admissible vector fields:

$$\Theta^k(\mathrm{D}_\omega) := \Big\{\theta \in C_0^k(\mathbb{R}^2,\mathbb{R}^2) \mid \theta\cdot n = 0 \text{ on } \partial\mathrm{D}_\omega,\ \theta = 0 \text{ on } \Xi\Big\}. \tag{3.181}$$

Finally, fixing a field $\theta \in \Theta^k(\mathrm{D}_\omega)$ we can define the admissible transformations for $t \geq 0$:

$$\Phi(t) = \mathrm{id}_{\mathbb{R}^n} + t\theta \tag{3.182}$$

With this definition, we can view t as the differentiation parameter. For a domain Ω_0 which stands for a reference domain, we define

$$\Omega_{0,t} := \Phi(t)(\Omega_0) \tag{3.183}$$

as being the transformed domain (3.183) (see Figure 35). Thus the shape derivative of the functional $\mathcal{J}(\Omega)$ with respect to the parameter t through the family of transformations $\Phi(t)$ is simply defined by

$$\mathcal{J}(\Omega_{0,t}) = \mathcal{J}(\Omega_0) + t\mathcal{J}'(\Omega_0) + o(t). \tag{3.184}$$

We end this introduction section with the definition of the *material derivative* of a field, with respect to such a perturbation of a domain. Let $(u_t)_{t\geq 0}$ be a family of fields defined on the family of transformed domain $(\Omega_{0,t})_{t\geq 0}$. We want to define what a derivative is with respect to the parameter t for such a family. In order to do this, we first transport u_t on the fixed reference domain $\Omega_{0,t}$, by composing it with the transformation $\Phi(t)$. Thus $u_t \circ \Phi(t)$ is defined on Ω_0. Provided that the following expansion exists, we define the *material derivative* of u_t at 0, denoted by $\dot{u}$, as being the field defined on Ω_0 satisfying

$$u_t \circ \Phi(t) = u_0 + t\dot{u} + o(t), \tag{3.185}$$

where u_0 and $\dot{u}$ do not depend on t. For a more general class of transformation, we should have defined the material derivative of a family of fields $(u_\theta)_\theta$ defined on $\Phi(\theta)(\Omega_0)$, denoted by $\dot{u}(\theta)$, as being the linear form on θ satisfying

$$u_\theta \circ \Phi(\theta) = u_0 + \dot{u}(\theta) + o(\theta). \tag{3.186}$$

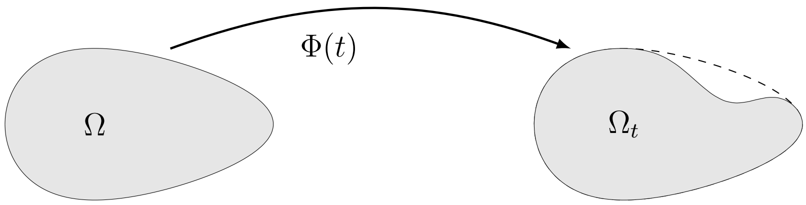

Figure 35: Shape transformation of a domain Ω by the transformation $\Phi(t)$ for $t > 0$. The resulting domain is denoted by Ω_t.

3.4.2 Shape transformation of the FSI problem

First we define for $0 \le t$ small enough the transformation

$$\Phi_t := \mathrm{id}_{\mathbb{R}^n} + tV, \tag{3.187}$$

for a fixed $V \in \Theta^k(\mathrm{D}_\omega)$, $k \ge 1$, with D_ω defined in (3.180), and Θ^k in (3.181). Let us name with the lower index t the new fields and variables induced by the problem written for the domains

$$\Omega_{0,t} := \Phi_t(\Omega_0) \quad \text{and} \quad \Omega^c_{0,t} := \Phi_t(\Omega^c_0), \quad \text{and} \quad \Gamma_{0,t} = \Phi_t(\Gamma_0), \tag{3.188}$$

where Ω_0, defined in Section 3.2, represents the initial shape of the elastic body attached to the rigid support ω, and Ω^c_0 is its open complementary in D_ω (see Figure 36). Let $(\mathrm{u}_t, \mathrm{p}_t, \mathrm{w}_t, \mathrm{s}_t)$ be the unique solution of the coupled Fluid Structure problem posed for the perturbed elastic body $\Omega_{0,t}$ as follows

$$\left\{\begin{array}{rcllr}
-\operatorname{div}\varsigma(\mathrm{u}_t,\mathrm{p}_t) + \boldsymbol{\epsilon}(\mathrm{u}_t\cdot\nabla)\mathrm{u}_t & = & f & \text{in} & \Omega_{F,t},\\
\operatorname{div}\ \mathrm{u}_t & = & 0 & \text{in} & \Omega_{F,t},\\
\mathrm{u}_t & = & 0 & \text{on} & \partial\Omega_{F,t},\\
-\operatorname{div}\Sigma(\mathrm{w}_t) + \nabla s_t & = & g & \text{in} & \Omega_{0,t},\\
\operatorname{div}\mathrm{w}_t & = & 0 & \text{in} & \Omega_{0,t},\\
\mathrm{w}_t & = & 0 & \text{on} & \partial\omega,\\
(\Sigma(\mathrm{w}_t) - \mathrm{s}_t I_d)n_{0,t} & = & (\varsigma(\mathrm{u}_t,\mathrm{p}_t)\circ T_t)\operatorname{cof}(\nabla T_t)n_{0,t} & \text{on} & \Gamma_{0,t},
\end{array}\right. \tag{3.189}$$

where the map T_t is defined by $T_t := \mathrm{id} + \mathrm{w}_t$, and is one to one from $\Omega_{0,t}$ to $\Omega_{S,t}$ for a w_t small enough, and where

$$\Omega_{S,t} := T_t(\Omega_{0,t}), \tag{3.190}$$

$$\Omega_{F,t} := \mathrm{D}_\omega \setminus \overline{\Omega_{S,t}}. \tag{3.191}$$

Thus $\Omega_{S,t}$ and $\Omega_{F,t}$ represent respectively the shape of the elastic body and the incompressible fluid after resolution of the coupled problem.

Before calculating material derivatives with the velocity method in Section 3.4.4, in which we will need to transport the fields onto fixed domain, we have to tackle a first difficulty. The families of fluid velocity and pressure fields $(\mathrm{u}_t, \mathrm{p}_t)_{t\ge 0}$ are defined on domains $\Omega_{F,t}$ depending on t, which are furthermore unknown because they depend on the family of displacement w_t. Therefore we want to transport fluid equations onto the reference configurations $\Omega^c_{0,t}$. For this, we apply what we have done at the end of Section 3.2.1. Let us consider a linear lifting $\mathcal{R}_t$:

$$\mathcal{R}_t \ : \ H^{3-1/2}(\Gamma_{0,t}) \longrightarrow H^3(\Omega^c_{0,t}), \tag{3.192}$$

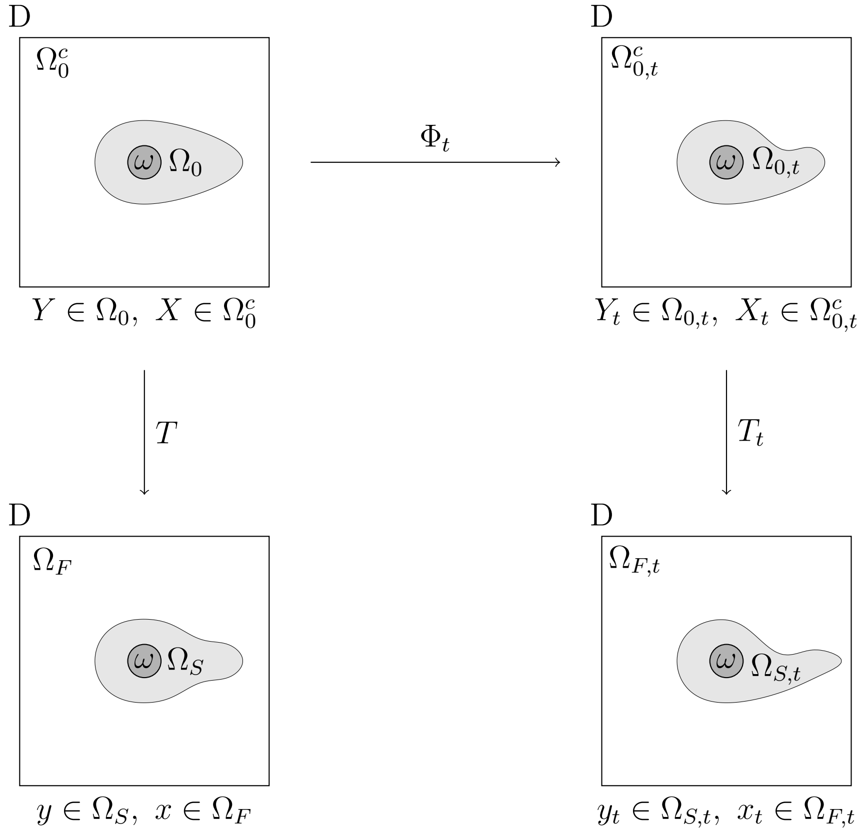

Figure 36: The geometries of the fluid-elasticity system submitted to transformation Φ_t and the resolution of the coupled problems, characterised by T_t.

and the Trace map

$$\gamma_t \ : \ H^3(\Omega_{0,t}) \longrightarrow H^{3-1/2}(\Gamma_{0,t}), \tag{3.193}$$

in such a way that we can introduce the following map defined on $\Omega_{0,t}^c$:

$$T_t := \mathrm{id} + \mathcal{R}_t(\gamma_t(\mathrm{w}_t)), \tag{3.194}$$

which is one to one from $\Omega_{0,t}^c$ to $\Omega_{F,t}$ for a w_t small enough. Thus we have defined a bijective map $T_t : \Omega_{0,t} \times \Omega_{0,t}^c \to \Omega_{S,t} \times \Omega_{F,t}$. For $t = 0$ (*i.e.* the coupled problem posed on the initial elastic domain Ω_0), all the fields and domains are written without the lower index t. The names of spatial variables depend on the domains they are related with, and are defined Figure 36. By defining T_t this way, the difficulty we meet is the following. The operator $\mathcal{R}_t$ and γ_t we deal with depend on t. To overcome this, we favor another definition of T_t.

New definition of T. We recall that for all $0 \leq t$, w_t is the solution displacement of the fluid-structure problem, belonging to $H^3(\Omega_{0,t})$. T_t was defined by $T_t = \mathrm{id} - \mathcal{R}_t(\gamma_t(\mathrm{w}_t))$, which can be represented this way:

$$\begin{tikzcd} H^3(\Omega_{0,t}) \arrow[r, "\gamma_t"] \arrow[dr, "T_t - Id"'] & H^{3-1/2}(\Gamma_{0,t}) \arrow[d, "\mathcal{R}_t"] \\ & H^3(\Omega_{0,t}^c) \end{tikzcd} \tag{3.195}$$

Now wet set a new definition for T_t

$$T_t = \mathrm{id} + \mathcal{R}(\gamma(\mathrm{w}_t \circ \Phi_t)) \circ \Phi_t^{-1}, \tag{3.196}$$

where Φ_t is defined in (3.187), and $\mathcal{R}$ and γ are respectively the lifting and trace operators which do not depend on t any more, and are defined by

$$\mathcal{R} \ : \ H^{3-1/2}(\Gamma_0) \longrightarrow H^3(\Omega_0^c), \tag{3.197}$$

and

$$\gamma \ : \ H^3(\Omega_0) \longrightarrow H^{3-1/2}(\Gamma_0). \tag{3.198}$$

We can represent T_t as follows

$$\begin{tikzcd} H^3(\Omega_{0,t}) \arrow[r, "\circ\Phi_t"] \arrow[dr, "T_t-\mathrm{id}"'] & H^3(\Omega_0) \arrow[r, "\gamma"] & H^{3-1/2}(\Gamma_0) \arrow[d, "\mathcal{R}"] \\ & H^3(\Omega_{0,t}^c) & H^3(\Omega_0^c) \arrow[l, "\circ\Phi_t^{-1}"'] \end{tikzcd} \tag{3.199}$$

3.4.3 Formulation in a fixed domain

Now we can write the variational formulation of the Navier-Stokes system written on $\Omega_{F,t}$ defined in (3.191), and then we transport it onto the reference domain $\Omega_{0,t}^c$, in the same way as in [Gra02]. Let $(\mathrm{u}_t, \mathrm{p}_t, \mathrm{w}_t, \mathrm{s}_t)$ be the solution of (3.189). We recall that $\varsigma(\mathrm{u}_t, \mathrm{p}_t) := 2\nu\nabla^s \mathrm{u}_t - \mathrm{p}_t \mathrm{I}$, and because of the incompressibility condition (if u_t is regular enough), we have $\mathrm{div}(\nabla \mathrm{u}_t^\top) = \nabla(\mathrm{div}\, \mathrm{u}_t) = 0$, so that $\mathrm{div}\, \varsigma(\mathrm{u}_t, \mathrm{p}_t) = \mathrm{div}(\nu\nabla \mathrm{u}_t - \mathrm{p}_t \mathrm{I})$. We have that $\mathrm{u}_t \in (H_0^1(\Omega_{F,t}))^2$ and $\mathrm{p}_t \in L^2(\Omega_{F,t})$ satisfies for all $\tilde{z} \in (H_0^1(\Omega_{F,t}))^2$ and for all $\tilde{\beta} \in L^2(\Omega_{F,t})$:

$$\begin{cases} \nu \displaystyle\int_{\Omega_{F,t}} \nabla \mathrm{u}_t \cdot \nabla \tilde{z} - \int_{\Omega_{F,t}} \mathrm{p}_t \,\mathrm{div}(\tilde{z}) + \int_{\Omega_{F,t}} \boldsymbol{\epsilon}(\mathrm{u}_t \cdot \nabla)\mathrm{u}_t \cdot \tilde{z} = \int_{\Omega_{F,t}} f \cdot \tilde{z}, \\ \displaystyle\int_{\Omega_{F,t}} \tilde{\beta}\, \mathrm{div}(\mathrm{u}_t) = 0. \end{cases} \tag{3.200}$$

We define

$$\mathrm{v}_t := \mathrm{u}_t \circ T_t, \tag{3.201}$$

$$\mathrm{q}_t := \mathrm{p}_t \circ T_t, \tag{3.202}$$

where T_t is defined in (3.196). We set $\tilde{z} = z \circ T_t^{-1}$ and $\tilde{\beta} = \beta \circ T_t^{-1}$ in equation (3.200), where $z \in (H_0^1(\Omega_{0,t}^c))^2$ and $\beta \in L^2(\Omega_{0,t}^c)$. We obtain with a change of variable T_t that $(\mathrm{v}_t, \mathrm{q}_t)$ satisfies the following problem:

$$\begin{cases} \text{Find } (\mathrm{v}_t, \mathrm{q}_t) \in (H_0^1(\Omega_{0,t}^c))^2 \times L^2(\Omega_{0,t}^c) \text{ such that for all } (z, \beta) \in (H_0^1(\Omega_{0,t}^c))^2 \times L^2(\Omega_{0,t}^c): \\ \nu \displaystyle\int_{\Omega_{0,t}^c} \nabla(\mathrm{v}_t) F(T_t) \cdot \nabla z - \int_{\Omega_{0,t}^c} \mathrm{q}_t (G(T_t) \cdot \nabla z) + \int_{\Omega_{0,t}^c} \boldsymbol{\epsilon}(\mathrm{v}_t \cdot G(T_t)\nabla)\mathrm{v}_t \cdot z = \int_{\Omega_{0,t}^c} f_t J(T_t) \cdot z, \\ \displaystyle\int_{\Omega_{0,t}^c} \beta(G(T_t) \cdot \nabla \mathrm{v}_t) = 0, \end{cases} \tag{3.203}$$

where $f_t := f \circ T_t$ and

$$F(T_t) = (\nabla T_t)^{-1} \,\mathrm{cof}(\nabla T_t), \tag{3.204}$$

$$G(T_t) = \mathrm{cof}(\nabla T_t), \tag{3.205}$$

$$J(T_t) = \det(\nabla T_t). \tag{3.206}$$

Problem (3.203) is related to the following boundary value problem:

$$\begin{cases} -\nu \operatorname{div}((\nabla \mathrm{v}_t) F(T_t)) + G(T_t)\nabla \mathrm{q}_t + \boldsymbol{\epsilon}(\mathrm{v}_t \cdot G(T_t)\nabla)\mathrm{v}_t = (f \circ T_t)J(T_t) & \text{in } \Omega^c_{0,t}, \\ \operatorname{div}(G(T_t)^\top \mathrm{v}_t) = 0 & \text{in } \Omega^c_{0,t}, \\ \mathrm{v}_t = 0 & \text{on } \Gamma_{0,t}. \end{cases} \tag{3.207}$$

With these definitions of v_t and q_t given in (3.201) and (3.202), we can compute as we did in Section 3.2.2 the surface force applied on the structure and depending on these new variables. This gives

$$(\varsigma(\mathrm{u}_t, \mathrm{p}_t) \circ T_t)\,\mathrm{cof}(\nabla T_t) n_{0,t} = (\nu(\nabla \mathrm{v}_t)F(T_t) - \mathrm{q}_t G(T_t)) n_{0,t} \quad \text{on } \Gamma_{0,t}. \tag{3.208}$$

Thus we find the complete Fluid Structure Interaction problem for $(\mathrm{v}_t, \mathrm{q}_t, \mathrm{w}_t, \mathrm{s}_t)$,

$$\left\{ \begin{array}{rcllr} -\nu \operatorname{div}((\nabla \mathrm{v}_t)F(T_t)) + G(T_t)\nabla \mathrm{q}_t & = & (f \circ T_t)J(T_t) & \text{in} & \Omega^c_{0,t}, \\ \operatorname{div}(G(T_t)^\top \mathrm{v}_t) & = & 0 & \text{in} & \Omega^c_{0,t}, \\ \mathrm{v}_t & = & 0 & \text{on} & \partial\Omega^c_{0,t}, \\ -\operatorname{div} \sigma(\mathrm{w}_t) + \nabla \mathrm{s}_t & = & g & \text{in} & \Omega_{0,t}, \\ \operatorname{div} \mathrm{w}_t & = & 0 & \text{in} & \Omega_{0,t}, \\ \mathrm{w}_t & = & 0 & \text{on} & \partial\omega, \\ (\sigma(\mathrm{w}_t) - \mathrm{s}_t \mathrm{I}) n_{0,t} & = & \nu(\nabla \mathrm{v}_t)F(T_t) n_{0,t} & & \\ & & -\mathrm{q}_t G(T_t) n_{0,t} & \text{on} & \Gamma_{0,t}. \end{array} \right. \tag{3.209}$$

In the next section, we calculate formally the problems satisfied by the material derivatives of $(\mathrm{v}_t, \mathrm{q}_t, \mathrm{w}_t, \mathrm{s}_t)$.

3.4.4 Material derivatives of solutions

In this section we investigate the form of the boundary value problems that must be satisfied by the material derivatives of the family of solutions $(\mathrm{v}_t, \mathrm{q}_t, \mathrm{w}_t, \mathrm{s}_t)$. As we have seen in the introduction of Section 3.4, we need to transport the fields which are defined on the transformed domains $\Omega_{0,t}$ and $\Omega^c_{0,t}$ onto the reference domains Ω_0 and Ω^c_0.

3.4.4.1 Fluid equations

In Section 3.4.3, we have written the Navier-Stokes equation transported onto the reference domain $\Omega^c_{0,t}$, by setting new variables $\mathrm{v}_t = \mathrm{u}_t \circ T_t$ and $\mathrm{p}_t = \mathrm{q}_t \circ T_t$ (see (3.201) and (3.202)). We obtained the following problem: find $(\mathrm{v}_t, \mathrm{q}_t) \in (H^1_0(\Omega^c_{0,t}))^2 \times L^2_0(\Omega^c_{0,t})$ such that for all test functions $(\mathfrak{v}, \mathfrak{q}) \in (H^1_0(\Omega^c_{0,t}))^2 \times L^2_0(\Omega^c_{0,t})$

$$\begin{cases} \nu \displaystyle\int_{\Omega^c_{0,t}} \nabla(\mathrm{v}_t) F(T_t) \cdot \nabla \mathfrak{v} - \int_{\Omega^c_{0,t}} \mathrm{q}_t (G(T_t) \cdot \nabla \mathfrak{v}) + \int_{\Omega^c_{0,t}} \boldsymbol{\epsilon}(\mathrm{v}_t \cdot G(T_t)\nabla)\mathrm{v}_t \cdot \mathfrak{v} = \langle f_t J(T_t), \mathfrak{v} \rangle_{H^{-1}, H^1_0}, \\ \displaystyle\int_{\Omega^c_{0,t}} \mathfrak{q}(G(T_t) \cdot \nabla \mathrm{v}_t) = 0, \end{cases} \tag{3.210}$$

where we recall that $F(T_t) = (\nabla T_t)^{-1}\operatorname{cof}(\nabla T_t)$, $G(T_t) = \operatorname{cof}(\nabla T_t)$, and $J(T_t) = \det(\nabla T_t)$ (see (3.204), (3.205), and (3.206)), with T_t defined equation (3.196) for w_t being the displacement solution of the structure part of problem (3.209). We define for all $\mathrm{v}, \mathfrak{v}$ in $(H_0^1(\Omega_{0,t}^c))^2$ and for all q in $L_0^2(\Omega_{0,t}^c)$:

$$a_{F,t}(\mathrm{w}_t; \mathrm{v}, \mathfrak{v}) := \nu \int_{\Omega_{0,t}^c} \nabla(\mathrm{v})F(T_t) \cdot \nabla\mathfrak{v} + \int_{\Omega_{0,t}} \boldsymbol{\epsilon}(\mathrm{v} \cdot G(T_t)\nabla)\mathrm{v} \cdot \mathfrak{v}, \tag{3.211}$$

$$b_{F,t}(\mathrm{w}_t; \mathfrak{v}, \mathrm{q}) := -\int_{\Omega_{0,t}^c} \mathrm{q}(G(T_t) \cdot \nabla\mathfrak{v}), \tag{3.212}$$

$$f_{F,t}(\mathrm{w}_t; \mathfrak{v}) := \int_{\Omega_{0,t}^c} J(T_t) f \circ T_t \cdot \mathfrak{v}, \tag{3.213}$$

so that (3.210) can be written

$$\begin{cases} \text{Find } (\mathrm{v}_t, \mathrm{q}_t) \text{ in } (H_0^1(\Omega_{0,t}^c))^2 \times L_0^2(\Omega_{0,t}^c) \text{ such that:} \\ a_{F,t}(\mathrm{w}_t; \mathrm{v}_t, \mathfrak{v}) + b_{F,t}(\mathrm{w}_t; \mathfrak{v}, \mathrm{q}_t) = f_{F,t}(\mathrm{w}_t; \mathfrak{v}), \quad \forall \mathfrak{v} \in (H_0^1(\Omega_{0,t}^c))^2, \\ \qquad b_{F,t}(\mathrm{w}_t; \mathrm{v}_t, \mathfrak{q}) = 0, \quad \forall \mathfrak{q} \in L_0^2(\Omega_{0,t}^c). \end{cases} \tag{3.214}$$

Let us define

$$\mathfrak{g}_t := \det(\nabla\Phi_t), \tag{3.215}$$

and

$$\mathfrak{J}_t := \nabla\Phi_t, \tag{3.216}$$

where Φ_t is defined in (3.187). Let $(\mathfrak{v}, \mathfrak{q}) \in (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c)$. We rewrite the problem (3.210) with the test functions $(\mathfrak{v} \circ \Phi_t^{-1}, (\mathfrak{g}_t^{-1}\mathfrak{q}) \circ \Phi_t^{-1})$, where Φ_t is defined by (3.187) and is such that $\Phi_t(\Omega_0^c) = \Omega_{0,t}^c$. We have the following relations

$$\mathfrak{J}_t^{-1}(F(T_t) \circ \Phi_t)\mathfrak{J}_t^{-\top}\mathfrak{g}_t = F(T_t \circ \Phi_t) \tag{3.217}$$

$$G(T_t) \circ \Phi_t \mathfrak{J}_t^{-\top}\mathfrak{g}_t = G(T_t \circ \Phi_t) \tag{3.218}$$

$$J(T_t) \circ \Phi_t \mathfrak{g}_t = J(T_t \circ \Phi_t), \tag{3.219}$$

where $\mathfrak{g}_t$ and $\mathfrak{J}_t$ are defined in (3.215) and (3.216). Then we transport the integrals from (3.210) onto Ω_0^c by means of the change of variable $X_t = \Phi_t(X)$. After a simplification using (3.217), (3.218), and (3.219), we obtain

$$\begin{cases} \nu \displaystyle\int_{\Omega_0^c} \nabla(\mathrm{v}_t \circ \Phi_t)F(T_t \circ \Phi_t) \cdot \nabla\mathfrak{v} - \int_{\Omega_0^c} (\mathrm{q}_t \circ \Phi_t)(G(T_t \circ \Phi_t) \cdot \nabla\mathfrak{v}) \\ \qquad + \displaystyle\int_{\Omega_0^c} \boldsymbol{\epsilon}(\mathrm{v}_t \circ \Phi_t \cdot G(T_t \circ \Phi_t)\nabla)\mathrm{v}_t \circ \Phi_t \cdot \mathfrak{v} = \int_{\Omega_0^c} J(T_t \circ \Phi_t) f \circ T_t \circ \Phi_t \cdot \mathfrak{v}, \\ \displaystyle\int_{\Omega_0^c} (G(T_t \circ \Phi_t) \cdot \nabla\mathrm{v}_t)\mathfrak{q}\, \mathfrak{g}_t^{-1} = 0. \end{cases} \tag{3.220}$$

We define for all $\mathrm{v}, \mathfrak{v}$ in $H_0^1(\Omega_0^c)$ and for all q in $L_0^2(\Omega_0^c)$:

$$a_F^t(\mathrm{w}_t; \mathrm{v}, \mathfrak{v}) := \nu \int_{\Omega_0^c} \nabla(\mathrm{v})F(T_t \circ \Phi_t) \cdot \nabla\mathfrak{v} + \int_{\Omega_0} \boldsymbol{\epsilon}(\mathrm{v} \cdot G(T_t \circ \Phi_t)\nabla)\mathrm{v} \cdot \mathfrak{v}, \tag{3.221}$$

$$b_F^t(\mathrm{w}_t; \mathfrak{v}, \mathrm{q}) := -\int_{\Omega_0^c} \mathrm{q}(G(T_t \circ \Phi_t) \cdot \nabla\mathfrak{v})\mathfrak{g}_t^{-1}, \tag{3.222}$$

$$f_F^t(\mathrm{w}_t; \mathfrak{v}) := \int_{\Omega_0^c} J(T_t \circ \Phi_t) f \circ T_t \circ \Phi_t \cdot \mathfrak{v}, \tag{3.223}$$

and we introduce

$$\mathrm{v}_t := \mathrm{v}^t \circ \Phi_t^{-1}, \tag{3.224}$$

$$\mathrm{q}_t := \mathfrak{g}_t^{-1}\mathrm{q}^t \circ \Phi_t^{-1}, \tag{3.225}$$

Then (3.220) can be written for v^t and q^t as follows

$$\begin{cases} \text{Find } (\mathrm{v}^t, \mathrm{q}^t) \text{ in } (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \text{ such that:} \\ a_F^t(\mathrm{w}_t; \mathrm{v}^t, \mathfrak{v}) + b_F^t(\mathrm{w}_t; \mathfrak{v}, \mathrm{q}^t) = f_F^t(\mathrm{w}_t; \mathfrak{v}), \quad \forall \mathfrak{v} \in (H_0^1(\Omega_0^c))^2, \\ \qquad b_F^t(\mathrm{w}_t; \mathrm{v}^t, \mathfrak{q}) = 0, \quad \forall \mathfrak{q} \in L_0^2(\Omega_0^c). \end{cases} \tag{3.226}$$

We denote by $\dot{T}$ the the material derivative of T_t defined by

$$\dot{T}(X) = \frac{d}{dt}\bigg|_{t=0} (T_t \circ \Phi_t(X)) \quad \forall X \in \mathrm{D}, \tag{3.227}$$

and by V the *velocity field* of the transformation given by, according to (3.187),

$$V(X) = \frac{d}{dt}\bigg|_{t=0} (\Phi_t(X)), \quad \forall X \in \mathrm{D}. \tag{3.228}$$

We have that

$$\frac{d}{dt}\bigg|_{t=0} \det(\nabla\Phi_t) = \operatorname{div} V \quad \text{ and } \quad \frac{d}{dt}\bigg|_{t=0} \det(\nabla(\Phi_t^{-1}) = -\operatorname{div} V, \tag{3.229}$$

from the definition of Φ_t in (3.187), and differentiation formula given in Appendix 3.7 equation (3.360). Now we can derivate this problem with respect to the variable t, and evaluate at $t = 0$. We introduce the following bilinear et linear forms (the map $a'_F(v, \mathfrak{v})$ is not linear with respect to v in the case $\boldsymbol{\epsilon} = 1$, i.e. with the Navier-Stokes equations)

$$a'_F(v, \mathfrak{v}) = \nu \int_{\Omega_0^c} (\nabla v) DF(\dot{T}) \cdot \nabla\mathfrak{v} + \int_{\Omega_{0,t}} \boldsymbol{\epsilon}(v \cdot DG(\dot{T})\nabla) v \cdot \mathfrak{v}, \tag{3.230}$$

$$b'_F(\mathrm{q}, \mathfrak{v}) = -\int_{\Omega_0^c} \mathrm{q}((DG(\dot{T}) - (\operatorname{div} V) G(T)) \cdot \nabla\mathfrak{v}), \tag{3.231}$$

$$l'_F(\mathfrak{v}) = \int_{\Omega_0^c} \Big(J(T)(\nabla(f)\circ T)\dot{T} + DJ(\dot{T}) f\circ T\Big) \cdot \mathfrak{v}, \tag{3.232}$$

where

$$T = T_0, \quad \text{ i.e. at } t = 0, \tag{3.233}$$

and where $DF(\dot{T})$, $DG(\dot{T})$, and $DJ(\dot{T})$ are computed in Appendix 3.7 Section 3.7.1, and given by expressions (3.371), (3.372), and (3.373). Namely

$$DF(\dot{T}) = \frac{d}{dt}\bigg|_{t=0} (F(T_t)) = \operatorname{cof}(\nabla T)^\top \left[\operatorname{tr}\left((\nabla T)^{-1}\nabla\dot{T}\right) \mathrm{I} - 2[\nabla\dot{T}(\nabla T)^{-1}]^s\right] (\nabla T)^{-\top}, \tag{3.234}$$

$$DG(\dot{T}) = \frac{d}{dt}\bigg|_{t=0} (G(T_t)) = \operatorname{cof}(\nabla T) \left[\operatorname{tr}\left((\nabla T)^{-1}\nabla\dot{T}\right) \mathrm{I} - [(\nabla T)^{-1}\nabla\dot{T}]^\top\right], \tag{3.235}$$

$$DJ(\dot{T}) = \frac{d}{dt}\bigg|_{t=0} (J(T_t)) = \operatorname{tr}(\operatorname{cof}(\nabla T)^\top \nabla\dot{T}). \tag{3.236}$$

By defining the material derivates $\dot{\mathrm{v}}$ and $\dot{\mathrm{q}}$ by

$$\dot{\mathrm{v}} := \frac{d}{dt}\Big|_{t=0}(\mathrm{v}^t) = \frac{d}{dt}\Big|_{t=0}(\mathrm{v}_t \circ \Phi_t), \tag{3.237}$$

$$\dot{\mathrm{q}} := \frac{d}{dt}\Big|_{t=0}(\mathrm{q}^t) = \frac{d}{dt}\Big|_{t=0}(\mathfrak{g}_t\ \mathrm{q}_t \circ \Phi_t), \tag{3.238}$$

we have that the material derivatives $\dot{\mathrm{v}}$ and $\dot{\mathrm{q}}$ satisfy the following problem

$$\begin{cases} \text{Find } (\dot{\mathrm{v}}, \dot{\mathrm{q}}) \in (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \text{ such that for all } (\mathfrak{v}, \mathfrak{q}) \in (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c)\text{:} \\ \nu \displaystyle\int_{\Omega_0^c} (\nabla\dot{\mathrm{v}})F(T)\cdot\nabla\mathfrak{v} - \int_{\Omega_0^c} \dot{\mathrm{q}}(G(T)\cdot\nabla\mathfrak{v}) + \int_{\Omega_0^c} \boldsymbol{\epsilon}[(\dot{\mathrm{v}}\cdot G(T)\nabla)\mathrm{v} + (\mathrm{v}\cdot G(T)\nabla)\dot{\mathrm{v}}]\cdot\mathfrak{v} \\ \qquad\qquad\qquad\qquad\qquad\qquad = l'_F(\mathfrak{v}) - a'_F(\mathrm{v},\mathfrak{v}) - b'_F(\mathrm{q},\mathfrak{v}), \\ \displaystyle\int_{\Omega_0^c} [(DG(\dot{T}) - (\operatorname{div} V)G(T))\cdot\nabla\mathrm{v} + G(T)\cdot\nabla\dot{\mathrm{v}}]\mathfrak{q} = 0, \end{cases} \tag{3.239}$$

where a'_F, b'_F, l'_F are given in (3.230), (3.231), and (3.232), and depend on T and $\dot{T}$.

3.4.4.2 Incompressible Elasticity

With the notations introduced right above, the surface force applied by the fluid on the structure can be expressed with respect to v_t and q_t by $(\nu(\nabla\mathrm{v}_t)F(T_t) - \mathrm{q}_t G(T_t))n_{0,t}$ according to expression (3.208). Let us then write the variational formulation of the structure problem.

$$\begin{cases} \text{Find } (\mathrm{w}_t, \mathrm{s}_t) \in (H^1(\Omega_{0,t}))^2 \times L_0^2(\Omega_{0,t}) \text{ with } \mathrm{w}_t = 0 \text{ on } \partial\omega \text{ such that:} \\ \displaystyle\int_{\Omega_{0,t}} \sigma(\mathrm{w}_t)\cdot\nabla^s\mathfrak{w} - \int_{\Omega_{0,t}} \mathrm{s}_t \operatorname{div}\mathfrak{w} = \int_{\Omega_{0,t}} g\cdot\mathfrak{w} + \int_{\Gamma_{0,t}} \mathfrak{w}\cdot(\nu(\nabla\mathrm{v}_t)F(T_t) - \mathrm{q}_t G(T_t))n_{0,t}d\Gamma_{0,t} \\ \qquad\qquad\qquad\qquad\qquad\qquad \forall\mathfrak{w} \in (H^1(\Omega_{0,t}))^2 \text{ with } \mathfrak{w} = 0 \text{ on } \partial\omega, \\ \displaystyle\int_{\Omega_{0,t}} \mathfrak{s}\operatorname{div}\mathrm{w}_t = 0, \quad \forall\mathfrak{s} \in L_0^2(\Omega_{0,t}). \end{cases} \tag{3.240}$$

By defining

$$a_{S,t}(\mathrm{w}_t, \mathfrak{w}) = \int_{\Omega_{0,t}} \sigma(\mathrm{w}_t)\cdot\nabla^s\mathfrak{w}, \tag{3.241}$$

$$b_{S,t}(\mathfrak{w}, \mathrm{s}_t) = \int_{\Omega_{0,t}} \mathrm{s}_t \operatorname{div}\mathfrak{w}, \tag{3.242}$$

$$f_{S,t}(\mathrm{w}_t; \mathrm{v}_t; \mathrm{q}_t; \mathfrak{w}) = \int_{\Omega_{0,t}} g\cdot\mathfrak{w} + \int_{\Gamma_{0,t}} \mathfrak{w}\cdot(\nu(\nabla\mathrm{v}_t)F(T_t) - \mathrm{q}_t G(T_t))n_{0,t}d\Gamma_{0,t}, \tag{3.243}$$

we can rewrite problem (3.240) as follows

$$\begin{cases} \text{Find } (\mathrm{w}_t, \mathrm{s}_t) \in (H^1(\Omega_{0,t}))^2 \times L_0^2(\Omega_{0,t}) \text{ with } \mathrm{w}_t = 0 \text{ on } \partial\omega \text{ such that:} \\ a_{S,t}(\mathrm{w}_t, \mathfrak{w}) + b_{S,t}(\mathfrak{w}, \mathrm{s}_t) = f_{S,t}(\mathrm{w}_t; \mathrm{v}_t; \mathrm{q}_t; \mathfrak{w}), \quad \forall\mathfrak{w} \in (H^1(\Omega_{0,t}))^2 \text{ with } \mathfrak{w} = 0 \text{ on } \partial\omega, \\ b_{S,t}(\mathrm{w}_t, \mathfrak{s}) = 0, \quad \forall\mathfrak{s} \in L_0^2(\Omega_{0,t}). \end{cases} \tag{3.244}$$

We want to derivate this problem with respect to t. For this purpose, let $(\mathfrak{w}, \mathfrak{s})$ be in $(H^1(\Omega_0))^2 \times L_0^2(\Omega_0)$. We insert $(\mathfrak{w}\circ\Phi_t^{-1}, (\mathfrak{g}_t^{-1}\mathfrak{s})\circ\Phi_t^{-1})$ as test functions into (3.240), where $\mathfrak{g}_t$is defined in (3.215), and then we transport the integrals onto Ω_0 or Γ_0 by means of the change of variable $Y_t = \Phi_t(Y)$. We recall that we have (see e.g. [Cia88]):

$$n_{0,t} d\Gamma_{0,t} = [\det(\nabla\Phi_t)\nabla\Phi_t^{-\top} n_0] d\Gamma_0, \tag{3.245}$$

where $d\Gamma_0$ and $d\Gamma_{0,t}$ are the length elements of the surfaces Γ_0 and $\Gamma_{0,t}$ respectively, and n_0 and $n_{0,t}$ are the normal vectors to Γ_0 and $\Gamma_{0,t}$ respectively. We also recall that $\mathrm{v}_t = \mathrm{v}^t \circ \Phi_t^{-1}$ (see expression (3.224)), and consequently we have

$$\nabla \mathrm{v}_t = (\nabla \mathrm{v}^t)\mathfrak{J}^{-1}, \tag{3.246}$$

where $\mathfrak{J}_t$ is defined in (3.216). Thus the surface term in (3.240) is transported as follows

$$\begin{aligned}\int_{\Gamma_{0,t}} &\mathfrak{w} \circ \Phi_t^{-1} \cdot (\nu(\nabla \mathrm{v}_t)F(T_t) - \mathrm{q}_t G(T_t)) n_{0,t} d\Gamma_{0,t} = \\ &\int_{\Gamma_0} \mathfrak{w} \cdot (\nu(\nabla \mathrm{v}^t)\mathfrak{J}^{-1}(F(T_t)\circ\Phi_t)\mathfrak{J}^{-\top}\mathfrak{g}_t - \mathfrak{g}_t^{-1}\mathrm{q}^t(G(T_t)\circ\Phi_t)\mathfrak{g}_t\mathfrak{J}_t^{-\top}) n_0 d\Gamma_0,\end{aligned} \tag{3.247}$$

where we recall that (see (3.202))

$$\mathrm{q}_t \circ \Phi_t = \mathfrak{g}_t^{-1}\mathrm{q}^t. \tag{3.248}$$

In view of (3.217) and (3.218) we have that $\mathfrak{J}_t^{-1}(F(T_t)\circ\Phi_t)\mathfrak{J}_t^{-\top}\mathfrak{g}_t = F(T_t\circ\Phi_t)$ and $G(T_t)\circ\Phi_t\mathfrak{J}_t^{-\top}\mathfrak{g}_t = G(T_t\circ\Phi_t)$. Hence from (3.247) we have

$$\begin{aligned}\int_{\Gamma_{0,t}} &\mathfrak{w} \circ \Phi_t^{-1} \cdot (\nu(\nabla \mathrm{v}_t)F(T_t) - \mathrm{q}_t G(T_t)) n_{0,t} d\Gamma_{0,t} = \\ &\int_{\Gamma_0} \mathfrak{w} \cdot (\nu(\nabla \mathrm{v}^t)F(T_t\circ\Phi_t) - \mathfrak{g}_t^{-1}\mathrm{q}^t G(T_t\circ\Phi_t)) n_0 d\Gamma_0.\end{aligned} \tag{3.249}$$

This brings us to define, for all $\mathrm{w}, \mathfrak{w}$ in $(H^1_{0,\partial\omega}(\Omega_0))^2$, where $H^1_{0,\partial\omega}(\Omega_0)$ is defined by

$$H^1_{0,\partial\omega}(\Omega_0) := \{u \in H^1(\Omega_0) \mid u = 0 \text{ on } \partial\omega\}, \tag{3.250}$$

and for all s in $L^2_0(\Omega_0)$:

$$a^t_S(\mathrm{w},\mathfrak{w}) = \int_{\Omega_0} \mathbf{C}[(\nabla \mathrm{w})\mathfrak{J}_t^{-1}]^s \cdot [(\nabla\mathfrak{w})\mathfrak{J}_t^{-1}]^s \mathfrak{g}_t, \tag{3.251}$$

$$b^t_S(\mathfrak{w},\mathrm{s}) = -\int_{\Omega_0} \mathrm{s}(\mathrm{I}\cdot(\nabla\mathfrak{w})\mathfrak{J}_t^{-1}), \tag{3.252}$$

$$f^t_S(\mathrm{w};\mathrm{v};\mathrm{q};\mathfrak{w}) = \int_{\Omega_0} g\circ\Phi_t\cdot\mathfrak{w} + \int_{\Gamma_0} \mathfrak{w}\cdot(\nu(\nabla \mathrm{v})F(T_t\circ\Phi_t) - \mathrm{q}G(T_t\circ\Phi_t)\mathfrak{g}_t^{-1}) n_0, \tag{3.253}$$

where for a matrix A, its symmetric part A^s is defined in (3.62). We write (3.240) with

$$\mathrm{w}_t := \mathrm{w}^t \circ \Phi_t^{-1}, \tag{3.254}$$

$$\mathrm{s}_t := \mathfrak{g}_t^{-1}\mathrm{s}^t \circ \Phi_t^{-1}, \tag{3.255}$$

where w^t and s^t are solutions of

$$\begin{cases}\text{Find } (\mathrm{w}^t,\mathrm{s}^t) \text{ in } (H^1_{0,\partial\omega}(\Omega_0))^2 \times L^2_0(\Omega_0) \text{ such that:} \\ a^t_S(\mathrm{w}^t,\mathfrak{w}) + b^t_S(\mathfrak{w},\mathrm{s}^t) = f^t_S(\mathrm{w}^t;\mathrm{v}^t;\mathrm{q}^t;\mathfrak{w}), \quad \forall\mathfrak{w}\in(H^1_{0,\partial\omega}(\Omega_0))^2, \\ \qquad b^t_S(\mathrm{w}^t,\mathfrak{s}) = 0, \quad \forall\mathfrak{s}\in L^2_0(\Omega_0),\end{cases} \tag{3.256}$$

with v^t and q^t solutions of (3.226).

Afterwards we can differentiate this problem with respect to t. Recalling that $\sigma(\mathrm{w}) = \mathbf{C}\nabla^s\mathrm{w}$ (see (3.22)-(3.23)), we define the useful bilinear and linear forms:

$$a'_S(\mathrm{w}, \mathfrak{w}) = \int_{\Omega_0} (\sigma(\mathrm{w}) \cdot \nabla^s \mathfrak{w}) \operatorname{div} V - \mathbf{C}(\nabla \mathrm{w} \nabla V)^s \cdot \nabla^s \mathfrak{w} - \sigma(\mathrm{w}) \cdot (\nabla \mathfrak{w} \nabla V)^s \, dY, \quad (3.257)$$

$$l'_S(\mathfrak{w}) = \int_{\Omega_0} (g \operatorname{div} V + \nabla g V) \cdot \mathfrak{w} \, dY, \quad (3.258)$$

$$b'_S(\mathrm{s}, \mathfrak{w}) = -\int_{\Omega_0} \mathrm{s} \left[-(I \cdot \nabla \mathfrak{w} \nabla V) \right] dY, \quad (3.259)$$

where V is defined in (3.228). We define the material derivatives $\dot{\mathrm{w}}$ and $\dot{\mathrm{s}}$ as follows:

$$\dot{\mathrm{w}} := \frac{d}{dt}\Big|_{t=0} (\mathrm{w}^t) = \frac{d}{dt}\Big|_{t=0} (\mathrm{w}_t \circ \Phi_t), \quad (3.260)$$

$$\dot{\mathrm{s}} := \frac{d}{dt}\Big|_{t=0} (\mathrm{s}^t) = \frac{d}{dt}\Big|_{t=0} (\mathfrak{g}_t \, \mathrm{s}_t \circ \Phi_t). \quad (3.261)$$

From the definitions of T_t in (3.196) and of $\dot{T}$ in (3.227), we have

$$\dot{T} = V + \mathcal{R}\gamma(\dot{\mathrm{w}}). \quad (3.262)$$

It remains to derivate with respect to t the term in (3.249)

$$\int_{\Gamma_0} \mathfrak{w} \cdot (\nu(\nabla \mathrm{v}^t) F(T_t \circ \Phi_t) - \mathfrak{g}_t^{-1} \mathrm{q}^t G(T_t \circ \Phi_t)) n_0 d\Gamma_0. \quad (3.263)$$

of problem (3.256). This gives rise to a term which is non linear with respect to w and linear with respect to $\dot{\mathrm{w}}$:

$$\begin{aligned} \mathcal{N}'_i(\mathrm{w}, \dot{\mathrm{w}}, \mathfrak{w}) = \int_{\Gamma_0} \mathfrak{w} \cdot \Big(& \nu(\nabla \mathrm{v}) DF(\dot{T}) - \mathrm{q} DG(\dot{T}) + \nu(\nabla \dot{\mathrm{v}}) F(T) \\ & - \dot{\mathrm{q}} G(T) - \mathrm{q} G(T)(-\operatorname{div} V) \Big), \end{aligned} \quad (3.264)$$

where $DF(\dot{T})$ and $DG(\dot{T})$ are defined in (3.234) and (3.235) respectively. Thus we obtain that the material derivatives $\dot{\mathrm{w}}$ defined in (3.260) and $\dot{\mathrm{s}}$ defined in (3.261) are solutions of the problem:

$$\begin{cases} \text{Find } (\dot{\mathrm{w}}, \dot{\mathrm{s}}) \in (H^1(\Omega_0))^2 \times L^2_0(\Omega_0) \text{ with } \dot{\mathrm{w}} = 0 \text{ on } \partial\omega \text{ such that:} \\ \displaystyle\int_{\Omega_0} \sigma(\dot{\mathrm{w}}) \cdot \nabla^s \mathfrak{w} \, dx - \int_{\Omega_0} \dot{\mathrm{s}} \operatorname{div} \mathfrak{w} = l'_S(\mathfrak{w}) - a'_S(\mathrm{w}, \mathfrak{w}) - b'_S(\mathrm{s}, \mathfrak{w}) + \mathcal{N}'_i(\mathrm{w}, \dot{\mathrm{w}}, \mathfrak{w}), \\ \qquad\qquad\qquad\qquad \forall \mathfrak{w} \in (H^1(\Omega_0))^2 \text{ with } \mathfrak{w} = 0 \text{ on } \partial\omega, \\ \displaystyle\int_{\Omega_0} \mathfrak{s} \left(I \cdot (\nabla \dot{\mathrm{w}} - \nabla \mathrm{w} \nabla V) \right) = 0, \quad \forall \mathfrak{s} \in L^2_0(\Omega_0). \end{cases} \quad (3.265)$$

3.4.5 Shape derivative of the cost functional

In this section, we compute the shape derivative of functionals depending on the FSI problem. In Section 3.4.5.1, we start with the example of an energy type functional, and then we present the calculations for a general volumic shape functional in Section 3.4.5.2.

3.4.5.1 An energy type functional

Let u and w be the velocity and displacement solutions of problem (3.189) for $t = 0$. Let us consider the following energy shape functional

$$\mathcal{J}(\Omega_0) = \int_{\Omega_F} |\nabla^s_x(\mathrm{u})|^2 dx + \int_{\Omega_0} |\nabla^s_Y(\mathrm{w})|^2 dY, \tag{3.266}$$

where $\nabla^s(\cdot)$ is defined in (3.9), and the norm of a matrix is defined in (3.63). Thus the shape functional evaluated on the domain $\Omega_{0,t}$ is given by

$$\mathcal{J}(\Omega_{0,t}) = \int_{\Omega_{F,t}} |\nabla^s_{x_t}(\mathrm{u}_t)|^2 dx_t + \int_{\Omega_{0,t}} |\nabla^s_{Y_t}(\mathrm{w}_t)|^2 dY_t. \tag{3.267}$$

We first develop the part of the functional depending on the displacement w_t:

$$\begin{aligned}
\mathcal{J}_S(\Omega_{0,t}) &= \int_{\Omega_{0,t}} |\nabla^s_{Y_t}(\mathrm{w}_t)|^2 dY_t, \\
&= \int_{\Omega_0} |\nabla^s_{Y_t}(\mathrm{w}_t)|^2 \circ \Phi_t \det(\nabla\Phi_t) dY, \\
&= \int_{\Omega_0} \left| \left[\nabla_Y(\mathrm{w}_t \circ \Phi_t)\nabla(\Phi_t)^{-1} \right]^s \right|^2 \det(\nabla\Phi_t) dY,
\end{aligned} \tag{3.268}$$

where Φ_t is defined in (3.187).

Then, we can calculate the derivative of $\mathcal{J}_S$ at 0 in the direction V, which is the velocity fields of the transformation Φ_t (see (3.187) and (3.228)). We recall that the matrix scalar product is $A \cdot B = A_{ij}B_{ij}$. Thus

$$\mathcal{J}'_S(\Omega_0) = 2\int_{\Omega_0} \nabla^s \mathrm{w} \cdot (\nabla\dot{\mathrm{w}} - \nabla\mathrm{w}\nabla V)\, dY + \int_{\Omega_0} |\nabla^s \mathrm{w}|^2 \operatorname{div}(V) dY, \tag{3.269}$$

where $\dot{\mathrm{w}}$ is the *material derivative* of w defined in (3.260), and where the derivative of $\det(\nabla\Phi_t)$ at 0 is given in (3.229) and is equal to $\operatorname{div}(V)$.

Now we develop the part of the functional depending on the fluid velocity. As we did in the previous sections, we introduce the field

$$\mathrm{v}_t := \mathrm{u}_t \circ T_t \tag{3.270}$$

defined on $\Omega^c_{0,t}$, and then we transport the integrals from $\Omega_{F,t}$ to $\Omega^c_{0,t}$:

$$\begin{aligned}
\mathcal{J}_F(\Omega_{0,t}) &= \int_{\Omega_{F,t}} |\nabla^s_{x_t}(\mathrm{u}_t)|^2 dx_t \\
&= \int_{\Omega_0^c} |\nabla^s_{x_t}(\mathrm{u}_t)|^2 \circ (T_t \circ \Phi_t) \det(\nabla(T_t \circ \Phi_t)) dX \\
&= \int_{\Omega_0^c} \left| \left[\nabla_{X_t}(\mathrm{u}_t \circ T_t)(\nabla_{X_t} T_t)^{-1} \right]^s \right|^2 \circ \Phi_t \det(\nabla(T_t \circ \Phi_t)) dX \\
&= \int_{\Omega_0^c} \left| \left[\nabla_X(\mathrm{v}_t \circ \Phi_t)\nabla_X(T_t \circ \Phi_t)^{-1} \right]^s \right|^2 \det(\nabla(T_t \circ \Phi_t)) dX.
\end{aligned} \tag{3.271}$$

We can calculate the derivative of $\mathcal{J}_F$ at 0 with respect to t.

$$\mathcal{J}'_F(\Omega_0) = \int_{\Omega_0^c} \left| \left[\nabla\mathrm{v}(\nabla T)^{-1} \right]^s \right|^2 \operatorname{tr}(\operatorname{cof}(\nabla T)^\top \nabla\dot{T}) dX$$

$$+ 2\int_{\Omega_0^c} \left[\nabla \mathrm{v}(\nabla T)^{-1}\right]^s \cdot \left(\nabla\dot{\mathrm{v}} - \nabla \mathrm{v}(\nabla T)^{-1}\nabla\dot{T}\right) \mathrm{cof}(\nabla T)^\top dX, \tag{3.272}$$

where $\dot{\mathrm{v}}$ and $\dot{T}$ are the material derivatives of v and T defined in (3.237) and (3.227), with $T = T_{t=0}$. The term $\mathrm{tr}(\mathrm{cof}(\nabla T)^\top \nabla\dot{T})$ in (3.272) occurs from the differentiation of the term $\det(\nabla(T_t \circ \Phi_t))$ in (3.271). The term $\left(\nabla\dot{\mathrm{v}} - \nabla \mathrm{v}(\nabla T)^{-1}\nabla\dot{T}\right) \mathrm{cof}(\nabla T)^\top$ in (3.272) comes from the differentiation of $|[\nabla_X(\mathrm{v}_t \circ \Phi_t)\nabla_X(T_t \circ \Phi_t)^{-1}]^s|^2$ in (3.271), which is thereafter multiplied by $\det(\nabla T)$. We recall in Appendix 3.7 the formulas for the derivatives of the determinant and inverse maps for matrices (see (3.360) and (3.361)).

Finally the shape derivative of the energy type functional is written as:

$$\begin{aligned}\mathcal{J}'(\Omega_0) = 2\int_{\Omega_0} \nabla^s \mathrm{w} \cdot (\nabla\dot{\mathrm{w}} - \nabla \mathrm{w}\nabla V)\, dY + \int_{\Omega_0} |\nabla^s \mathrm{w}|^2 \,\mathrm{div}(V) dY \\ + 2\int_{\Omega_0^c} \left[\nabla \mathrm{v}(\nabla T)^{-1}\right]^s \cdot \left(\nabla\dot{\mathrm{v}} - \nabla \mathrm{v}(\nabla T)^{-1}\nabla\dot{T}\right) \mathrm{cof}(\nabla T)^\top dX \\ + \left|\left[\nabla \mathrm{v}(\nabla T)^{-1}\right]^s\right|^2 \mathrm{tr}(\mathrm{cof}(\nabla T)^\top \nabla\dot{T}) dX.\end{aligned} \tag{3.273}$$

Now we give the shape derivative of a general abstract shape functional.

3.4.5.2 General shape functional

We consider a functional of the form

$$\mathcal{J}(\Omega_0) = \mathcal{J}_S(\Omega_0) + \mathcal{J}_F(\Omega_0) = \int_{\Omega_0} j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y))\, dY + \int_{\Omega_F} j_F(x, \mathrm{u}(x), \nabla \mathrm{u}(x))\, dx, \tag{3.274}$$

where $j_S = j_S(Y, \mathrm{w}, \nabla\mathrm{w})$ and $j_F = j_F(x, \mathrm{u}, \nabla\mathrm{u})$ are differentiable functions. Thus the shape functional evaluated on the domain $\Omega_{0,t}$ is given by

$$\begin{aligned}\mathcal{J}(\Omega_{0,t}) = \mathcal{J}_S(\Omega_{0,t}) + \mathcal{J}_F(\Omega_{0,t}) = \int_{\Omega_{0,t}} j_S(Y_t, \mathrm{w}_t(Y_t), \nabla \mathrm{w}_t(Y))\, dY_t \\ + \int_{\Omega_{F,t}} j_F(x_t, \mathrm{u}_t(x_t), \nabla \mathrm{u}_t(x))\, dx_t.\end{aligned} \tag{3.275}$$

First we consider the shape derivative of $\mathcal{J}_S$ with respect to t. After transporting the integral from $\Omega_{0,t}$ to Ω_0, we obtain

$$\mathcal{J}_S(\Omega_{0,t}) = \int_{\Omega_0} j_S\left(\Phi_t(Y), \mathrm{w}_t \circ \Phi_t(Y), (\nabla \mathrm{w}_t) \circ \Phi_t(Y)\right) \det(\nabla\Phi_t)\, dY. \tag{3.276}$$

Thus the shape derivative of $\mathcal{J}_S$ is given by

$$\begin{aligned}\mathcal{J}_S'(\Omega_0) = \int_{\Omega_0} j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y))\, \mathrm{div}\, V\, dY \\ + \int_{\Omega_0} D_1 j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y)) V\, dY \\ + \int_{\Omega_0} D_2 j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y)) \dot{\mathrm{w}} v\end{aligned}$$

$$+ \int_{\Omega_0} D_3 j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y))(\nabla \dot{\mathrm{w}} - \nabla \mathrm{w} \nabla V)\, dY, \tag{3.277}$$

where $\dot{\mathrm{w}}$ is the material derivative of w_t at $t = 0$ given in (3.260), and V the *velocity field* of the transformation defined in (3.228), and where D_1, D_2, and D_3 stand for differential on each argument of j_S.

Secondly we consider the shape derivative of $\mathcal{J}_F$ with respect to t. We perform a change of variable $X_t = T_t \circ \Phi_t(X)$, in order to rewrite the integrals from $\Omega_{F,t}$ to Ω_0^c. This gives

$$\mathcal{J}_F(\Omega_{0,t}) = \int_{\Omega_0^c} j_F(T_t \circ \Phi_t(X), \mathrm{u}_t \circ T_t \circ \Phi_t(X), (\nabla \mathrm{u}_t) \circ T_t \circ \Phi_t(X)) \det(\nabla(T_t \circ \Phi_t(X)))\, dX. \tag{3.278}$$

We calculate the shape derivative of $\mathcal{J}_F$, setting

$$\mathrm{v} = \mathrm{u} \circ T. \tag{3.279}$$

This gives

$$\begin{aligned}
\mathcal{J}'_F(\Omega_0) &= \int_{\Omega_0^c} j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) \operatorname{tr}(\operatorname{cof}(\nabla T)^\top \nabla \dot{T})\, dX \\
&+ \int_{\Omega_0^c} D_1 j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) \dot{T} \det(\nabla T)\, dX \\
&+ \int_{\Omega_0^c} D_2 j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) \dot{\mathrm{v}} \det(\nabla T)\, dX \\
&+ \int_{\Omega_0^c} D_3 j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1})(\nabla \dot{\mathrm{v}} - \nabla \mathrm{v}(\nabla T)^{-1} \nabla \dot{T}) \operatorname{cof}(\nabla T)^\top\, dX.
\end{aligned} \tag{3.280}$$

The term $\operatorname{tr}(\operatorname{cof}(\nabla T)^\top \nabla \dot{T})$ in (3.280) comes from the differentiation of $\det(\nabla(T_t \circ \Phi_t(X)))$ in (3.278). The terms $\dot{T}$ and $\dot{\mathrm{v}}$ in (3.280) are respectively the results of the differentiation through the chain rule of the terms $T_t \circ \Phi_t(X)$ and $\mathrm{u}_t \circ T_t \circ \Phi_t(X)$ in (3.278). For the last term $(\nabla \dot{\mathrm{v}} - \nabla \mathrm{v}(\nabla T)^{-1} \nabla \dot{T}) \operatorname{cof}(\nabla T)^\top$ in (3.280) deriving from $(\nabla \mathrm{u}_t) \circ T_t \circ \Phi_t(X)$ in (3.278), we can write

$$\begin{aligned}
(\nabla \mathrm{u}_t) \circ T_t \circ \Phi_t(X) &= (\nabla(\mathrm{u}_t \circ T_t \circ \Phi_t))(X)(\nabla(T_t \circ \Phi_t))^{-1}(X), \\
&= (\nabla(\mathrm{v}_t \circ \Phi_t))(X)(\nabla(T_t \circ \Phi_t))^{-1}(X),
\end{aligned} \tag{3.281}$$

with $\mathrm{v}_t = \mathrm{u}_t \circ T_t$ (see (3.270)), and from the definitions of $\dot{\mathrm{v}}$ and $\dot{T}$ given in (3.237) and (3.227), we find by the differentiation with respect to t of (3.281), the last term of (3.280). From there, we can write in the following proposition the formula of the shape derivative of the abstract shape functional $\mathcal{J}(\Omega_0)$ defined by (3.274), which is denoted by $\mathcal{J}'(\Omega_0)$.

Proposition 3.12. *Let $\mathcal{J}(\Omega_0)$ be the shape functional defined by* (3.274)*, where j_S and j_F are differentiable functions. Then, the shape derivative of $\mathcal{J}(\Omega_0)$, with respect to t by the velocity method computed for the transformation Φ_t defined in* (3.187)*, and evaluated at $t = 0$, is given by*

$$\begin{aligned}
\mathcal{J}'(\Omega_0) &= \int_{\Omega_0} j_S(Y, \mathrm{w}, \nabla \mathrm{w}) \operatorname{div} V\, dY \\
&+ \int_{\Omega_0} D_1 j_S(Y, \mathrm{w}, \nabla \mathrm{w}) V\, dY
\end{aligned}$$

$$
\begin{aligned}
&+ \int_{\Omega_0} D_2 j_S(Y, \mathrm{w}, \nabla \mathrm{w}) \dot{\mathrm{w}}\, dY \\
&+ \int_{\Omega_0} D_3 j_S(Y, \mathrm{w}, \nabla \mathrm{w})(\nabla \dot{\mathrm{w}} - \nabla \mathrm{w} \nabla V)\, dY \\
&+ \int_{\Omega_0^c} j_F(T, \mathrm{v}, \nabla \mathrm{v} (\nabla T)^{-1}) \operatorname{tr}(\operatorname{cof}(\nabla T)^\top \nabla \dot{T})\, dX \\
&+ \int_{\Omega_0^c} D_1 j_F(T, \mathrm{v}, \nabla \mathrm{v} (\nabla T)^{-1}) \dot{T} \det(\nabla T)\, dX \\
&+ \int_{\Omega_0^c} D_2 j_F(T, \mathrm{v}, \nabla \mathrm{v} (\nabla T)^{-1}) \dot{\mathrm{v}} \det(\nabla T)\, dX \\
&+ \int_{\Omega_0^c} D_3 j_F(T, \mathrm{v}, \nabla \mathrm{v} (\nabla T)^{-1})(\nabla \dot{\mathrm{v}} - \nabla \mathrm{v} (\nabla T)^{-1} \nabla \dot{T}) \operatorname{cof}(\nabla T)^\top\, dX. \qquad (3.282)
\end{aligned}
$$

In the next section, we propose a method allowing us to simplify expression (3.282).

3.5 Adjoint method, or Céa's method

In this Section, we present the *adjoint method*, or *Céa's method* introduced in [Céa86], used for a formal and useful calculation of the shape derivative of a shape functional. This method allows to guess straightforwardly the *adjoint states* we need to introduce in order to simplify the expression of the shape derivative. Notably it enables to write this derivative in such a way that it does not depend on the material derivatives of the solutions anymore. After the introduction to this method, we apply it to the FSI problem. We refer to [All07] Section 6.4.3 for a more detailed presentation of Céa's method, also called *Lagrangian method*.

3.5.1 Presentation of the method

Let Ω_0 be an admissible domain of the fluid-structure problem, standing for the elastic material (see Figure 33). We denote by Ω any perturbation of Ω_0 which can be characterised by vector field, or equivalently a transformation field. For example we can consider $\Omega = (\mathrm{id}_{\mathbb{R}^2} + tV)(\Omega_0)$, for $V \in \Theta^k(\mathrm{D}_\omega)$ and for $t > 0$. First we define the following functional space:

$$
\mathcal{V} := (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \times (H_{0,\partial\omega}^1(\Omega_0))^2 \times L_0^2(\Omega_0). \qquad (3.283)
$$

We will denote by $\mathcal{X}_0$ the quadruplet $(\mathrm{v}, \mathrm{q}, \mathrm{w}, \mathrm{s})$ solution of the fluid-structure problem with initial data Ω_0, and by $\mathcal{Y}$ a test quadruplet $(\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s})$. Let's rewrite the fluid-structure optimization problem with these notations. We denote by $\mathbb{M}^2$ the space of squared matrices of $\mathbb{R}^n$. Let $A : \mathcal{U}_{ad} \times \mathbb{M}^2 \times \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ be a differentiable map, bilinear on $\mathcal{V} \times \mathcal{V}$, and $L : \mathcal{U}_{ad} \times \mathbb{M}^2 \times \mathcal{V} \to \mathbb{R}$ be a differentiable map, linear on $\mathcal{V}$. Finally let $\mathfrak{F} : \mathcal{V} \to \mathbb{M}^2$ be a non linear differentiable map. We write $\mathcal{X}_\Omega$ the solution of the following problem:

$$
\text{Find } \mathcal{X}_\Omega \in \mathcal{V} \text{ such that:} \quad A\Big(\Omega; \mathfrak{F}(\mathcal{X}_\Omega); \mathcal{X}_\Omega, \mathcal{Y}\Big) = L\Big(\Omega; \mathfrak{F}(\mathcal{X}_\Omega); \mathcal{Y}\Big), \quad \forall \mathcal{Y} \in \mathcal{V}. \qquad (3.284)
$$

Now we define a shape functional:

$$
\mathcal{J}(\Omega) = j(\Omega, \mathcal{X}_\Omega). \qquad (3.285)
$$

This suggests the definition of the following Lagrangian for all Ω and for all $\mathcal{X}, \mathcal{Y} \in \mathcal{V}$:

$$\mathcal{L}\Big(\Omega, \mathcal{X}, \mathcal{Y}\Big) = j(\Omega, \mathcal{X}) + A\Big(\Omega; \mathfrak{F}(\mathcal{X}); \mathcal{X}, \mathcal{Y}\Big) - L\Big(\Omega; \mathfrak{F}(\mathcal{X}); \mathcal{Y}\Big). \tag{3.286}$$

By definition we have for all $\mathcal{Y} \in \mathcal{V}$:

$$\mathcal{L}\Big(\Omega, \mathcal{X}_\Omega, \mathcal{Y}\Big) = j(\Omega, \mathcal{X}_\Omega) \tag{3.287}$$

Thus the shape derivative of j is

$$j'(\Omega_0, \mathcal{X}_0) = \frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, \mathcal{X}_0, \mathcal{Y}\Big) + \left\langle \frac{\partial \mathcal{L}}{\partial \mathcal{X}}\Big(\Omega_0, \mathcal{X}_0, \mathcal{Y}\Big), \dot{\mathcal{X}}_0 \right\rangle, \tag{3.288}$$

where $\dot{\mathcal{X}}_0 = \partial_\Omega \mathcal{X}_0$ is the material derivative of $\mathcal{X}_0$. Let $\mathcal{Y}_0$ be the solution of the following problem:

$$\text{Find } \mathcal{Y}_0 \in \mathcal{V} \text{ such that:} \quad \left\langle \frac{\partial \mathcal{L}}{\partial \mathcal{X}}\Big(\Omega_0, \mathcal{X}_0, \mathcal{Y}_0\Big), \mathcal{Z} \right\rangle = 0 \quad \forall \mathcal{Z} \in \mathcal{V}, \tag{3.289}$$

we called $\mathcal{Y}_0$ the *adjoint solution*, or *adjoint state*, and we finally have

$$\mathcal{J}'(\Omega_0) = j'(\Omega_0, \mathcal{X}_0) = \frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, \mathcal{X}_0, \mathcal{Y}_0\Big). \tag{3.290}$$

We can see that the shape derivative $\mathcal{J}'(\Omega_0)$ in expression (3.290) does not depend on the material derivative $\dot{\mathcal{X}}_0$, unlike expression (3.288). Let us give a slightly more detailed expression of $\mathcal{J}'(\Omega_0)$. We develop problem (3.289):

$$\begin{aligned}\left\langle \frac{\partial \mathcal{L}}{\partial \mathcal{X}}\Big(\Omega_0, \mathcal{X}_0, \mathcal{Y}\Big), \mathcal{Z} \right\rangle &= \left\langle \frac{\partial j}{\partial \mathcal{X}}\Big(\Omega_0, \mathcal{X}_0\Big), \mathcal{Z} \right\rangle + A\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{Z}, \mathcal{Y}\Big) \\ &+ \left\langle \frac{\partial A}{\partial \mathfrak{F}}\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{X}_0, \mathcal{Y}\Big)\mathfrak{F}'(\mathcal{X}_0), \mathcal{Z} \right\rangle - \left\langle \frac{\partial L}{\partial \mathfrak{F}}\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{Y}\Big)\mathfrak{F}'(\mathcal{X}_0), \mathcal{Z} \right\rangle, \end{aligned} \tag{3.291}$$

where we have used the fact that A is linear with respect to $\mathcal{Z}$, and we develop the shape derivative

$$\frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, \mathcal{X}_0, \mathcal{Y}_0\Big) = \frac{\partial j}{\partial \Omega}(\Omega_0, \mathcal{X}_0) + \frac{\partial A}{\partial \Omega}\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{X}_0, \mathcal{Y}_0\Big) - \frac{\partial L}{\partial \Omega}\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{Y}_0\Big). \tag{3.292}$$

Finally we can write the shape derivative as follows:

$$j'(\Omega_0) = \frac{\partial j}{\partial \Omega}(\Omega_0, \mathcal{X}_0) + \frac{\partial A}{\partial \Omega}\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{X}_0, \mathcal{Y}_0\Big) - \frac{\partial L}{\partial \Omega}\Big(\Omega; \mathfrak{F}(\mathcal{X}_0); \mathcal{Y}_0\Big). \tag{3.293}$$

Let us apply this method to the FSI problem. That is we need to define what are the parametrized bilinear and linear forms A and L, the map $\mathfrak{F}$, and the Lagrangian $\mathcal{L}$.

3.5.2 Application to the fluid-structure problem

We first present in a compact and formal way how to apply the adjoint method to the FSI problem. We postponed detailed calculations to Sections 3.5.3 and 3.5.4.

Let v_t, q_t, w_t, and s_t be the solutions of the following problem written in the transformed configuration:

$$\begin{cases} \text{Find } (\mathrm{v}_t, \mathrm{q}_t) \text{ in } (H_0^1(\Omega_{0,t}^c))^2 \times L_0^2(\Omega_{0,t}^c) \text{ and } (\mathrm{w}_t, \mathrm{s}_t) \text{ in } (H_{0,\partial\omega}^1(\Omega_{0,t}))^2 \times L_0^2(\Omega_{0,t}) \text{ such that:} \\ a_{F,t}(\mathrm{w}_t; \mathrm{v}_t, \mathfrak{v}) + b_{F,t}(\mathrm{w}_t; \mathfrak{v}, \mathrm{q}_t) = f_{F,t}(\mathrm{w}_t; \mathfrak{v}), \quad \forall \mathfrak{v} \in (H_0^1(\Omega_{0,t}^c))^2, \\ \qquad b_{F,t}(\mathrm{w}_t; \mathrm{v}_t, \mathfrak{q}) = 0, \quad \forall \mathfrak{q} \in L_0^2(\Omega_{0,t}^c), \\ a_{S,t}(\mathrm{w}_t, \mathfrak{w}) + b_{S,t}(\mathfrak{w}, \mathrm{s}_t) = f_{S,t}(\mathrm{w}_t; \mathrm{v}_t; \mathrm{q}_t; \mathfrak{w}), \quad \forall \mathfrak{w} \in (H_{0,\partial\omega}^1(\Omega_{0,t}))^2, \\ \qquad b_{S,t}(\mathrm{w}_t, \mathfrak{s}) = 0, \quad \forall \mathfrak{q} \in L_0^2(\Omega_{0,t}^c), \end{cases} \tag{3.294}$$

where $a_{F,t}$, $b_{F,t}$, and $f_{F,t}$ are defined in (3.211), (3.212), and (3.213), and $a_{S,t}$, $b_{S,t}$, and $f_{S,t}$ are defined in (3.241), (3.242), and (3.243). By setting

$$\mathrm{v}^t := \mathrm{v}_t \circ \Phi_t, \tag{3.295}$$

$$\mathrm{w}^t := \mathrm{w}_t \circ \Phi_t, \tag{3.296}$$

$$\mathrm{q}^t := \mathfrak{g}_t \mathrm{q}_t \circ \Phi_t, \tag{3.297}$$

$$\mathrm{s}^t := \mathfrak{g}_t \mathrm{s}_t \circ \Phi_t, \tag{3.298}$$

where we recall that $\mathfrak{g}_t$ is defined in (3.215), we have that $(\mathrm{v}^t, \mathrm{w}^t, \mathrm{q}^t, \mathrm{s}^t)$ is solution of the following problem

$$\begin{cases} \text{Find } (\mathrm{v}^t, \mathrm{q}^t) \text{ in } (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \text{ and } (\mathrm{w}^t, \mathrm{s}^t) \text{ in } (H_{0,\partial\omega}^1(\Omega_0))^2 \times L_0^2(\Omega_0) \text{ such that:} \\ a_F^t(\mathrm{w}^t; \mathrm{v}^t, \mathfrak{v}) + b_F^t(\mathrm{w}^t; \mathfrak{v}, \mathrm{q}^t) = f_F^t(\mathrm{w}^t; \mathfrak{v}), \quad \forall \mathfrak{v} \in (H_0^1(\Omega_0^c))^2, \\ \qquad b_F^t(\mathrm{w}^t; \mathrm{v}^t, \mathfrak{q}) = 0, \quad \forall \mathfrak{q} \in L_0^2(\Omega_0^c), \\ a_S^t(\mathrm{w}^t, \mathfrak{w}) + b_S^t(\mathfrak{w}, \mathrm{s}^t) = f_S^t(\mathrm{w}^t; \mathrm{v}^t; \mathrm{q}^t; \mathfrak{w}), \quad \forall \mathfrak{w} \in (H_{0,\partial\omega}^1(\Omega_0))^2, \\ \qquad b_S^t(\mathrm{w}^t, \mathfrak{s}) = 0, \quad \forall \mathfrak{s} \in L_0^2(\Omega_0^c). \end{cases} \tag{3.299}$$

where a_F^t, b_F^t, and f_F^t are defined in (3.221), (3.222), and (3.223), and a_S^t, b_S^t, and f_S^t are defined in (3.251), (3.252), and (3.253).

We consider the abstract shape functional (see (3.274))

$$\begin{aligned} \mathcal{J}(\Omega_{0,t}) &= \mathcal{J}_{S,t}(\mathrm{w}_t) + \mathcal{J}_{F,t}(\mathrm{w}_t, \mathrm{v}_t) \\ &= \int_{\Omega_{0,t}} j_S(Y_t, \mathrm{w}_t(Y_t), \nabla \mathrm{w}_t(Y_t))\, dY_t + \int_{\Omega_{0,t}} j_F(x_t, \mathrm{v}_t(x_t), \nabla \mathrm{v}_t(x_t) \nabla (T_t)^{-1})\, dx_t. \end{aligned} \tag{3.300}$$

Once again a change of variable with (3.295)-(3.298) gives (see also (3.276) and (3.278))

$$\begin{aligned} \mathcal{J}(\Omega_{0,t}) &= \mathcal{J}_S^t(\mathrm{w}^t) + \mathcal{J}_F^t(\mathrm{w}^t, \mathrm{v}^t) \\ &= \int_{\Omega_0} j_S \left(\Phi_t(Y), \mathrm{w}^t, (\nabla \mathrm{w}^t) \nabla (\Phi_t)^{-1}(Y)\right) \det(\nabla \Phi_t)\, dY \\ &\quad + \int_{\Omega_0^c} j_F(T_t \circ \Phi_t(X), \mathrm{v}^t \circ \Phi_t(X), (\nabla \mathrm{v}^t) \nabla \Phi_t^{-1} \nabla (T_t)^{-1} \circ \Phi_t(X)) \det(\nabla \Phi_t(X))\, dX. \end{aligned} \tag{3.301}$$

From there, we define the Lagrangian (3.286)

$$\begin{aligned}\mathcal{L}(t, \mathrm{v}, \mathrm{q}, \mathfrak{v}, \mathfrak{q}, \mathrm{w}, \mathrm{s}, \mathfrak{w}, \mathfrak{s}) = &\mathcal{J}_F^t(\mathrm{w}, \mathrm{v}) + \mathcal{J}_S^t(\mathrm{w}) \\ &+ a_F^t(\mathrm{w}; \mathrm{v}, \mathfrak{v}) + b_F^t(\mathrm{w}; \mathfrak{v}, \mathrm{q}) - f_F^t(\mathrm{w}; \mathfrak{v}) \\ &+ b_F^t(\mathrm{w}; \mathrm{v}, \mathfrak{q}) \\ &+ a_S^t(\mathrm{w}, \mathfrak{w}) + b_S^t(\mathfrak{w}, \mathrm{s}) - f_S^t(\mathrm{w}; \mathrm{v}; \mathrm{q}; \mathfrak{w}) \\ &+ b_S^t(\mathrm{w}, \mathfrak{s}).\end{aligned} \tag{3.302}$$

Partial derivatives are involved in the definition of the adjoint states. We have that

$$\langle \frac{\partial \mathcal{L}}{\partial \mathrm{q}}(t, \mathrm{v}, \mathrm{q}, \mathfrak{v}, \mathfrak{q}, \mathrm{w}, \mathrm{s}, \mathfrak{w}, \mathfrak{s}), d\rangle = D_{\mathrm{q}} b_F^t(\mathrm{w}; \mathfrak{v}, \mathrm{q}) \cdot d - D_{\mathrm{q}} f_S^t(\mathrm{w}; \mathrm{v}; \mathrm{q}; \mathfrak{w}) \cdot d \tag{3.303}$$

$$\langle \frac{\partial \mathcal{L}}{\partial \mathrm{s}}(t, \mathrm{v}, \mathrm{q}, \mathfrak{v}, \mathfrak{q}, \mathrm{w}, \mathrm{s}, \mathfrak{w}, \mathfrak{s}), e\rangle = D_{\mathrm{s}} b_S^t(\mathfrak{w}, \mathrm{s}) \cdot e \tag{3.304}$$

$$\begin{aligned}\langle \frac{\partial \mathcal{L}}{\partial \mathrm{v}}(t, \mathrm{v}, \mathrm{q}, \mathfrak{v}, \mathfrak{q}, \mathrm{w}, \mathrm{s}, \mathfrak{w}, \mathfrak{s}), v\rangle = &D_{\mathrm{v}} \mathcal{J}_F^t(\mathrm{w}, \mathrm{v}) \cdot v + D_{\mathrm{v}} a_F^t(\mathrm{w}; \mathrm{v}, \mathfrak{v}) \cdot v + D_{\mathrm{v}} b_F^t(\mathrm{w}; \mathrm{v}, \mathfrak{q}) \cdot v \\ &- D_{\mathrm{v}} f_S^t(\mathrm{w}; \mathrm{v}; \mathrm{q}; \mathfrak{w}) \cdot v\end{aligned} \tag{3.305}$$

$$\begin{aligned}\langle \frac{\partial \mathcal{L}}{\partial \mathrm{w}}(t, \mathrm{v}, \mathrm{q}, \mathfrak{v}, \mathfrak{q}, \mathrm{w}, \mathrm{s}, \mathfrak{w}, \mathfrak{s}), w\rangle = &D_{\mathrm{w}} \mathcal{J}_F^t(\mathrm{w}, \mathrm{v}) \cdot w + D_{\mathrm{w}} \mathcal{J}_S^t(\mathrm{w}) \cdot w \\ &+ D_{\mathrm{w}} a_F^t(\mathrm{w}; \mathrm{v}, \mathfrak{v}) \cdot w + D_{\mathrm{w}} b_F^t(\mathrm{w}; \mathfrak{v}, \mathrm{q}) \cdot w - D_{\mathrm{w}} f_F^t(\mathrm{w}; \mathfrak{v}) \cdot w \\ &+ D_{\mathrm{w}} b_F^t(\mathrm{w}; \mathrm{v}, \mathfrak{q}) \cdot w \\ &+ D_{\mathrm{w}} a_S^t(\mathrm{w}, \mathfrak{w}) \cdot w - D_{\mathrm{w}} f_S^t(\mathrm{w}; \mathrm{v}; \mathrm{q}; \mathfrak{w}) \cdot w \\ &+ D_{\mathrm{w}} b_S^t(\mathrm{w}, \mathfrak{s}) \cdot w.\end{aligned} \tag{3.306}$$

According to (3.289), we would like to find $(\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s})$ such that for all (v, d, w, e):

$$\langle \frac{\partial \mathcal{L}}{\partial \mathrm{v}}, v\rangle + \langle \frac{\partial \mathcal{L}}{\partial \mathrm{q}}, d\rangle + \langle \frac{\partial \mathcal{L}}{\partial \mathrm{w}}, w\rangle + \langle \frac{\partial \mathcal{L}}{\partial \mathrm{s}}, e\rangle = 0 \tag{3.307}$$

For visualizing the coupled terms in $(\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s})$, the problem can be gathered and presented in the following matrix

$$\begin{array}{cc} \begin{array}{c} \mathfrak{v} \\ \mathfrak{q} \\ \mathfrak{w} \\ \mathfrak{s} \end{array} & \begin{pmatrix} D_{\mathrm{v}} a_F^t & D_{\mathrm{q}} b_F^t & D_{\mathrm{w}} a_F^t + D_{\mathrm{w}} b_F^t - D_{\mathrm{w}} f_F^t & 0 \\ D_{\mathrm{v}} b_F^t & 0 & D_{\mathrm{w}} b_F^t & 0 \\ -D_{\mathrm{v}} f_S^t & -D_{\mathrm{q}} f_S^t & D_{\mathrm{w}} a_S^t - D_{\mathrm{w}} f_S^t & D_{\mathrm{s}} b_S^t \\ 0 & 0 & D_{\mathrm{w}} b_S^t & 0 \end{pmatrix} \\ & \begin{array}{cccc} \quad v \quad & \quad d \quad & \qquad\qquad w \qquad\qquad & \quad e \end{array} \end{array} \tag{3.308}$$

In the following section, we give the explicit calculus of the differentiation of the Lagrangian. In our case presented in the current section, the shape functional $\mathcal{J}$ depends on the domain through the parameter t, that we have introduced in order to simplify calculations. Thus, by using the method described in Section 3.5.1, we compute derivatives with respect to the variable t instead of Ω. Finally, expression (3.290) is rewritten, and we will simplify the shape derivative of the shape functional $\mathcal{J}(\Omega_0)$ by using the following expression

$$\mathcal{J}'(\Omega_0) = j'(0, \mathrm{v}, \mathrm{q}, \mathrm{w}, \mathrm{s}) = \frac{\partial \mathcal{L}}{\partial t}\Big(0, \mathrm{v}, \mathrm{q}, \mathrm{w}, \mathrm{s}, \mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s}\Big). \tag{3.309}$$

3.5.3 Definition of a Lagrangian, calculus of its derivatives

We consider the shape functional defined by (3.274) that we can rewrite as

$$\mathcal{J}(\Omega_0) = \int_{\Omega_0^c} j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) \det(\nabla T)\, dX + \int_{\Omega_0} j_S(Y, \mathrm{w}, \nabla \mathrm{w})\, dY. \tag{3.310}$$

We want to explicitly construct the related Lagrangian of $\mathcal{J}(\Omega_0)$ as in (3.286). Then we will turn to the calculation of its derivatives with respect to $(\mathrm{v}, \mathrm{q}, \mathrm{w}, \mathrm{s})$ as well as with respect to the parameter t which are required for computing the shape derivative of $\mathcal{J}$ (see (3.288)).

3.5.3.1 Shape functional and its related Lagrangian

Writing $\mathcal{J}$ on a perturbed domain $\Omega_{0,t}$ leads to (see Section 3.4.5.2)

$$\mathcal{J}(\Omega_{0,t}) = \int_{\Omega_{0,t}^c} j_F(T_t, \mathrm{v}_t, \nabla \mathrm{v}_t(\nabla T_t)^{-1}) \det(\nabla T_t)\, dX_t + \int_{\Omega_{0,t}} j_S(Y_t, \mathrm{w}_t, \nabla \mathrm{w}_t)\, dY_t. \tag{3.311}$$

where T_t is defined in (3.196), with $\mathrm{w}_t \in (H^1_{0,\partial\omega}(\Omega_{0,t}))^2$ displacement solution of the problem (3.240), and where $\mathrm{v}_t \in (H^1_0(\Omega^c_{0,t}))^2$ is the velocity solution on the reference domain of the problem (3.210). We want to apply Cea's method presented in Section 3.5.1 to find the adjoint states needed for the calculation of the shape derivative of $\mathcal{J}$. For this we need to define a Lagrangian having independent variables. The map T_t depends both on the parameter t, through the map Φ_t, and on the field w_t. To make a distinction between these two dependencies, we introduce the map $T_{t,\mathrm{w}}$ defined by

$$\begin{array}{llll} \mathfrak{T}: & \mathbb{R}_+ \times (H^1_{0,\partial\omega})^2(\Omega_0) & \longrightarrow & H^1(\mathrm{D}_\omega) \\ & (t, \mathrm{w}) & \longmapsto & T_{t,\mathrm{w}} := \mathrm{id} + \mathcal{R}(\gamma(\mathrm{w})) \circ \Phi_t^{-1}. \end{array} \tag{3.312}$$

In this manner, the map $\mathfrak{T}$ depends on functions w belonging to the fixed space $(H^1_{0,\partial\omega}(\Omega_0))^2$. Furthermore, we recover the definition of T_t given in (3.196) with the use of map $\mathfrak{T}$ as follows

$$T_t = T_{t,\mathrm{w}_t \circ \Phi_t}. \tag{3.313}$$

We introduce the following notation for a given function u:

$$u_{\star t} = u \circ \Phi_t^{-1} \quad \text{and} \quad u^{\star t} = u \circ \Phi_t, \tag{3.314}$$

in order to simplify the notation. First we introduce the following natural Lagrangian, defined from the shape functional and the variational equations (3.210) and (3.240), for $0 \leq t$, for all (v, q) and $(\mathfrak{v}, \mathfrak{q})$ in $(H^1_0(\Omega^c_{0,t}))^2 \times L^2_0(\Omega^c_{0,t})$, and for all (w, s) and $(\mathfrak{w}, \mathfrak{s})$ in $(H^1_{0,\partial\omega}(\Omega_{0,t}))^2 \times L^2_0(\Omega_{0,t})$. According to (3.286), and in view of (3.210), (3.240), and (3.311), we have:

$$\begin{aligned} \tilde{\mathcal{L}}(t, (\mathrm{v}, \mathrm{q}), (\mathfrak{v}, \mathfrak{q}), (\mathrm{w}, \mathrm{s}), (\mathfrak{w}, \mathfrak{s})) &= \int_{\Omega^c_{0,t}} j_F(T_{t,\mathrm{w}^{\star t}}, \mathrm{v}, \nabla \mathrm{v} \nabla (T_{t,\mathrm{w}^{\star t}})^{-1}) J(T_{t,\mathrm{w}^{\star t}}) \\ &+ \int_{\Omega_{0,t}} j_S(Y_t, \mathrm{w}, \nabla \mathrm{w}) \\ &+ \int_{\Omega^c_{0,t}} [\nu(\nabla \mathrm{v}) F(T_{t,\mathrm{w}^{\star t}}) \cdot \nabla \mathfrak{v} - \mathrm{q}(G(T_{t,\mathrm{w}^{\star t}}) \cdot \nabla \mathfrak{v}) \\ &\qquad + \boldsymbol{\epsilon}(\mathrm{v} \cdot G(T_{t,\mathrm{w}^{\star t}}) \nabla) \mathrm{v} \cdot \mathfrak{v} - (f \circ T_{t,\mathrm{w}^{\star t}} \cdot \mathfrak{v}) J(T_{t,\mathrm{w}^{\star t}})] \end{aligned}$$

$$
\begin{aligned}
&+\int_{\Omega_{0,t}^c} \mathfrak{q}(G(T_{t,\mathrm{w}^{\star t}})\cdot\nabla \mathrm{v})\\
&+\int_{\Omega_{0,t}}[\sigma(\mathrm{w})\cdot\nabla^s\mathfrak{w}-\mathrm{s}\,\mathrm{div}(\mathfrak{w})-g\cdot(\mathfrak{w})]-\int_{\Gamma_{0,t}}\mathfrak{w}\cdot(\nu(\nabla\mathrm{v})F(T_{t,\mathrm{w}^{\star t}})-\mathrm{q}G(T_{t,\mathrm{w}^{\star t}}))n_{0,t}\\
&+\int_{\Omega_{0,t}}\mathfrak{s}\,\mathrm{div}(\mathrm{w}),
\end{aligned}
\tag{3.315}
$$

where F, G, and J are given in (3.204), (3.205), and (3.206). Defined this way, the variables of $\tilde{\mathcal{L}}$ are not independent because the function spaces depends on t. Let's rewrite this Lagrangian by transporting the integral on the fixed domains Ω_0 and Ω_0^c with the changes of variable $X_t = \Phi_t(X)$ and $Y_t = \Phi_t(Y)$. We recall

$$\mathfrak{g}_t = \det(\nabla\Phi_t), \tag{3.316}$$

and that

$$\mathfrak{J}_t := \nabla\Phi_t. \tag{3.317}$$

For $0 \le t$, for all (v,q) and $(\mathfrak{v},\mathfrak{q})$ in $(H_0^1(\Omega_0^c))^2\times L_0^2(\Omega_0^c)$, and for all (w,s) and $(\mathfrak{w},\mathfrak{s})$ in $(H^1_{0,\partial\omega}(\Omega_0))^2\times L_0^2(\Omega_0)$, we define the new Lagrangian $\mathcal{L}$:

$$
\begin{aligned}
&\mathcal{L}(t,(\mathrm{v},\mathrm{q}),(\mathfrak{v},\mathfrak{q}),(\mathrm{w},\mathrm{s}),(\mathfrak{w},\mathfrak{s})) :=\\
&\qquad\tilde{\mathcal{L}}\left(t,(\mathrm{v}_{\star t},(\mathfrak{g}_t^{-1}\mathrm{q})_{\star t}),(\mathfrak{v}_{\star t},(\mathfrak{g}_t^{-1}\mathfrak{q})_{\star t}),(\mathrm{w}_{\star t},(\mathfrak{g}_t^{-1}\mathrm{s})_{\star t}),(\mathfrak{w}_{\star t},(\mathfrak{g}_t^{-1}\mathfrak{s})_{\star t})\right).
\end{aligned}
\tag{3.318}
$$

By setting:

$$T^t_{\mathrm{w}} := T_{t,\mathrm{w}}\circ\Phi_t \tag{3.319}$$

with the transported expression of $\tilde{\mathcal{L}}$, in view of (3.315), and because we have

$$\nabla(\mathrm{v}\circ\Phi_t^{-1}) = \nabla\mathrm{v}\nabla\Phi_t^{-1} = \nabla\mathrm{v}\mathfrak{J}_t^{-1}, \tag{3.320}$$

and

$$(\mathrm{v}_t\cdot G(T_t)\nabla)\mathrm{v}_t\cdot z = \nabla\mathrm{v}_t G(T_t)^\top\mathrm{v}_t\cdot z, \tag{3.321}$$

we can write:

$$
\begin{aligned}
\mathcal{L}(t,(\mathrm{v},\mathrm{q}),(\mathfrak{v},\mathfrak{q}),(\mathrm{w},\mathrm{s}),(\mathfrak{w},\mathfrak{s})) &= \int_{\Omega_0^c} j_F(T^t_{\mathrm{w}},\mathrm{v},\nabla\mathrm{v}\nabla(T^t_{\mathrm{w}})^{-1})J(T_{t,\mathrm{w}})^{\star t}\mathfrak{g}_t\\
&+\int_{\Omega_0} j_S(\Phi_t,\mathrm{w},\nabla\mathrm{w}\mathfrak{J}_t^{-1})\mathfrak{g}_t\\
&+\int_{\Omega_0^c}\Big[\nu(\nabla\mathrm{v})\mathfrak{J}_t^{-1}F(T_{t,\mathrm{w}})^{\star t}\cdot(\nabla\mathfrak{v})\mathfrak{J}_t^{-1}\mathfrak{g}_t+\boldsymbol{\epsilon}(\nabla\mathrm{v}\mathfrak{J}_t^{-1}\mathfrak{g}_t(G(T_{t,\mathrm{w}})^{\star t})^\top)\mathrm{v}\cdot\mathfrak{v}\\
&\qquad -\mathrm{q}(G(T_{t,\mathrm{w}})^{\star t}\cdot(\nabla\mathfrak{v})\mathfrak{J}_t^{-1})\Big]\\
&-\int_{\Omega_0^c}(f\circ T^t_{\mathrm{w}}\cdot\mathfrak{v})J(T_{t,\mathrm{w}})^{\star t}\mathfrak{g}_t+\int_{\Omega_0^c}\mathfrak{q}G(T_{t,\mathrm{w}})^{\star t}\cdot(\nabla\mathrm{v})\mathfrak{J}_t^{-1}\\
&+\int_{\Omega_0}\Big[\mathbf{C}((\nabla\mathrm{w})\mathfrak{J}_t^{-1})^s\cdot((\nabla\mathfrak{w})\mathfrak{J}_t^{-1})^s\mathfrak{g}_t-\mathrm{s}(\mathrm{I}\cdot(\nabla\mathfrak{w})\mathfrak{J}_t^{-1})-(g^{\star t}\cdot\mathfrak{w})\mathfrak{g}_t\Big]\\
&-\int_{\Gamma_0}\mathfrak{w}\cdot\left(\nu(\nabla\mathrm{v})\mathfrak{J}_t^{-1}F(T_{t,\mathrm{w}})^{\star t}\mathfrak{g}_t-\mathrm{q}G(T_{t,\mathrm{w}})^{\star t}\right)\mathfrak{J}_t^{-\top}n_0+\int_{\Omega_0}\mathfrak{s}(\mathrm{I}\cdot(\nabla\mathrm{w})\mathfrak{J}_t^{-1}).
\end{aligned}
\tag{3.322}
$$

We simplify this expression with notation and calculi led in Appendix 3.7, giving that

$$\mathfrak{J}_t^{-1}F(T_{t,\mathrm{w}})^{\star t}\mathfrak{J}_t^{-\top}\mathfrak{g}_t = F(T^t_{\mathrm{w}}), \tag{3.323}$$

$$G(T_{t,\mathrm{w}})^{\star t}\mathfrak{J}_t^{-\top} = \mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t), \tag{3.324}$$
$$J(T_{t,\mathrm{w}})^{\star t}\mathfrak{g}_t = J(T_{\mathrm{w}}^t) \tag{3.325}$$

We obtain also in view of (3.321) that:

$$\begin{aligned}
\mathcal{L}(t,(\mathrm{v},\mathrm{q}),(\mathfrak{v},\mathfrak{q}),(\mathrm{w},\mathrm{s}),(\mathfrak{w},\mathfrak{s})) &= \int_{\Omega_0^c} j_F(T_{\mathrm{w}}^t,\mathrm{v},\nabla\mathrm{v}\nabla(T_{\mathrm{w}}^t)^{-1})J(T_{\mathrm{w}}^t)\\
&+\int_{\Omega_0} j_S(\Phi_t,\mathrm{w},\nabla\mathrm{w}\mathfrak{J}_t^{-1})\mathfrak{g}_t\\
&+\int_{\Omega_0^c}\Big[\nu(\nabla\mathrm{v})F(T_{\mathrm{w}}^t)\cdot\nabla\mathfrak{v} - \mathrm{q}(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t)\cdot\nabla\mathfrak{v}) + \boldsymbol{\epsilon}(\mathrm{v}\cdot G(T_{\mathrm{w}}^t)\nabla)\mathrm{v}\cdot\mathfrak{v}\\
&\quad+\int_{\Omega_0^c}\mathfrak{q}(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t)\cdot\nabla\mathrm{v}) - (f\circ T_{\mathrm{w}}^t\cdot\mathfrak{v})J(T_{\mathrm{w}}^t)\Big]\\
&+\int_{\Omega_0}\Big[\mathbf{C}((\nabla\mathrm{w})\mathfrak{J}_t^{-1})^s\cdot((\nabla\mathfrak{w})\mathfrak{J}_t^{-1})^s\mathfrak{g}_t - \mathrm{s}(\mathrm{I}\cdot(\nabla\mathfrak{w})\mathfrak{J}_t^{-1}) - (g^{\star t}\cdot\mathfrak{w})\mathfrak{g}_t\Big]\\
&\quad-\int_{\Gamma_0}\mathfrak{w}\cdot(\nu(\nabla\mathrm{v})F(T_{\mathrm{w}}^t) - \mathrm{q}\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t))n_0 + \int_{\Omega_0}\mathfrak{s}(\mathrm{I}\cdot(\nabla\mathrm{w})\mathfrak{J}_t^{-1}).
\end{aligned}\tag{3.326}$$

We define the transported solutions of Stokes problem

$$\mathrm{v}^t = \mathrm{v}_t\circ\Phi_t, \tag{3.327}$$
$$\mathrm{q}^t = \mathfrak{g}_t q_t\circ\Phi_t, \tag{3.328}$$

and the transported solutions of the incompressible elasticity problem

$$\mathrm{w}^t = \mathrm{w}_t\circ\Phi_t, \tag{3.329}$$
$$\mathrm{s}^t = \mathfrak{g}_t s_t\circ\Phi_t. \tag{3.330}$$

According to (3.287), we find $(\mathrm{v}^t,\mathrm{q}^t,\mathrm{w}^t,\mathrm{s}^t)$ such that, for all $(\mathfrak{v},\mathfrak{q})$ in $(H_0^1(\Omega_0^c))^2\times L_0^2(\Omega_0^c)$, and for all $(\mathfrak{w},\mathfrak{s})$ in $(H_{0,\partial\omega}^1(\Omega_0))^2\times L_0^2(\Omega_0)$:

$$\mathcal{L}(t,(\mathrm{v}^t,\mathrm{q}^t),(\mathfrak{v},\mathfrak{q}),(\mathrm{w}^t,\mathrm{s}^t),(\mathfrak{w},\mathfrak{s})) = J(\Omega_{0,t}), \tag{3.331}$$

where $\mathcal{L}$ is given by (3.326).

3.5.3.2 Derivatives of the Lagrangian

In the following, we calculate formally the partial derivative of the Lagrangian $\mathcal{L}$. This Lagrangian depends on nine variables, which we do not write for a sake of readability. To have no ambiguity, we say that we write the derivatives evaluated at $t\in\mathbb{R}_+$, $(\mathrm{v},\mathrm{q}),(\mathfrak{v},\mathfrak{q})\in(H_0^1(\Omega_0^c))^2\times L_0^2(\Omega_0^c)$, and $(\mathrm{w},\mathrm{s}),(\mathfrak{w},\mathfrak{s})\in(H_{0,\partial\omega}^1(\Omega_0))^2\times L_0^2(\Omega_0)$. For $d\in L_0^2(\Omega_0^c)$ and $e\in L_0^2(\Omega_0)$, we have

$$\langle\frac{\partial\mathcal{L}}{\partial\mathfrak{q}},d\rangle = \int_{\Omega_0^c} d(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t)\cdot\nabla\mathrm{v}), \tag{3.332}$$
$$\langle\frac{\partial\mathcal{L}}{\partial\mathfrak{s}},e\rangle = \int_{\Omega_0} e(\mathrm{I}\cdot(\nabla\mathrm{w})\mathfrak{J}_t^{-1}). \tag{3.333}$$

Let h be in $(H_0^1(\Omega_0^c))^2$, we have

$$\langle\frac{\partial\mathcal{L}}{\partial\mathfrak{v}},h\rangle = \nu\int_{\Omega_0^c}(\nabla\mathrm{v})F(T_{\mathrm{w}}^t)\cdot\nabla h - \mathrm{q}(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t)\cdot\nabla h)$$

$$+ \boldsymbol{\epsilon}(\mathrm{v} \cdot G(T_{\mathrm{w}}^t)\nabla)\mathrm{v} \cdot h - (f \circ T_{\mathrm{w}}^t \cdot h)J(T_{\mathrm{w}}^t). \tag{3.334}$$

Let k be in $H^1_{0,\partial\omega}(\Omega_0)$, we have

$$\begin{aligned}\langle \frac{\partial \mathcal{L}}{\partial \mathfrak{w}}, k\rangle = &\int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w})\mathfrak{J}_t^{-1})^s \cdot ((\nabla k)\mathfrak{J}_t^{-1})^s \mathfrak{g}_t - (g^{\star t} \cdot k)\mathfrak{g}_t - \int_{\Omega_0} \mathrm{s}(\mathrm{I} \cdot (\nabla k)\mathfrak{J}_t^{-1}) \\ &- \int_{\Gamma_0} k \cdot (\nu(\nabla \mathrm{v})F(T_{\mathrm{w}}^t) - \mathrm{q}\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t))n_0. \end{aligned} \tag{3.335}$$

If $\mathrm{w} = \mathrm{w}^t$, then $\langle \partial_{\mathfrak{s}}\mathcal{L}, e\rangle = 0$ for all e in $L^2_0(\Omega_0)$. If additionally we have $\mathrm{v} = \mathrm{v}^t$, then $\langle \partial_{\mathfrak{q}}\mathcal{L}, d\rangle = 0$ for all d in $L^2_0(\Omega_0^c)$. If $\mathrm{v} = \mathrm{v}^t$, $\mathrm{q} = \mathrm{q}^t$, and $\mathrm{w} = \mathrm{w}^t$, then $\langle \partial_{\mathfrak{v}}\mathcal{L}, h\rangle = 0$ for all h in $H^1_0(\Omega_0^c)$. If $\mathrm{v} = \mathrm{v}^t$, $\mathrm{q} = \mathrm{q}^t$, $\mathrm{w} = \mathrm{w}^t$, and $\mathrm{s} = \mathrm{s}^t$, then $\langle \partial_{\mathfrak{w}}\mathcal{L}, k\rangle = 0$ for all k in $H^1_{\partial\omega=0}(\Omega_0)$. We see that the expressions (3.332), (3.333), (3.334) and (3.335) allow to get back the initial fluid-structure problem written on the initial domains Ω_0 and Ω_0^c, and give us the primal solutions.

Now we write the dual problems. Let $d \in L^2_0(\Omega_0^c)$ and $e \in L^2_0(\Omega_0)$, we derivate the Lagrangian with respect to the variables q and s:

$$\langle \frac{\partial \mathcal{L}}{\partial \mathrm{q}}, d\rangle = -\int_{\Omega_0^c} d(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t) \cdot \nabla \mathfrak{v}) + \int_{\Gamma_0} \mathfrak{w} \cdot d(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t))n_0, \tag{3.336}$$

$$\langle \frac{\partial \mathcal{L}}{\partial \mathrm{s}}, e\rangle = -\int_{\Omega_0} e(\mathrm{I} \cdot (\nabla \mathfrak{w})\mathfrak{J}_t^{-1}). \tag{3.337}$$

Let h be in $H^1_0(\Omega_0^c)$, we compute the derivative of the Lagrangian with respect to the variable v. In order to simplify the expression of this derivative, we simply write $D_\alpha j_F$ and $D_\alpha j_S$ instead of $D_\alpha j_F(T_{\mathrm{w}}^t, \mathrm{v}, \nabla \mathrm{v}\nabla(T_{\mathrm{w}}^t)^{-1})$ and $D_\alpha j_S(\Phi_t, \mathrm{w}, \nabla \mathrm{w}\mathfrak{J}^{-1})$ respectively, for $\alpha = 1, 2, 3$.

$$\begin{aligned}\langle \frac{\partial \mathcal{L}}{\partial \mathrm{v}}, h\rangle = &\int_{\Omega_0^c} \left[(D_2 j_F)h + (D_3 j_F)\nabla h \nabla(T_{\mathrm{w}}^t)^{-1}\right] J(T_{\mathrm{w}}^t) \\ &+ \int_{\Omega_0^c} \nu(\nabla h)F(T_{\mathrm{w}}^t) \cdot \nabla \mathfrak{v} + \boldsymbol{\epsilon}[(\nabla h G(T_{\mathrm{w}}^t)^\top \mathrm{v} + \nabla \mathrm{v} G(T_{\mathrm{w}}^t)^\top h) \cdot \mathfrak{v}] \\ &- \int_{\Gamma_0} \mathfrak{w} \cdot \nu(\nabla h)F(T_{\mathrm{w}}^t)n_0 + \int_{\Omega_0^c} \mathfrak{q}(\mathfrak{g}_t^{-1}G(T_{\mathrm{w}}^t) \cdot \nabla h). \end{aligned} \tag{3.338}$$

Let k be in $H^1_{0,\partial\omega}(\Omega_0)$:

$$\begin{aligned}\langle \frac{\partial \mathcal{L}}{\partial \mathrm{w}}, k\rangle = &\int_{\Omega_0^c} (j_F)D_{\mathrm{w}}J(T_{\mathrm{w}}^t)k + \left[(D_1 j_F)D_{\mathrm{w}}(T_{\mathrm{w}}^t)k + (D_3 j_F)\nabla \mathrm{v} D_{\mathrm{w}}(\nabla(T_{\mathrm{w}}^t)^{-1})k\right] J(T_{\mathrm{w}}^t) \\ &+ \int_{\Omega_0} (D_2 j_S)k\mathfrak{g}_t + (D_3 j_S)\nabla k \mathfrak{J}_t^{-1}\mathfrak{g}_t \\ &+ \int_{\Omega_0^c} (\nu \nabla \mathrm{v} D_{\mathrm{w}}F(T_{\mathrm{w}}^t)k - \mathrm{q}\mathfrak{g}_t^{-1}D_{\mathrm{w}}G(T_{\mathrm{w}}^t)k) \cdot \nabla \mathfrak{v} + \boldsymbol{\epsilon}(\mathrm{v} \cdot D_{\mathrm{w}}G(T_{\mathrm{w}}^t)\nabla)\mathrm{v} \cdot \mathfrak{v} \\ &- \int_{\Omega_0^c} (D_{\mathrm{w}}(f \circ T_{t,\mathrm{w}}{}^{\star t})k \cdot \mathfrak{v})J(T_{\mathrm{w}}^t) + (f \circ T_{\mathrm{w}}^t \cdot \mathfrak{v})D_{\mathrm{w}}J(T_{\mathrm{w}}^t)k \\ &+ \int_{\Omega_0^c} (\mathfrak{g}_t^{-1}D_{\mathrm{w}}G(T_{\mathrm{w}}^t)k \cdot \nabla \mathrm{v})\mathfrak{q} \\ &+ \int_{\Omega_0} \mathbf{C}((\nabla k)\mathfrak{J}_t^{-1})^s \cdot ((\nabla \mathfrak{w})\mathfrak{J}_t^{-1})^s \mathfrak{g}_t + \int_{\Omega_0} \mathfrak{s}(\mathrm{I} \cdot (\nabla k)\mathfrak{J}_t^{-1}) \end{aligned}$$

$$- \int_{\Gamma_0} \mathfrak{w} \cdot \left(\nu \nabla \mathrm{v} D_{\mathrm{w}} F(T^t_{\mathrm{w}}) k - \mathrm{q} \mathfrak{g}_t^{-1} D_{\mathrm{w}} G(T^t_{\mathrm{w}}) k \right) n_0, \tag{3.339}$$

where the derivatives $D_{\mathrm{w}}(\cdot)$ with respect to the variable w are given in Appendix 3.7. Finally we calculate partial derivative of the Lagrangian with respect to the variable t, referring once again to 3.7 for the expressions of the t variable derivatives $D_t(\cdot)$. We recall that we have

$$\frac{d}{dt} \det(\nabla \Phi_t) = \operatorname{div} V_t \tag{3.340}$$

where V_t is defined by

$$V_t(X) = \frac{d}{dt} \left(\Phi_t(X) \right), \quad \forall X \in \mathrm{D}, \tag{3.341}$$

and that

$$\frac{d}{dt} \mathfrak{J}_t^{-1} = -\mathfrak{J}_t^{-1} \nabla V_t \mathfrak{J}_t^{-1}, \tag{3.342}$$

$$\frac{d}{dt} \mathfrak{g}_t = \operatorname{tr}(\operatorname{cof}(\mathfrak{J}_t)^\top \nabla V_t). \tag{3.343}$$

Thus we obtain

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial t} = & \int_{\Omega_0^c} (j_F) \partial_t J(T^t_{\mathrm{w}}) + (D_1 j_F) \partial_t (T^t_{\mathrm{w}}) J(T^t_{\mathrm{w}}) + (D_3 j_F) \nabla \mathrm{v} \partial_t (\nabla (T^t_{\mathrm{w}})^{-1}) J(T^t_{\mathrm{w}}) \\
& + \int_{\Omega_0} (j_S) \operatorname{div} V_t + (D_1 j_S) V_t \mathfrak{g}_t + (D_3 j_S) \nabla \mathrm{w} D_t \mathfrak{J}_t^{-1} \mathfrak{g}_t \\
& + \int_{\Omega_0^c} (\nu \nabla \mathrm{v} \partial_t F(T^t_{\mathrm{w}}) - \mathrm{q} \partial_t (\mathfrak{g}_t^{-1} G(T^t_{\mathrm{w}}))) \cdot \nabla \mathfrak{v} + \boldsymbol{\epsilon}(\mathrm{v} \cdot \partial_t G(T^t_{\mathrm{w}}) \nabla) \mathrm{v} \cdot \mathfrak{v} \\
& \qquad - \int_{\Omega_0^c} [(f \circ T^t_{\mathrm{w}} \cdot \mathfrak{v}) \partial_t J(T^t_{\mathrm{w}}) + (\partial_t (f \circ T^t_{\mathrm{w}}) \cdot \mathfrak{v}) J(T^t_{\mathrm{w}})] \\
& \qquad + \int_{\Omega_0^c} (\partial_t (\mathfrak{g}_t^{-1} G(T^t_{\mathrm{w}})) \cdot \nabla \mathrm{v}) \mathfrak{q} \\
& - \int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w}) \mathfrak{J}_t^{-1} \nabla V_t \mathfrak{J}_t^{-1})^s \cdot ((\nabla \mathfrak{w}) \mathfrak{J}_t^{-1})^s \mathfrak{g}_t - \int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w}) \mathfrak{J}_t^{-1})^s \cdot ((\nabla \mathfrak{w}) \mathfrak{J}_t^{-1} \nabla V_t \mathfrak{J}_t^{-1})^s \mathfrak{g}_t \\
& \qquad + \int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w}) \mathfrak{J}_t^{-1})^s \cdot ((\nabla \mathfrak{w}) \mathfrak{J}_t^{-1})^s \operatorname{tr}(\operatorname{cof}(\mathfrak{J}_t)^\top \nabla V_t) - \int_{\Omega_0} \mathfrak{s} (\mathrm{I} \cdot (\nabla \mathrm{w}) \mathfrak{J}_t^{-1} \nabla V_t \mathfrak{J}_t^{-1}) \\
& \qquad - \int_{\Gamma_0} \mathfrak{w} \cdot (\nu \nabla \mathrm{v} \partial_t F(T^t_{\mathrm{w}}) - \mathrm{q} \partial_t (\mathfrak{g}_t^{-1} G(T^t_{\mathrm{w}}))) n_0,
\end{aligned} \tag{3.344}$$

where we recall that $T^t_{\mathrm{w}} = T_{t,\mathrm{w}} \circ \Phi_t = \Phi_t + \mathcal{R}(\gamma(\mathrm{w}))$ (see formula (3.312)), and ∂_t denotes the partial derivative with respect to the variable t, where $T_{t,\mathrm{w}}$ is considered as a function of the variable t and the variable w. Then this formula can be simplified by noticing that finally, $\partial_t T_{t,\mathrm{w}} = V_t$ where V_t is defined in (3.341), and taking into account the derivative formulas (3.363), (3.364), and (3.365) given in Appendix Section 3.7.1. The simplified formula will appear in Theorem 3.14.

3.5.4 Definition of the adjoint states

Formally , we have (see (3.288))

$$\mathcal{J}'(\Omega_0) = \begin{pmatrix} \partial_t \\ \partial_{\mathrm{v}} \\ \partial_{\mathrm{q}} \\ \partial_{\mathrm{w}} \\ \partial_{\mathrm{s}} \end{pmatrix} \mathcal{L}(0, (\mathrm{v}^0, \mathrm{q}^0), (\mathfrak{v}, \mathfrak{q}), (\mathrm{w}^0, \mathrm{s}^0), (\mathfrak{w}, \mathfrak{s})) \cdot \begin{pmatrix} 1 \\ \dot{\mathrm{v}} \\ \dot{\mathrm{q}} \\ \dot{\mathrm{w}} \\ \dot{\mathrm{s}} \end{pmatrix} \tag{3.345}$$

Let us write the adjoint equations. For this, the partial derivatives of the Lagrangian calculated in the previous section are evaluated at $t = 0$, at $(\mathrm{v}, \mathrm{q}) = (\mathrm{v}^0, \mathrm{q}^0)$ the solution of problem (3.210) written for $t = 0$, at $(\mathrm{w}, \mathrm{s}) = (\mathrm{w}^0, \mathrm{s}^0)$ the solution of problem (3.240) written for $t = 0$. This being done, we obtain from equations (3.336), (3.337), (3.338), and (3.339) that for all $(\mathfrak{v}, \mathfrak{q}), (h, d) \in (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c)$, and for all $(\mathfrak{w}, \mathfrak{s}), (k, e) \in (H_{0,\partial\omega}^1(\Omega_0))^2 \times L_0^2(\Omega_0)$:

$$
\begin{aligned}
\langle \frac{\partial \mathcal{L}}{\partial \mathrm{q}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), d\rangle &= -\int_{\Omega_0^c} d(G(T) \cdot \nabla \mathfrak{v}) + \int_{\Gamma_0} \mathfrak{w} \cdot d\, G(T) n_0, && (3.346)\\
\langle \frac{\partial \mathcal{L}}{\partial \mathrm{s}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), e\rangle &= -\int_{\Omega_0} e \operatorname{div} \mathfrak{w}, && (3.347)\\
\langle \frac{\partial \mathcal{L}}{\partial \mathrm{v}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), h\rangle &= \int_{\Omega_0^c} (D_2 j_F) h J(T) + (D_3 j_F) \nabla h \nabla(T)^{-1} J(T) + \int_{\Omega_0^c} \mathfrak{q}(G(T) \cdot \nabla h)\\
&\quad + \int_{\Omega_0^c} \nu(\nabla h) F(T) \cdot \nabla \mathfrak{v} + \boldsymbol{\epsilon}[(\nabla h G(T)^\top \mathrm{v} + \nabla \mathrm{v} G(T)^\top h) \cdot \mathfrak{v}] && (3.348)\\
&\quad - \int_{\Gamma_0} \mathfrak{w} \cdot (\nu(\nabla h) F(T)) n_0, && (3.349)\\
\langle \frac{\partial \mathcal{L}}{\partial \mathrm{w}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), k\rangle &= \int_{\Omega_0} (D_2 j_s) k + (D_3 j_s) \nabla k\\
&\quad + \int_{\Omega_0^c} (j_F) D_\mathrm{w} J(T) k + (D_1 j_F)(D_\mathrm{w}(T) k) J + (D_3 j_F) \nabla \mathrm{v} D_\mathrm{w}(\nabla(T)^{-1}) k J\\
&\quad + \int_{\Omega_0^c} \nu(\nabla \mathrm{v})(D_\mathrm{w} F(T) k) \cdot \nabla \mathfrak{v} - q((D_\mathrm{w} G(T) k) \cdot \nabla \mathfrak{v}) + \boldsymbol{\epsilon}(\mathrm{v} \cdot D_\mathrm{w} G(T) k \nabla) \mathrm{v} \cdot \mathfrak{v}\\
&\quad - \int_{\Omega_0^c} ((\nabla f) \circ T D_\mathrm{w}(T) k \cdot \mathfrak{v}) J + (f \circ T \cdot \mathfrak{v}) D_\mathrm{w} J(T) k + \int_{\Omega_0^c} (D_\mathrm{w} G(T) k \cdot \nabla \mathrm{v}) \mathfrak{q}\\
&\quad + \int_{\Omega_0} \mathbf{C}(\nabla k)^s \cdot (\nabla \mathfrak{w})^s - \int_{\Gamma_0} \mathfrak{w} \cdot (\nu(\nabla \mathrm{v}) D_\mathrm{w} F(T) k - q D_\mathrm{w} G(T) k) n_0 && (3.350)\\
&\quad + \int_{\Omega_0} \mathfrak{s} \operatorname{div} k, && (3.351)
\end{aligned}
$$

where $T = T^0$, $J = J(T^0)$, $G = G(T^0)$, and $F = F(T^0)$, and once again we have written $D_\alpha j_F$ and $D_\alpha j_S$ instead of $D_\alpha j_F(T, \mathrm{v}, \nabla \mathrm{v} \nabla(T)^{-1})$ and $D_\alpha j_S(Y, \mathrm{w}, \nabla \mathrm{w})$ respectively, for $\alpha = 1, 2, 3$.

With these expressions, we can write in the following proposition the problem satisfied by the adjoint states defined by the adjoint method presented in Section 3.5.1, associated to the shape functional $\mathcal{J}$ defined in (3.310) and to the Fluid-Structure Interaction problem (3.44).

Proposition 3.13. *Let $\mathcal{L}$ be the Lagrangian defined in* (3.326)*, associated to the shape functional $\mathcal{J}$ defined in* (3.310) *and to the Fluid-Structure Interaction problem* (3.44)*. Let $(\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s})$ be the adjoint state solution defined by the adjoint method, allowing to simplify the expression of the shape derivative of $\mathcal{J}$. Then $(\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s})$ is the solution of the variational problem defined by*

$$
\begin{cases}
\textit{Find } (\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s}) \textit{ in } (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \times (H_{0,\partial\omega}^1(\Omega_0))^2 \times L_0^2(\Omega_0) \textit{ such that:}\\
\langle \frac{\partial \mathcal{L}}{\partial \mathrm{q}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), d\rangle + \langle \frac{\partial \mathcal{L}}{\partial \mathrm{s}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), e\rangle\\
\qquad + \langle \frac{\partial \mathcal{L}}{\partial \mathrm{v}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), h\rangle + \langle \frac{\partial \mathcal{L}}{\partial \mathrm{w}}((\mathfrak{v}, \mathfrak{q}), (\mathfrak{w}, \mathfrak{s})), k\rangle = 0,\\
\textit{for all } (h, d, k, e) \textit{ in } (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \times (H_{0,\partial\omega}^1(\Omega_0))^2 \times L_0^2(\Omega_0),
\end{cases}
\qquad (3.352)
$$

given by expressions (3.346)*,* (3.347)*,* (3.349)*, and* (3.351)*.*

From there, we can simply the formula (3.282) of the shape derivative $\mathcal{J}'(\Omega_0)$, using the adjoint states defined in Proposition 3.13. The final formula will be written in Theorem 3.14.

3.5.5 Simplified formula for the shape derivative $\mathcal{J}'(\Omega_0)$

The method we have just presented in Section 3.5 is a formal method. Indeed, we have defined a Lagrangian and carried out several derivative calculations without any justification. To be rigorous, we should show the differentiability with respect to the variable t of the solutions of the fluid-structure interaction problem, that is to say their shape differentiability, and justify that the adjoint problems defined in Section 3.5.4 are well defined (which should be shown in the same way as in Section 3.3 for the Fluid-Structure Interaction problem). These justifications are part of the ongoing work and the perspectives for the continuation of this thesis.

In the meantime, assuming that the adjoint problems do have a unique solution, and that we have the shape differentiability of the considered fields, we can simplify the formula of the shape derivative $\mathcal{J}'(\Omega_0)$ given by (3.282) obtained in Section 3.4.5.2. For this, we follow what is done in Section 3.5.1, using formulas (3.309) and (3.344). This leads to the following theorem.

Theorem 3.14. *Let $\mathcal{J}(\Omega_0)$ be the shape functional defined by* (3.310)*. Let* $(\mathrm{v}, \mathrm{q}, \mathrm{w}, \mathrm{s}) \in (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \times (H^1_{0,\partial\omega}(\Omega_0))^2 \times L_0^2(\Omega_0)$ *be the solution of the Fluid-Structure Interaction problem* (3.44)*, and* $(\mathfrak{v}, \mathfrak{q}, \mathfrak{w}, \mathfrak{s}) \in (H_0^1(\Omega_0^c))^2 \times L_0^2(\Omega_0^c) \times (H^1_{0,\partial\omega}(\Omega_0))^2 \times L_0^2(\Omega_0)$ *be the adjoint states solution of the adjoint problem* (3.352)*. Then the shape derivative of $\mathcal{J}(\Omega_0)$ can be written as follows:*

$$\begin{aligned}
\mathcal{J}'(\Omega_0) = &\int_{\Omega_0^c} j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) DJ(V) + D_1 j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) V J(T) \\
&+ \int_{\Omega_0^c} D_3 j_F(T, \mathrm{v}, \nabla \mathrm{v}(\nabla T)^{-1}) \nabla \mathrm{v}(-\nabla T^{-1} \nabla V \nabla T^{-1}) J(T^t_{\mathrm{w}}) \\
&+ \int_{\Omega_0} j_S(Y, \mathrm{w}, \nabla \mathrm{w}) \operatorname{div} V + D_1 j_S(Y, \mathrm{w}, \nabla \mathrm{w}) V + D_3 j_S(Y, \mathrm{w}, \nabla \mathrm{w}) \nabla \mathrm{w}(-\nabla V) \\
&+ \int_{\Omega_0^c} (\nu \nabla \mathrm{v} DF(V) - \mathrm{q}(-\operatorname{div}(V) G(T) + DG(V))) \cdot \nabla \mathfrak{v} + \boldsymbol{\epsilon}(\mathrm{v} \cdot DG(V) \nabla) \mathrm{v} \cdot \mathfrak{v} \\
&\qquad - \int_{\Omega_0^c} [(f \circ T \cdot \mathfrak{v}) DJ(V) + (D_t(f \circ T) \cdot \mathfrak{v}) J(T)] \\
&\qquad + \int_{\Omega_0^c} (-\operatorname{div}(V) G(T) + DG(V)) \cdot \nabla \mathrm{v})\mathfrak{q} \\
&- \int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w}) \nabla V)^s \cdot ((\nabla \mathfrak{w}))^s - \int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w}))^s \cdot ((\nabla \mathfrak{w}) \nabla V)^s \\
&\qquad + \int_{\Omega_0} \mathbf{C}((\nabla \mathrm{w}))^s \cdot ((\nabla \mathfrak{w}))^s \operatorname{div}(V) - \int_{\Omega_0} \mathfrak{s}(\mathrm{I} \cdot (\nabla \mathrm{w}) \nabla V) \\
&\qquad - \int_{\Gamma_0} \mathfrak{w} \cdot (\nu \nabla \mathrm{v} DF(V) - \mathrm{q}(-\operatorname{div}(V) G(T) + DG(V))) n_0,
\end{aligned} \tag{3.353}$$

where $T := T_0$ is given by (3.196)*, V is the velocity of the transformation Φ_t given by* (3.228)*, and $DJ(V)$, $DG(V)$, and $DFJ(V)$ are given in expressions* (3.375)*,* (3.376)*, and* (3.377) *in Section 3.7.1.1.*

3.6 Conclusion

In this chapter, we have presented a Fluid Structure Interaction model, for which we define a shape optimization problem. The purpose is to optimize an abstract shape functional $\mathcal{J}(\Omega_0)$, defined by

$$\mathcal{J}(\Omega_0) = \int_{\Omega_0} j_S(Y, \mathrm{w}(Y), \nabla \mathrm{w}(Y))\, dY + \int_{\Omega_F} j_F(x, \mathrm{u}(x), \nabla \mathrm{u}(x))\, dx, \tag{3.354}$$

depending on the initial elastic domain Ω_0 of the FSI problem, and where u is the velocity field of the fluid whereas w is the displacement field of the elastic structure. We have calculated the shape derivative of $\mathcal{J}(\Omega_0)$ by using the velocity method, together with an adjoint method. We still have to answer two fundamental questions.

The first question deals with the shape differentiability of the solutions of the FSI problem. Indeed the expressions of the shape derivatives we have calculated provided that this shape differentiability is established. For this, we are currently working on a proof of the shape differentiability relying on an application of the Implicit Function theorem. This method is described in [HP06] Chapter 5 for a Laplacian problem with Dirichlet or Neumann boundary conditions.

The second question deals with the proof of the existence of minimizers for $\mathcal{J}(\Omega_0)$, for $\Omega_0 \in \mathcal{U}_{\mathrm{ad}}$, where $\mathcal{U}_{\mathrm{ad}}$ is a class of admissible domain. For this, we plan to apply direct methods of the calculus of variations. Namely consider a minimizing sequence of domains $\Omega_{0,n}$, and show that its limit is a minimizer for $\mathcal{J}$.

We need to find a class $\mathcal{U}_{\mathrm{ad}}$ being compact with respect to some convergence, and show that the functional $\mathcal{J}$ is lower semi continuous with respect to this convergence. We also need to show that the FSI problem is continuous, which is done by addressing the question of the shape differentiability. Finally we need to show that the functional $\mathcal{J}$ is coercive, namely there exist two positive constants C_1 and C_2 such that

$$\mathcal{J}(\Omega_0) \geq C_1 \|\mathrm{u}_{\Omega_0}\|^2 + C_2 \|\mathrm{w}_{\Omega_0}\|^2,$$

for some suitable norms, where u_{Ω_0} and w_{Ω_0} are respectively the velocity and the displacement solutions of the FSI problem posed on Ω_0.

We are working on the proof of this second question. We have chosen to lead the study described above for $\mathcal{U}_{\mathrm{ad}}$ being a class of admissible Lipschitz domain, with a bounded Lipschitz character. The advantage to deal with such a class of domain, is that it offers a compactness property for several kinds of convergences, such as the *Hausdorff* convergence, the *characteristic functions* convergence, and the *compact* convergence (see e.g., [HP06]).

Furthermore, in order to prove that $\mathcal{J}$ is coercive, we need to prove that the constants involved in the estimations of the solutions of FSI problems posed on a domain Ω_0, are uniform with respect $\Omega_0 \in \mathcal{U}_{\mathrm{ad}}$. We are currently working on the H^3-norm estimates of problems (3.50), (3.54), and the fixed point procedure (see Section 3.3.4) for controlling with respect to Ω_0 all the constants and estimates.

3.7 Appendix

3.7.1 Derivatives of J, G, and F maps

Let A_α be a differentiable squared matrix field in $\mathbb{R}^{n\times n}$ depending on the variable $\alpha \in \mathbb{V}$, where $\mathbb{V}$ is a normed vector space endowed with the norm $\|\cdot\|_{\mathbb{V}}$. We define the following maps depending on A_α:

$$\bar{J}(A_\alpha) := \det(A_\alpha), \tag{3.355}$$
$$\bar{G}(A_\alpha) := \operatorname{cof}(A_\alpha), \tag{3.356}$$
$$\bar{F}(A_\alpha) := A_\alpha^{-1}\operatorname{cof}(A_\alpha), \tag{3.357}$$

where $\operatorname{cof}(A_\alpha)$ is the cofactor matrix of A_α defined by

$$\operatorname{cof}(A_\alpha) = \det(A_\alpha)A_\alpha^{-T}. \tag{3.358}$$

We denote by $D_\alpha(A_\alpha)$ the Fréchet derivative of A at α, namely $D_\alpha(A_\alpha)$ is the continuous linear map from $\mathbb{V}$ to $\mathbb{R}^{n\times n}$ such that for all $d\alpha \in \mathbb{V}$:

$$A_{\alpha+d\alpha} = A_\alpha + D_\alpha(A_\alpha)(d\alpha) + o(\|d\alpha\|_{\mathbb{V}}). \tag{3.359}$$

We recall that the determinant $\det(\cdot)$, the inverse $(\cdot)^{-1}$, and the cofactor $\operatorname{cof}(\cdot)$ matrix maps are differentiable, and their derivatives are written as follows. Let $A, B \in \mathbb{R}^{n\times n}$, A being invertible, and $|B|$ is supposed to be sufficiently small so that $A+B$ is invertible. We have

$$\det(A+B) = \det(A) + \operatorname{tr}(\operatorname{cof}(A)^\top B) + o(|B|), \tag{3.360}$$
$$(A+B)^{-1} = A^{-1} - A^{-1}BA^{-1} + +o(|B|), \tag{3.361}$$
$$\operatorname{cof}(A+B) = \operatorname{cof}(A) + \left(\operatorname{tr}(\operatorname{cof}(A)^\top B)\mathrm{I} - \operatorname{cof}(A)B^\top\right)A^{-\top} + o(|B|). \tag{3.362}$$

Thus, from the definitions (3.355), (3.356), and (3.357), and in view of the chain rule, we have the following derivatives:

$$D_\alpha\bar{J}(A_\alpha)(d\alpha) = \operatorname{tr}(\operatorname{cof}(A_\alpha)^\top D_\alpha(A_\alpha)(d\alpha)) \tag{3.363}$$
$$D_\alpha\bar{G}(A_\alpha)(d\alpha) = \left[\operatorname{tr}(A_\alpha^{-1}D_\alpha(A_\alpha)(d\alpha))\mathrm{I} - A_\alpha^{-\top}D_\alpha(A_\alpha)(d\alpha)^\top\right]\operatorname{cof}(A_\alpha) \tag{3.364}$$
$$D_\alpha\bar{F}(A_\alpha)(d\alpha) = \operatorname{cof}(A_\alpha)^\top\left[\operatorname{tr}(A_\alpha^{-1}D_\alpha(A_\alpha)(d\alpha))\mathrm{I} - 2(D_\alpha(A_\alpha)(d\alpha)A_\alpha^{-1})^s\right]A_\alpha^{-\top}. \tag{3.365}$$

3.7.1.1 Derivatives with respect to t

Let Φ_t and T_t be the maps defined respectively in (3.187) and (3.196) in Section 3.4.2, by

$$\Phi_t := \mathrm{id}_{\mathbb{R}^n} + tV, \tag{3.366}$$

for a fixed $V \in \Theta^k(\mathrm{D}_\omega)$, and

$$T_t = \mathrm{id} + \mathcal{R}(\gamma(\mathrm{w}_t \circ \Phi_t)) \circ \Phi_t^{-1}. \tag{3.367}$$

Let F, G, and J the maps defined in (3.204), (3.205), and (3.206) by

$$F(T_t) = (\nabla T_t)^{-1}\operatorname{cof}(\nabla T_t), \tag{3.368}$$

$$G(T_t) = \mathrm{cof}(\nabla T_t), \tag{3.369}$$
$$J(T_t) = \det(\nabla T_t). \tag{3.370}$$

From the above calculations, we find the expressions (3.236), (3.235), and (3.234):

$$DJ(\dot{T}) = \mathrm{tr}(\mathrm{cof}(\nabla T)^\top \nabla \dot{T}), \tag{3.371}$$
$$DG(\dot{T}) = \mathrm{cof}(\nabla T)\left[\mathrm{tr}\left((\nabla T)^{-1}\nabla \dot{T}\right)\mathrm{I} - [(\nabla T)^{-1}\nabla \dot{T}]^\top\right], \tag{3.372}$$
$$DF(\dot{T}) = \mathrm{cof}(\nabla T)^\top\left[\mathrm{tr}\left((\nabla T)^{-1}\nabla \dot{T}\right)\mathrm{I} - 2[\nabla \dot{T}(\nabla T)^{-1}]^s\right](\nabla T)^{-\top}, \tag{3.373}$$

where, with $\dot{\mathrm{w}}$ defined in (3.260) we have

$$\dot{T} = \frac{d}{dt}\bigg|_{t=0}(T_t \circ \Phi_t) = V + \mathcal{R}\gamma(\dot{\mathrm{w}}). \tag{3.374}$$

Finally, we define the following expression needed in the writing of Theorem 3.14:

$$DJ(V) = \mathrm{tr}(\mathrm{cof}(\nabla T)^\top \nabla V), \tag{3.375}$$
$$DG(V) = \mathrm{cof}(\nabla T)\left[\mathrm{tr}\left((\nabla T)^{-1}\nabla V\right)\mathrm{I} - [(\nabla T)^{-1}\nabla V]^\top\right], \tag{3.376}$$
$$DF(V) = \mathrm{cof}(\nabla T)^\top\left[\mathrm{tr}\left((\nabla T)^{-1}\nabla V\right)\mathrm{I} - 2[\nabla V(\nabla T)^{-1}]^s\right](\nabla T)^{-\top}. \tag{3.377}$$

3.7.1.2 Derivatives with respect to w

We introduce the following notation for a given function u:

$$u_{\star t} = u \circ \Phi_t^{-1} \quad \text{and} \quad u^{\star t} = u \circ \Phi_t. \tag{3.378}$$

For w in $H^1_{0,\partial\omega}(\mathrm{D}_\omega)$, we had defined in (3.312)

$$T_{t,\mathrm{w}} = \mathrm{id} + \mathcal{R}\gamma(\mathrm{w}) \circ \Phi_t^{-1}, \tag{3.379}$$

in such a way that $T_{t,\mathrm{w}_t^{\star t}} = T_t$. We also set

$$T^t_{\mathrm{w}} := T_{t,\mathrm{w}} \circ \Phi_t \tag{3.380}$$

Then we have the rather simple expressions:

$$D_t(T^t_{\mathrm{w}_t^{\star t}}) = V_t + \mathcal{R}\gamma(D_t(\mathrm{w}_t \circ \Phi_t)), \tag{3.381}$$
$$D_t(T^t_{\mathrm{w}_t^{\star t}})_{|t=0} = V + \mathcal{R}\gamma(\dot{\mathrm{w}}), \tag{3.382}$$

and for $k \in H^1_{0,\partial\omega}$, we have

$$D_{\mathrm{w}}(T^t_{\mathrm{w}})k = \mathcal{R}\gamma(k). \tag{3.383}$$

From (3.363), (3.364), and (3.365) we can also deduce the values of $D_{\mathrm{w}}J(T^t_{\mathrm{w}})k$, $D_{\mathrm{w}}G(T^t_{\mathrm{w}})k$, and $D_{\mathrm{w}}F(T^t_{\mathrm{w}})k$, and the values of $D_tJ(T^t_{\mathrm{w}})$, $D_t(G(T^t_{\mathrm{w}})\mathfrak{g}_t^{-1})$, and $D_tF(T^t_{\mathrm{w}})$ in Section 3.5.3.2.

3.7.2 Various identities

We recall that

$$\mathfrak{g}_t := \det(\nabla\Phi_t), \tag{3.384}$$
$$\mathfrak{J}_t := \nabla\Phi_t. \tag{3.385}$$

We have the following identities

$$\mathfrak{J}_t^{-1}(F(T_t)\circ\Phi_t)\mathfrak{J}_t^{-\top}\mathfrak{g}_t = F(T_t\circ\Phi_t) \tag{3.386}$$
$$G(T_t)\circ\Phi_t\mathfrak{J}_t^{-\top}\mathfrak{g}_t = G(T_t\circ\Phi_t) \tag{3.387}$$
$$J(T_t)\circ\Phi_t\mathfrak{g}_t = J(T_t\circ\Phi_t). \tag{3.388}$$

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Appendix A

Elements of tensor calculus

Let u and v be two vectors of $\mathbb{R}^n$, A and B be two second order tensors of $\mathbb{R}^n$, and $\mathbf{T}$ be a fourth order tensor of $\mathbb{R}^n$. Let $\{\mathrm{e}_i\}_{i=1,\cdots,n}$ a base of $\mathbb{R}^n$), we write:

$$\mathbf{T}A = \mathbf{T}_{ijkl}A_{kl}\,\mathrm{e}_i \otimes \mathrm{e}_j, \tag{A.1}$$

$$AB = A_{ik}B_{kj}\,\mathrm{e}_i \otimes \mathrm{e}_j, \tag{A.2}$$

$$A \cdot B = A_{ij}B_{ij}, \tag{A.3}$$

$$Au = A_{ij}u_j\,\mathrm{e}_i, \tag{A.4}$$

$$u \cdot v = u_i v_i, \tag{A.5}$$

where $\mathrm{e}_i \otimes \mathrm{e}_j$ is a matrix such that $(\mathrm{e}_i \otimes \mathrm{e}_j)_{kl} = \delta_{ik}\delta_{jl}$. We define

$$u \otimes_s v := \frac{u \otimes v + v \otimes u}{2}. \tag{A.6}$$

For all tensor fields $\mathbf{A}$, we define the *volume averaging* of $\mathbf{A}$ over Ω by

$$\langle \mathbf{A} \rangle_\Omega := \frac{1}{V}\int_\Omega \mathbf{A}(y)dy, \tag{A.7}$$

where $V = |\Omega|$ denotes the area of the unit cell. If there is no ambiguity on the domain Ω, we simply write

$$\langle \mathbf{A} \rangle := \frac{1}{V}\int_\Omega \mathbf{A}(y)dy. \tag{A.8}$$

Cofactor matrix:

$$\mathrm{cof}(A) = \det(A)A^{-\top}$$

Identity tensors:

$$\mathrm{I} = \mathrm{e}_i \otimes \mathrm{e}_i, \tag{A.9}$$

$$\mathrm{I} \otimes \mathrm{I} = \mathrm{e}_i \otimes \mathrm{e}_i \otimes \mathrm{e}_j \otimes \mathrm{e}_j, \tag{A.10}$$

$$\mathbb{I} = \frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\mathrm{e}_i \otimes \mathrm{e}_j \otimes \mathrm{e}_k \otimes \mathrm{e}_l. \tag{A.11}$$

Divergence operator:

$$\mathrm{div}(A) := \frac{\partial A_{ij}}{\partial x_j}\mathrm{e}_i, = \nabla \cdot A.$$

Let $\mathbf{C}$ be a fourth order tensor standing for the elasticity tensor. Let u be a vector field of $\mathbb{R}^n$. We define the *strain* and the *stress* respectively as follows

$$e(u) = \frac{1}{2}\left(\nabla u + \nabla u^\top\right), \tag{A.12}$$

$$\sigma(u) = \mathbf{C}e(u). \tag{A.13}$$

Green's identity (divergence theorem):

$$\int_\Omega (\mathrm{div}(\sigma(u)) \cdot v + \sigma(u) \cdot e(v)) = \int_\Omega \mathrm{div}(\sigma(u)v) = \int_{\partial\Omega} \sigma(u)n \cdot v. \tag{A.14}$$

Detailed calculus of topological derivatives

The topological derivatives of the tensors $\mathbf{E}^h$ and $\mathbf{F}^h$, given in Section 1.2.4, can be used in a procedure of topological optimization the same as we did for the tensors $\mathbf{C}^h$ and $\mathbf{D}^h$ in Chapter 2. The methods for the calculation of these topological derivatives in the mixture case or in the case where the contrast vanishes are exactly the same as those developed in Sections 1.3.5, 1.3.3, and 1.3.4. However, in order to enable the reader easily to check the validity of the formulas – for example for an numerical use – we detail these calculations in this Appendix.

B.1 Topological derivative of the tensor $\mathbf{E}^h$

We recall the definition of $\mathbf{E}^h_\varepsilon$

$$(\mathbf{E}^h_\varepsilon)_{ijpqr} := \frac{2}{V}\int_{\mathcal{Y}} \gamma_\varepsilon \sigma(u^\varepsilon_{ij}) \cdot (e(\tilde{\tilde{u}}^\varepsilon_{pqr}) + \tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r). \tag{B.1}$$

We start simplifying the expression (1.71) with the help of equation (1.108) written for $\tilde{\tilde{u}}^\varepsilon_{pqr}$ with $\eta = \tilde{u}^\varepsilon_{ij}$, noting that $u^\varepsilon_{ij} = \tilde{u}^\varepsilon_{ij} + (\mathrm{e}_i \otimes_s \mathrm{e}_j)y$, and noting that $\langle \tilde{u}^\varepsilon_{ij} \rangle = 0$. We get

$$(\mathbf{E}^h_\varepsilon)_{ijpqr} = \frac{2}{V}\int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot (e(\tilde{\tilde{u}}^\varepsilon_{pqr}) + \tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) + \gamma_\varepsilon \sigma(u^\varepsilon_{pq}) \cdot (\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_r). \tag{B.2}$$

We calculate directly

$$\begin{aligned}\frac{V}{2}(\mathbf{E}^h_\varepsilon - \mathbf{E}^h)_{ijpqr} = &\int_{\mathcal{Y}} \qquad 0 \qquad\qquad\qquad\qquad\qquad\qquad + \sigma(\delta u^\varepsilon_{pq}) \cdot (\tilde{u}_{ij} \otimes_s \mathrm{e}_r) \\ &+ \int_{\mathcal{Y}} \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot (e(\delta\tilde{\tilde{u}}^\varepsilon_{pqr}) + \delta\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) + \sigma(u_{pq}) \cdot (\delta\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_r) \\ &+ (\gamma - 1)\int_{B_\varepsilon} \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot (e(\tilde{\tilde{u}}^\varepsilon_{pqr}) + \tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) + \sigma(u^\varepsilon_{pq}) \cdot (\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_r) \\ &+ \mathcal{R}(\varepsilon).\end{aligned} \tag{B.3}$$

where

$$\mathcal{R}(\varepsilon) = \int_{\mathcal{Y}} \sigma(\delta u^\varepsilon_{pq}) \cdot (\delta\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_r) = o(\varepsilon^2) \tag{B.4}$$

From (1.107) for $\varepsilon = 0$ and $\eta = \delta\tilde{\tilde{u}}^\varepsilon_{pqr}$ we have

$$\int_{\mathcal{Y}} \mathbf{C}(\mathrm{e}_i \otimes_s \mathrm{e}_j) \cdot e(\delta\tilde{\tilde{u}}^\varepsilon_{pqr}) = -\int_{\mathcal{Y}} \sigma(\tilde{u}_{ij}) \cdot e(\delta\tilde{\tilde{u}}^\varepsilon_{pqr}) = -\int_{\mathcal{Y}} \sigma(\delta\tilde{\tilde{u}}^\varepsilon_{pqr}) \cdot e(\tilde{u}_{ij}) \tag{B.5}$$

From (1.175) written for $\delta\tilde{\tilde{u}}^\varepsilon_{pqr}$, with $\eta = \tilde{u}_{ij}$, noting that $\langle \tilde{u}_{ij} \rangle = 0$, we have

$$
\begin{aligned}
-\int_{\mathcal{Y}} \sigma(\delta\tilde{\tilde{u}}^\varepsilon_{pqr}) \cdot e(\tilde{u}_{ij}) = &-\int_{\mathcal{Y}} (\sigma(\delta\tilde{u}^\varepsilon_{pq})) \cdot (\tilde{u}_{ij} \otimes_s \mathrm{e}_r) + \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) \cdot e(\tilde{u}_{ij}) \\
&- (1-\gamma) \int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}^\varepsilon_{pqr}) + \mathbf{C}(\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r)) \cdot e(\tilde{u}_{ij}) \\
&+ (1-\gamma) \int_{B_\varepsilon} \sigma(u^\varepsilon_{pq}) \cdot (\tilde{u}_{ij} \otimes_s \mathrm{e}_r)
\end{aligned}
\tag{B.6}
$$

Then we insert (B.6) into (B.3) (reminder: $u_{ij} = \tilde{u}_{ij} + (\mathrm{e}_i \otimes_s \mathrm{e}_j)y$)

$$
\begin{aligned}
\frac{V}{2}(\mathbf{E}^h_\varepsilon - \mathbf{E}^h)_{ijpqr} = &\int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) \cdot e(u_{ij}) + \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_r) \cdot e(u_{pq}) \\
&+ (\gamma-1) \int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}^\varepsilon_{pqr}) + \mathbf{C}\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) \cdot e(u_{ij}) \\
&+ (\gamma-1) \int_{B_\varepsilon} \sigma(u^\varepsilon_{pq}) \cdot (\delta\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_r) \\
&+ \mathcal{R}(\varepsilon).
\end{aligned}
\tag{B.7}
$$

We remark that the third term of the right hand side of equation (B.7) is $o(\varepsilon^2)$. We introduce the following adjoint states $\upsilon^r_{ij} \in \mathcal{V}$ and $\upsilon^r_{pq} \in \mathcal{V}$ satisfying

$$
\int_{\mathcal{Y}} \sigma(\upsilon^r_{ij}) \cdot e(\eta) = \int_{\mathcal{Y}} (\sigma(u_{ij}) - \mathbf{C}^h(\mathrm{e}_i \otimes_s \mathrm{e}_j)) \cdot (\eta \otimes_s \mathrm{e}_r), \tag{B.8}
$$

$$
\int_{\mathcal{Y}} \sigma(\upsilon^r_{pq}) \cdot e(\eta) = \int_{\mathcal{Y}} (\sigma(u_{pq}) - \mathbf{C}^h(\mathrm{e}_p \otimes_s \mathrm{e}_q)) \cdot (\eta \otimes_s \mathrm{e}_r), \tag{B.9}
$$

for any $\eta \in \mathcal{W}$.

We set $\eta = \delta\tilde{u}^\varepsilon_{pq}$ in (B.8), and $\eta = \delta\tilde{u}^\varepsilon_{ij}$ in (B.9), we set $\eta = \upsilon^r_{ij}$ in (1.148) and $\eta = \upsilon^r_{pq}$ in (1.148) written for $\delta\tilde{u}^\varepsilon_{ij}$. Taking into account that $\langle \delta\tilde{u}^\varepsilon_{pq} \rangle = 0$ and $\langle \delta\tilde{u}^\varepsilon_{ij} \rangle = 0$, we find

$$
\begin{aligned}
\frac{V}{2}(\mathbf{E}^h_\varepsilon - \mathbf{E}^h)_{ijpqr} = &(1-\gamma) \int_{B_\varepsilon} \sigma(u^\varepsilon_{pq}) \cdot e(\upsilon^r_{ij}) + (1-\gamma) \int_{B_\varepsilon} \sigma(u^\varepsilon_{ij}) \cdot e(\upsilon^r_{pq}) \\
&- (1-\gamma) \int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}^\varepsilon_{pqr}) + \mathbf{C}\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) \cdot e(u_{ij}) \\
&+ o(\varepsilon^2).
\end{aligned}
\tag{B.10}
$$

Finally, following the calculations led in Section 1.3.5, we obtain:

$$
\begin{aligned}
D_T(\mathbf{E}^h_{ijpqr}) = &\, 2\mathbb{P}\sigma(u_{pq}) \cdot e(\upsilon^r_{ij}) + 2\mathbb{P}\sigma(u_{ij}) \cdot e(\upsilon^r_{pq}) \\
&- 2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr}) + \mathbf{C}\tilde{u}_{pq} \otimes_s \mathrm{e}_r) \cdot e(u_{ij}).
\end{aligned}
\tag{B.11}
$$

B.2 Topological derivative of the tensor $\mathbf{F}^h$

Let $0 \le \varepsilon < \varepsilon_0$, we recall the definition of $\mathbf{F}^h_\varepsilon$:

$$
(\mathbf{F}^h_\varepsilon)_{ijkpqr} = \frac{1}{V} \int_{\mathcal{Y}} \gamma_\varepsilon \mathbf{C}(\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}^\varepsilon_{ijk})) \cdot (\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r + e(\tilde{\tilde{u}}^\varepsilon_{pqr})). \tag{B.12}
$$

We first simplify $\mathbf{F}_\varepsilon^h$ thanks to the identity (1.108), in view of $\langle \tilde{\tilde{u}}_{pqr}^\varepsilon \rangle = 0$, and because $\mathbf{C}^h(\mathrm{e}_i \otimes_s \mathrm{e}_j)$ is a constant tensor. This gives

$$(\mathbf{F}_\varepsilon^h)_{ijkpqr} = \frac{1}{V}\int_{\mathcal{Y}} \gamma_\varepsilon \left(\mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}_{ijk}^\varepsilon)) \cdot (\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) + \sigma(u_{ij}^\varepsilon) \cdot (\tilde{\tilde{u}}_{pqr}^\varepsilon \otimes_s \mathrm{e}_k) \right). \quad \text{(B.13)}$$

Using (1.169) we directly compute the difference $V(\mathbf{F}_\varepsilon^h - \mathbf{F}^h)$, in view of the estimates used in Section 1.3.5:

$$\begin{aligned} V(\mathbf{F}_\varepsilon^h - \mathbf{F}^h)_{ijkpqr} = &\int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k + e(\delta\tilde{\tilde{u}}_{ijk}^\varepsilon)) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) + \sigma(\delta u_{ij}^\varepsilon) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) \\ &+ \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}_{ijk})) \cdot (\delta\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) + \sigma(u_{ij}) \cdot (\delta\tilde{\tilde{u}}_{pqr}^\varepsilon \otimes_s \mathrm{e}_k) \\ &+ (\gamma - 1)\int_{B_\varepsilon} \mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}_{ijk}^\varepsilon)) \cdot (\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) + \sigma(u_{ij}^\varepsilon) \cdot (\tilde{\tilde{u}}_{pqr}^\varepsilon \otimes_s \mathrm{e}_k) \\ &+ o(\varepsilon^2). \end{aligned} \quad \text{(B.14)}$$

From there, we recall from (1.175) that we have

$$\begin{aligned} \int_{\mathcal{Y}} \sigma(\delta\tilde{\tilde{u}}_{ijk}^\varepsilon) \cdot e(\eta) = &\int_{\mathcal{Y}} (\sigma(\delta\tilde{u}_{ij}^\varepsilon) - (\mathbf{C}_\varepsilon^h - \mathbf{C}^h)(\mathrm{e}_i \otimes_s \mathrm{e}_j)) \cdot (\eta \otimes \mathrm{e}_k) - \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k) \cdot e(\eta) \\ &+ (1-\gamma)\int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}_{ijk}^\varepsilon) + \mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k)) \cdot e(\eta) - (1-\gamma)\int_{B_\varepsilon} \sigma(u_{ij}^\varepsilon) \cdot (\eta \otimes \mathrm{e}_k). \end{aligned} \quad \text{(B.15)}$$

We introduce the following adjoint states $v_{Fijk} \in \mathcal{V}$ and $w_{Fijk} \in \mathcal{V}$, which satisfy for any $\eta \in \mathcal{W}$:

$$\int_{\mathcal{Y}} \sigma(v_{Fijk}) \cdot e(\eta) = \int_{\mathcal{Y}} (\sigma(u_{ij}) - \mathbf{C}^h(\mathrm{e}_i \otimes_s \mathrm{e}_j)) \cdot (\eta \otimes_s \mathrm{e}_k) \quad \text{(B.16)}$$

$$\int_{\mathcal{Y}} \sigma(w_{Fijk}) \cdot e(\eta) = \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k) \cdot e(\eta). \quad \text{(B.17)}$$

We simplify the term $\mathbf{C}e(\delta\tilde{\tilde{u}}_{ijk}^\varepsilon) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r)$ by setting $\eta = \delta\tilde{\tilde{u}}_{ijk}^\varepsilon$ in (B.17) written with indices ijk replaced by pqr, and setting $\eta = w_{Fpqr}$ in (B.15), and we simplify the term $\sigma(u_{ij}^\varepsilon) \cdot (\tilde{\tilde{u}}_{pqr}^\varepsilon \otimes_s \mathrm{e}_k)$ by setting $\eta = \delta\tilde{\tilde{u}}_{pqr}^\varepsilon$ in (B.16) and $\eta = v_{Fijk}$ in (B.15) written for pqr instead of ijk. We can develop the expression (B.14)

$$\begin{aligned} V(\mathbf{F}_\varepsilon^h - \mathbf{F}^h)_{ijkpqr} = &\int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r) + \sigma(\delta u_{ij}^\varepsilon) \cdot (\tilde{\tilde{u}}_{pqr} \otimes_s \mathrm{e}_k) \\ &+ \int_{\mathcal{Y}} \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}_{ijk})) \cdot (\delta\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) \\ (iii) \quad &+ (\gamma - 1)\int_{B_\varepsilon} \mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k + e(\tilde{\tilde{u}}_{ijk}^\varepsilon)) \cdot (\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) + \sigma(u_{ij}^\varepsilon) \cdot (\tilde{\tilde{u}}_{pqr}^\varepsilon \otimes_s \mathrm{e}_k) \\ (iv) \quad &+ \int_{\mathcal{Y}} \sigma(\delta\tilde{u}_{ij}^\varepsilon) \cdot (w_{Fpqr} \otimes_s \mathrm{e}_k) - \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k) \cdot e(w_{Fpqr}) \\ (v) \quad &+ (1-\gamma)\int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}_{ijk}^\varepsilon) + \mathbf{C}(\tilde{u}_{ij}^\varepsilon \otimes_s \mathrm{e}_k)) \cdot e(w_{Fpqr}) - (1-\gamma)\int_{B_\varepsilon} \sigma(u_{ij}^\varepsilon) \cdot (w_{Fpqr} \otimes_s \mathrm{e}_k) \\ (vi) \quad &+ \int_{\mathcal{Y}} \sigma(\delta\tilde{u}_{pq}^\varepsilon) \cdot (v_{Fijk} \otimes_s \mathrm{e}_r) - \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r) \cdot e(v_{Fijk}) \\ (vii) \quad &+ (1-\gamma)\int_{B_\varepsilon} (\sigma(\tilde{\tilde{u}}_{pqr}^\varepsilon) + \mathbf{C}(\tilde{u}_{pq}^\varepsilon \otimes_s \mathrm{e}_r)) \cdot e(v_{Fijk}) - (1-\gamma)\int_{B_\varepsilon} \sigma(u_{pq}^\varepsilon) \cdot (v_{Fijk} \otimes_s \mathrm{e}_r) \\ &+ o(f(\varepsilon)). \end{aligned} \quad \text{(B.18)}$$

First we develop the sum of lines (iii), (v), and (vii) of the right hand side of (B.18), taking into account that $v_{Fijk} - w_{Fijk} = \tilde{\tilde{u}}_{ijk}$:

$$\begin{aligned}(iii) + (v) + (vii) = {} & \pi\varepsilon^2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r) \\ & + \pi\varepsilon^2\mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot (v_{Fpqr}(\hat{y}) \otimes_s \mathrm{e}_k) \\ & + \pi\varepsilon^2\mathbb{P}\sigma(u_{pq})(\hat{y}) \cdot (v_{Fijk}(\hat{y}) \otimes_s \mathrm{e}_r) \\ & - \pi\varepsilon^2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot e(w_{Fpqr}) \\ & - \pi\varepsilon^2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot e(v_{Fijk}) \end{aligned} \tag{B.19}$$

We gather corresponding terms, and add and remove in the last line $e(v_{Fijk}) \pm \tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)$, this gives

$$\begin{aligned}(iii) + (v) + (vii) = {} & \pi\varepsilon^2\mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot (v_{Fpqr}(\hat{y}) \otimes_s \mathrm{e}_k) \\ & + \pi\varepsilon^2\mathbb{P}\sigma(u_{pq})(\hat{y}) \cdot (v_{Fijk}(\hat{y}) \otimes_s \mathrm{e}_r) \\ & - \pi\varepsilon^2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot (e(w_{Fpqr})(\hat{y}) - (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \\ & - \pi\varepsilon^2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot (e(w_{Fijk})(\hat{y}) - (\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \\ & - \pi\varepsilon^2\mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot (e(\tilde{\tilde{u}}_{ijk})(\hat{y}) + (\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)). \end{aligned} \tag{B.20}$$

We gather corresponding terms taking into account that $v_{Fijk} - w_{Fijk} = \tilde{\tilde{u}}_{ijk}$, and using the symmetry of all the involved tensors

$$\begin{aligned} V(\mathbf{F}^h_\varepsilon - \mathbf{F}^h)_{ijkpqr} = {} & (iii) + (v) + (vii) + o(\varepsilon^2) \\ & + \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}^\varepsilon_{ij} \otimes_s \mathrm{e}_k) \cdot (\tilde{u}_{pq} \otimes_s \mathrm{e}_r - e(w_{Fpqr})) + \sigma(\delta u^\varepsilon_{ij}) \cdot (v_{Fpqr} \otimes_s \mathrm{e}_k) \\ & + \int_{\mathcal{Y}} \mathbf{C}(\delta\tilde{u}^\varepsilon_{pq} \otimes_s \mathrm{e}_r) \cdot (\tilde{u}_{ij} \otimes_s \mathrm{e}_k - e(w_{Fijk})) + \sigma(\delta\tilde{u}^\varepsilon_{pq}) \cdot (v_{Fijk} \otimes_s \mathrm{e}_r). \end{aligned} \tag{B.21}$$

We recall that

$$\int_{\mathcal{Y}} \sigma(\delta\tilde{u}^\varepsilon_{ij}) \cdot e(\eta) = (1-\gamma)\int_{B_\varepsilon} \sigma(u^\varepsilon_{ij}) \cdot e(\eta), \tag{B.22}$$

and we introduce the following adjoint state $q_{F}{}^{r}_{ijk} \in \mathcal{V}$, which satisfies for any $\eta \in \mathcal{W}$:

$$\begin{aligned} \int_{\mathcal{Y}} \sigma(q_{F}{}^{r}_{ijk}) \cdot e(\eta) = {} & \int_{\mathcal{Y}} [\mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k - e(w_{Fijk})) - \langle \mathbf{C}(\tilde{u}_{ij} \otimes_s \mathrm{e}_k - e(w_{Fijk}))\rangle] \cdot (\eta \otimes_s \mathrm{e}_r) \\ & + \int_{\mathcal{Y}} (\mathbf{C}(v_{Fijk} \otimes_s \mathrm{e}_r)) \cdot e(\eta). \end{aligned} \tag{B.23}$$

Setting $\eta = \delta\tilde{u}^\varepsilon_{pq}$ into equation (B.23), and $\eta = q_{F}{}^{r}_{ijk}$ into the equation (B.22) written with pq indices, and proceeding the same interchanging indices ijk and pqr, we have

$$\begin{aligned} V(\mathbf{F}^h_\varepsilon - \mathbf{F}^h)_{ijkpqr} = {} & (iii) + (v) + (vii) + o(\varepsilon^2) \\ & + (1-\gamma)\int_{B_\varepsilon} \sigma(u^\varepsilon_{ij}) \cdot e(q_{F}{}^{k}_{pqr}) + (1-\gamma)\int_{B_\varepsilon} \sigma(u^\varepsilon_{pq}) \cdot e(q_{F}{}^{r}_{ijk}). \end{aligned} \tag{B.24}$$

We can write, starting gathering corresponding terms, regarding the equality $v_{Fijk} = \tilde{\tilde{u}}_{ijk} + w_{Fijk}$, and in view of the previous calculations:

$$V(\mathbf{F}^h_\varepsilon - \mathbf{F}^h)_{ijkpqr} = \pi\varepsilon^2\mathbb{P}\sigma(u_{ij}(\hat{y})) \cdot (v_{Fpqr}(\hat{y}) \otimes_s \mathrm{e}_k)$$

$$
\begin{aligned}
&+ \pi\varepsilon^2 \mathbb{P}\sigma(u_{pq}(\hat{y})) \cdot (v_{Fijk}(\hat{y}) \otimes_s \mathrm{e}_r) \\
&- \pi\varepsilon^2 \mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot (e(w_{Fpqr}) - (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \\
&- \pi\varepsilon^2 \mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot e(w_{Fijk} - (\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \\
&- \pi\varepsilon^2 \mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot (e(\tilde{\tilde{u}}_{ijk})(\hat{y}) + (\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \\
&- \pi\varepsilon^2 \mathbb{P}\sigma(u_{ij})(\hat{y}) \cdot e(q_{Fpqr^k})(\hat{y}) - \pi\varepsilon^2 \mathbb{P}\sigma(u_{pq})(\hat{y}) \cdot e(q_{Fijk^r})(\hat{y}) + o(\varepsilon^2).
\end{aligned}
\tag{B.25}
$$

Finally we have

$$
\begin{aligned}
(\mathbf{F}^h_\varepsilon - \mathbf{F}^h)_{ijkpqr} = {} & 2\frac{\pi\varepsilon^2}{V} \left[\mathbb{P}\sigma(u_{ij}(\hat{y})) \cdot (v_{Fpqr}(\hat{y}) \otimes_s \mathrm{e}_k - e(q_{Fpqr^k}))\right]^{\mathrm{sym}} \\
& - 2\frac{\pi\varepsilon^2}{V} \left[\mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot (e(w_{Fpqr}) - (\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r))\right]^{\mathrm{sym}} \\
& - \frac{\pi\varepsilon^2}{V} \mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot (e(\tilde{\tilde{u}}_{ijk})(\hat{y}) + (\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) + o(\varepsilon^2),
\end{aligned}
\tag{B.26}
$$

where for a sixth order tensor $\mathbf{F}$, we define

$$
\mathbf{F}^{\mathrm{sym}}_{ijkpqr} := \frac{1}{2}(\mathbf{F}_{ijkpqr} + \mathbf{F}_{pqrijk}). \tag{B.27}
$$

This expression can also be written as follows by simplifying lines 2 and 3 of (B.26)

$$
\begin{aligned}
(\mathbf{F}^h_\varepsilon - \mathbf{F}^h)_{ijkpqr} = {} & 2\frac{\pi\varepsilon^2}{V} \left[\mathbb{P}\sigma(u_{ij}(\hat{y})) \cdot (v_{Fpqr}(\hat{y}) \otimes_s \mathrm{e}_k - e(q_{Fpqr^k}))\right]^{\mathrm{sym}} \\
& - 2\frac{\pi\varepsilon^2}{V} \left[\mathbb{P}(\sigma(\tilde{\tilde{u}}_{ijk})(\hat{y}) + \mathbf{C}(\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) \cdot e(v_{Fpqr})\right]^{\mathrm{sym}} \\
& + \frac{\pi\varepsilon^2}{V} \mathbb{P}(\sigma(\tilde{\tilde{u}}_{pqr})(\hat{y}) + \mathbf{C}(\tilde{u}_{pq}(\hat{y}) \otimes_s \mathrm{e}_r)) \cdot (e(\tilde{\tilde{u}}_{ijk})(\hat{y}) + (\tilde{u}_{ij}(\hat{y}) \otimes_s \mathrm{e}_k)) + o(\varepsilon^2).
\end{aligned}
\tag{B.28}
$$