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Thèse de Doctorat

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UFC UNIVERSITÉ DE FRANCHE-COMTÉ

Contribution au noyau d'un logiciel de modélisation asymptotique symbolique

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Bin YANG

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Contribution to a kernel of a symbolic asymptotic modeling software

Dissertation

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By

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ABSTRACT

This thesis is dedicated to develop a kernel of a symbolic asymptotic modeling software package `MEMSALab` which will be used for automatic generation of asymptotic models for arrays of micro and nanosystems. Unlike traditional software packages aimed at numerical simulations by using pre-built models, the purpose of `MEMSALab` is to derive asymptotic models for input equations by taking into account their own features i.e. the scalar valued/vector valued solution, different estimates on the solutions and sources, thin structures, periodic structures, multiple nested scales etc.

We have proposed an approach called "*by extension-combination*" for the asymptotic modeling which allows an incremental model construction so that the wanted features can be included step by step. In this approach, the derivation starts from a so-called reference proof which is a periodic homogenization model derivation for a second order elliptic equation with periodic coefficient defined in a one-dimensional domain, then a complex model is constructed by extending and combining elementary models, each of which covers a specific feature, until all wanted features are taken into account. On the other hand, a theoretical framework for the computer-aided asymptotic model derivation is proposed. It relies on a combination of the asymptotic method used in the field of partial differential equations with term rewriting techniques coming from computer science. In this framework, the first order rewriting rules (FO-rules) are used to express mathematical rules and their application are controled by first order strategies. The design of FO-rules benefits from the grammar which is proposed for a systematic formulation of all needed mathematical objects, ie geometry domains, functions, operators etc, used in the model derivation. Then second order rewriting rules (SO-rules) and strategies are introduced to built elementary models by extending existing proofs and to combine them to built complex models. To avoid conflicts in the combination of extensions, each SO-rule is formulated as a combination of unit outward growths. Each unit outward growth is a composition of an *R-semantic conservation SO-rule* and an *Admissible parameterized SO-rule* corresponding to semantic conservation transformation and parametrization of the FO-rules. Thanks to the simple formulation of the unit outward growth, the behavior of their combination becomes possible to be studied. Then the rules for fluent combinations are proposed.

The interest of this approach is that if features of the input model are covered by the existing elementary models, the derivation can be generated by applying combination of the existing rules on the reference proof. This facilitates the pro-

gramming for new models.

Next, an homogenization model of the electrothermoelastic equation defined in a multi-layered thin domain has been derived following the reference proof by using extended mathematical rules and some extended steps. It contributes in two aspects. First, the model can be used for simulation embedded in an optimization loop. Second, it prepares the design of related extensions for its inclusion in MEMSALab.

At last, an optimization tool has been developed by combining a house-made optimization software package SIMBAD and COMSOL-MATLAB simulation and it has been applied for optimization of a SThM probe. General optimization principles have been summarized and an optimal design has been obtained.

Keywords: Multi-scale, Arrays, Nanosystem, Asymptotic model, Rewriting technique, extension-combination, Elementary model, Thin-domain, Feature, Optimization

Résumé

Cette thèse est consacrée au développement d'un noyau du logiciel MEMSALab de modélisation par calcul symbolique qui sera utilisé pour la génération automatique de modèles asymptotiques pour des matrices de micro et nanosystèmes. Contrairement à des logiciels traditionnels réalisant des simulations numériques utilisant des modèles prédéfinis, le principe de fonctionnement de MEMSALab est de construire des modèles asymptotiques qui transforment des équations aux dérivées partielles en tenant compte de leurs caractéristiques, à savoir : la nature scalaire ou vectorielle de la solution, les ordres des estimations des solutions et des sources, la périodicité de coefficients ou de géométries, la minceur de certaines parties, ou bien la présence d'échelles multiples imbriquées.

Nous avons proposé une méthode appelée "par extension-combinaison" pour la modélisation asymptotique, qui permet la construction de modèle de façon incrémentale de sorte que les caractéristiques désirées soient incluses étape par étape. Par cette approche, la construction d'un modèle utilise la démonstration d'un modèle qui sert de référence. Ce dernier est un modèle d'homogénéisation périodique d'une équation elliptique du second ordre avec coefficient périodique définie dans un domaine mono-dimensionnel. Un modèle complexe est ensuite réalisé par la combinaison d'extensions élémentaires de ce modèle, chaque extension tenant compte d'une caractéristique spécifique, jusqu'à ce que toutes les caractéristiques nécessaires soient prises en compte. Un cadre théorique a été proposé pour la formulation de cette méthode de façon à ce qu'elle puisse être mise en oeuvre de façon informatique. Il repose sur une combinaison de méthodes asymptotiques issues de la théorie des équations aux dérivés partielles et de techniques de réécriture issues de l'informatique. Dans ce cadre, les règles de réécriture du premier ordre sont utilisées pour exprimer des règles mathématiques et leur applications sont contrôlées par des stratégies du premier ordre. Ces règles et stratégies sont exprimées dans une grammaire qui permet de prendre en compte tous les objets mathématiques nécessaires, à savoir les domaines géométriques, les fonctions, les opérateurs etc... . Des règles de réécriture et des stratégies du second ordre servent à construire des extensions de la preuve de référence et à les combiner. Pour éviter les conflits dans la combinaison d'extensions, ces règles du second ordre sont formulées par des opérations simples ou par leurs combinaisons, introduites pour l'occasion, appelées "greffes". Grâce à ce concept, la combinaison devient une opération facile à réaliser. L'intérêt de cette approche est que si les caractéristiques du modèle d'entrée sont bien couvertes par les extensions élémentaires existantes, la construction du nouveau modèle asymptotique est générée par simple combinaison des extensions de la preuve de référence. Cela permet la construction et la programmation de nouveaux modèles.

Ensuite, un modèle d'homogénéisation de l'équation d'électro-thermo-mécanique

posée dans un domaine mince multicouche est établi en suivant les étapes de la construction du modèle de référence, mais utilisant des propriétés plus générales. Cette contribution conduit d'une part à un nouveau modèle qui peut être utilisé comme modèle simplifié qui peut être intégré dans un calcul d'optimisation pour accélérer les calculs. D'autre part, elle prépare l'implantation de la construction de ce modèle dans MEMSALab exprimée sous forme d'extensions élémentaires et de leurs combinaisons. Pour finir, un outil d'optimisation a été développé en combinant SIMBAD, une boite à outils logicielle pour l'optimisation et développée en interne, et COMSOL-MATLAB. Il a été appliqué pour étudier la conception optimale d'une classe de sondes de microscopie atomique thermique et a permis d'établir des règles générale pour leurs conception.

Mots-clés: Multi-échelle, réseau, nanosystèmes, modèle asymptotique, technique de réécriture, extension-combinaison, modèle primaire, mince-domaine, caractéristique, Optimisation

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1 Context of the thesis: micro-system arrays, asymptotic methods and their implementation

During the past two decades, in the field of micro and nanotechnologies, a number of devices involving arrays on a chip, or *MEMS*[1] *Arrays* have been fabricated. Typical ones are micro-conveyors, arrays of micro-cantilevers (used for atomic force microscopy, nano-lithography or data storage), arrays of micro-mirrors and micro-lenses (used in optical applications e.g. in video projectors and lithography masks, and in many applications such as filters for fiber optic and laser arrays), arrays of microneedles, micro-bolometers, etc, see Figure 1. These systems have common

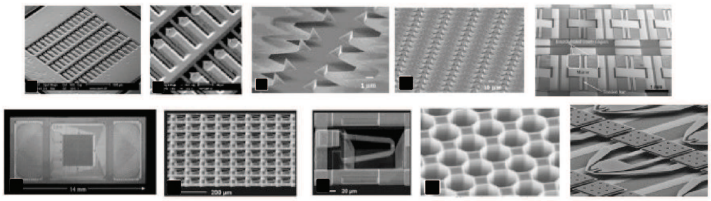


Figure 1: Examples of micro-system arrays

features: they are distributed, often spatially periodic, and they have multi-physics and various multi-scale characteristics. Because of the complex geometry of their cells, having possibly a multiscale structure, and their large number the direct simulation of the micro-system arrays by a numerical method as the Finite Element Method (FEM) turns out to be impractical. Extensive development of such systems requires design and simulation tools which motivates this work and more generally a research activity at the FEMTO-ST institute. It is worthwhile mentioning that the presented application is about scanning thermal microscopy and involves a relatively complex microsystem, but not an array. However, as the reader will see, the developed model fits well with the illustration needed by our approach.

Asymptotic methods. One possible solution is to use *asymptotic methods* and especially periodic homogenization methods. Asymptotic methods applied to partial differential equations (PDE, for short) are model reduction techniques, their purpose is to approximate the initial model, given as a PDE, by a second model of which the simulation by the FEM can be done in a reasonable time. They are very useful for complex system simulation and are of great interest in the software design community. They have experienced strong growth since 1980, with an increasing range of applications in all fields of physics and engineering: thermal,

[1] Micro-Electro-Mechanical Systems

solid and fluid mechanical, electromagnetism, etc. They have rigorous mathematical foundation and can lead to error estimates based on the small parameters involved in the approach. This is a valuable aspect from the model reliability point of view. They have been applied when a physical problem depends on one or more small parameters which can be some coefficients or can be related to the geometry. Their principle is to identify the asymptotic model obtained when the parameters tend to zero. For instance, this method applies in periodic homogenization, i.e. to systems consisting of a large number of periodic cells, the small parameter being the ratio of the cell size over the size of the complete system, see for instance [7, 30, 44]. Another well-developed case is when parts of a system are thin, e.g. thin elastic plates as in [26], that is to say that some of their dimensions are small compared to others. A third kind of use is that of strongly heterogeneous systems e.g. [15], i.e. when equation coefficients are much smaller in some parts of a system than in others. These three cases can be combined in many ways leading to a broad variety of configurations and models. In addition, it is possible to take into account several nested scales and the asymptotic characteristics can be different at each scale: thin structures to a scale, periodic structures to another, e.g. [11], [12], [13], [46], etc. It is also possible to cover cases where the asymptotic phenomena happen only in certain regions or even are localized to the boundary. Moreover, different physical phenomena can be taken into account: heat transfer, solid deformations, fluid flow, fluid-structure interaction or electromagnetics. In each model, the coefficients can be random or deterministic. Finally, different operating regimes can be considered as the static or the dynamic regimes, or the associated spectral problems. Today, there exists a vast literature covering an impressive variety of configurations.

Asymptotic methods, enjoy a number of advantages. The resulting models are generally much faster (often by several order of magnitude – depending on the kind of model simplification –) to simulate than the original one and are fully parameterized, which is not the case with other model order reduction approaches. In addition, they do not require any long numerical calculation for building them, so they can be inserted into identification and optimization loops of a design process. Finally, they are of general use and they can be rigorously applied whenever a model depends on one or several small parameters and the error between their solution and nominal model solution can be estimated.

There is a vast literature on asymptotic methods for PDEs both in applied mathematics and in many modeling areas. Many reference books have been published, and there are several journal devoted to them. (SIAM: Multi-scale Modeling and Simulation, Asymptotic Analysis, Networks and Heterogeneous Media, International Journal for Multi-scale Computational Engineering, Journal of Multi-scale Modeling, International Journal of Theoretical and Applied Multi-scale Mechanics

etc...).

Two-scale convergence. For periodic homogenization, several methods have been emerging over the years. In this thesis, we focus on the two-scale convergence. In 1989 in [52], the notion of two-scale convergence was introduced for periodic homogenization problems and this method was further developed in [1]. Independently, in 1990, the reference [3] introduced a dilation operation to study homogenization for a periodic medium with double porosity. This technique was used again in [16], [2] and [50]. M. Lenczner with his co-workers in [45]-[49] used the same idea to develop a complete framework yielding similar results for periodic homogenization as the two-scale convergence method. They introduced this new technique to address homogenization of spatially periodic analog electronic circuits in view of their application in arrays of MEMS. Then, J. Casado Diaz et al. [23], [24]-[25] combined it with the two-scale convergence to study perforated domains and thin structures. Then, the same concept was called *periodic unfolding method* by D. Cioranescu, A. Damlamian and G. Griso who have developed a number of their properties, including error estimates, in [25], [28], [37] [38] and [39]. This technique has been extensively developed by many other authors in a variety of applications. In particular, it has been applied to find models of complex structures combining other asymptotic features, as thin structure or strong heterogeneity of coefficients, with the periodic homogenization, see among others [11], [12], [13], or [46]. We notice that in [47], an attention has been paid to formulate the proofs of model derivation as a sequence of algebraic calculation without relying on abstract arguments.

Existing FEM simulation software and homogenization software. FEM simulation software packages have been developed and applied in a lot of fields in the recent decades. The comercial finite element analysis software packages `ABAQUS`, `ANSYS`, `COMSOL` and `CONVENTOR` are the most famous and widely used among the software simulation packages. They are used in the simulation of multi-physics, and in particular, `CONVENTOR` is specialized in the simulation of the micro-system arrays. On the other hand, free finite element analysis software packages, such as `Code Aster, FreeFem++`, have also been developed. Such software implement very limited number of multi-scale models. However, a number of homogenization software packages also exist. For example, `Helius` from Firehole, `MAC/GMC` from NASA, `CZone` from Engenuity, and `DIGIMAT` from eXstream Engineering. `Helius` and `DIGIMAT` are specialized in the analysis of the properties of composite materials by using different homogenization methods. The Multicontinuum Technology is used in `Helius`, and the Mean-Field homogenization method is used in `DIGIMAT`. In these homogenization software packages, the homogenized models are pre-computed case-by-case. They can cover a limited number of pos-

sible models, which remains a tiny fraction of possible cases, with regards to the wide variety of possible physical features and geometrical configurations.

Drawbacks of the asymptotic methods, motivation of the thesis. Commercial software already available on the market, such as `MDS`, `DIGIMAT`, `Firehole`, `Czone` mentioned above, are well connected with classical finite element software and their efficiency is clearly established. Of course, the homogenized models being implemented are specific to a physical field, and new models might be derived if another physics has to be taken into account. Other asymptotic features, as for instance those considered in this paper, are not used in the above-mentionned software. To take them into account would considerably multiply the number of possible models and render ineffective a model-by-model approach.

In addition to the problem of the number of possible models generated by combining various asymptotic methods, another limitation to their dissemination in engineering software is that each new configuration requires new long handmade calculations that may be based on several techniques. In the literature, each published paper focuses on a special case regarding geometry or physics, and no academic work is oriented in an effort to deal with a more general picture. Moreover, even if a large number of models combining various features have already been derived, the set of already addressed problems represents only a tiny fraction of these could be derived from all possible asymptotic feature combinations based on existing techniques.

Summing up, we can say that on the one hand, periodic homogenization models are well disseminated in some engineering communities, and that on the other hand transfering, in software for engineers, models built from combination of several asymptotic methods is not yet done, and seems to be not achievable in a model-by-model approach. We consider that this challenge can be formulated as a scientific problem that deserves to be posed and we propose first components of solution. Namely, we establish a mathematical framework for combining asymptotic methods of different natures and thus for producing, aided by a computer, a wide variety of complex models. The proposed solution combines principles of asymptotic model derivations, also called proofs, and *rewriting* methods issued from computer science.

2 Contributions of the thesis

Contrary to the approach followed in the homogenization software packages, our approach is more general: we rely on a *systematic* application of asymptotic meth-

ods, and we aim to implement them in a software package, called MEMSALab[2], that constructs approximated models. The architecture of MEMSALab is shown in Figure 2. It is designed to complement a FEM software package that has an internal formal representation of PDEs as `COMSOL` or `FreeFEM++`. It envisionned functioning consists in three steps completed with an optimization tool. The first step, by the *FEM software/ MEMSALab interface,* is a transfer, from a FEM software package, of a PDE (or a system of PDEs) and its translation in the grammar of the symbolic computation language used in the kernel of MEMSALab. In the second step, the multi-scale model (MSM) is symbolically derived and the result is saved. In the third step, by the *MEMSALab / FEM Software interface,* the MSM is translated back to the format of the FEM software package and its simulation is launched. The parameter updating and optimization tool is interfaced with the FEM software package.

This thesis, contributes only to some of these aspects, namely, the kernel of MEMSALab i.e. the MSM constructor is highlighted by yellow color in Figure 2 as described in Section 2.1, and the optimization tools for the application of MSM, introduced in Section 2.2. The latter has been done for an application to a class of systems governed by thermoelectroelasticity equations ie for scanning probes used in thermal microscopy. Moreover, an asymptotic model has been built that has indeed a wider range of applications as explained in Section 2.2. Its derivation follows the rules for being implemented in *MEMSALab*.

2.1 MEMSALab software design

Underlying principles of MEMSALab. Our design methodology consists of three aspects.

1. The first one is to establish a general mathematical theoretical framework for the multi-scale model derivations. In this unified framework, the derivations – in a setting of different physical features and geometries – could be different in details, but the *skeleton* of the derivations remains "the same". The mathematical proofs underling the model derivations are written in an algebraic way, few abstract reasoning is used. The algebraic nature of the proofs is crucial, since it allows implementation of the proofs as symbolic transformations.

2. The second aspect is the design and the implementation of a symbolic transformation tool to implement the multi-scale model derivations. The designer formulates the mathematical properties as well the elementary derivations (i.e. the skeleton proofs) with this tool.

[2]For MEMS Arrays

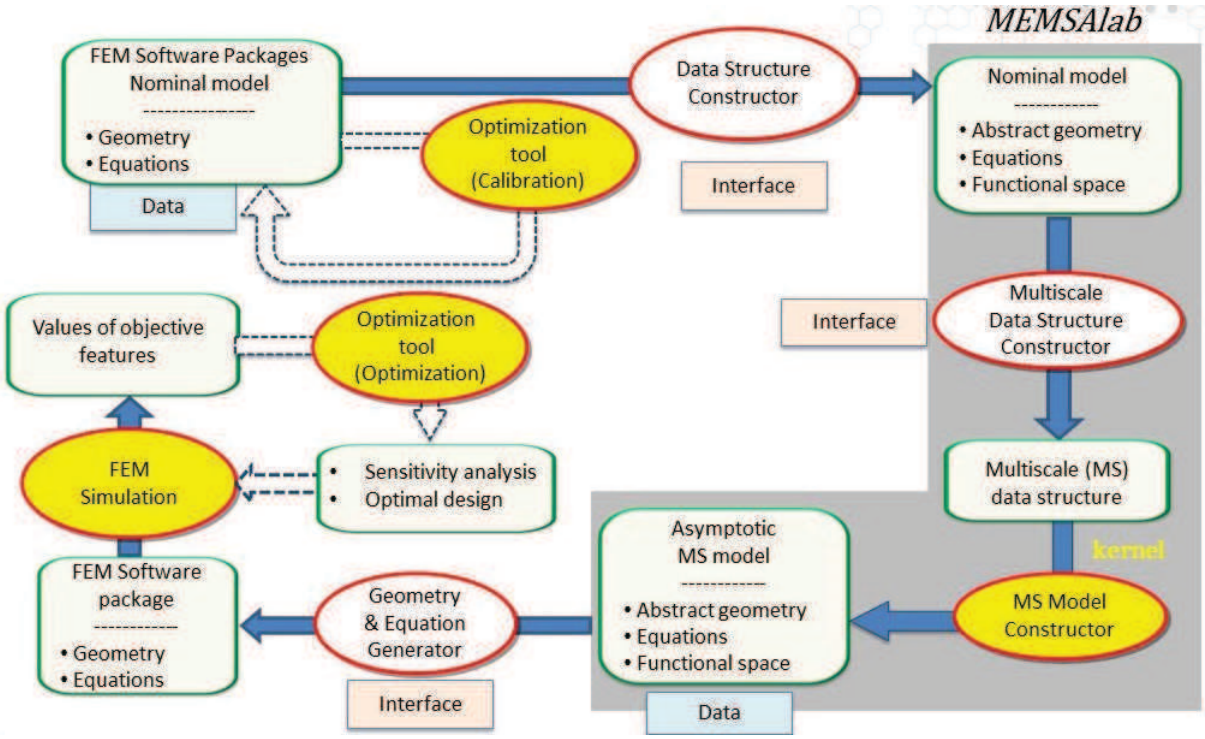


Figure 2: MEMSLab software architecture.

3. Since only the elementary derivations of the general framework are implemented in MEMSALab, the third aspect of our design methodology consists in developing an *extension mechanism* allowing the combination of the already implemented derivations. This is a systematic way to build complex models by reusing and combining already existing proofs.

Main steps of model derivation. The mathematical framework is this developed in [47] based on the two-scale transform also called the periodic unfolding operator. We think that it has the potential to be adapted to a large number of configurations without major change in the flow of the proofs, but we are aware that a lot of specific steps have to be changed/added. Basically, the model derivation by this approach has the three following steps commonly shared by most of the asymptotic methods:

1. Asymptotic expansions of the solutions, in a two-scale sense in our work, are assumed with regards to norm estimates, which are admitted in the current state. Then, weak limits of two-scale transforms of first-order derivatives are derived.

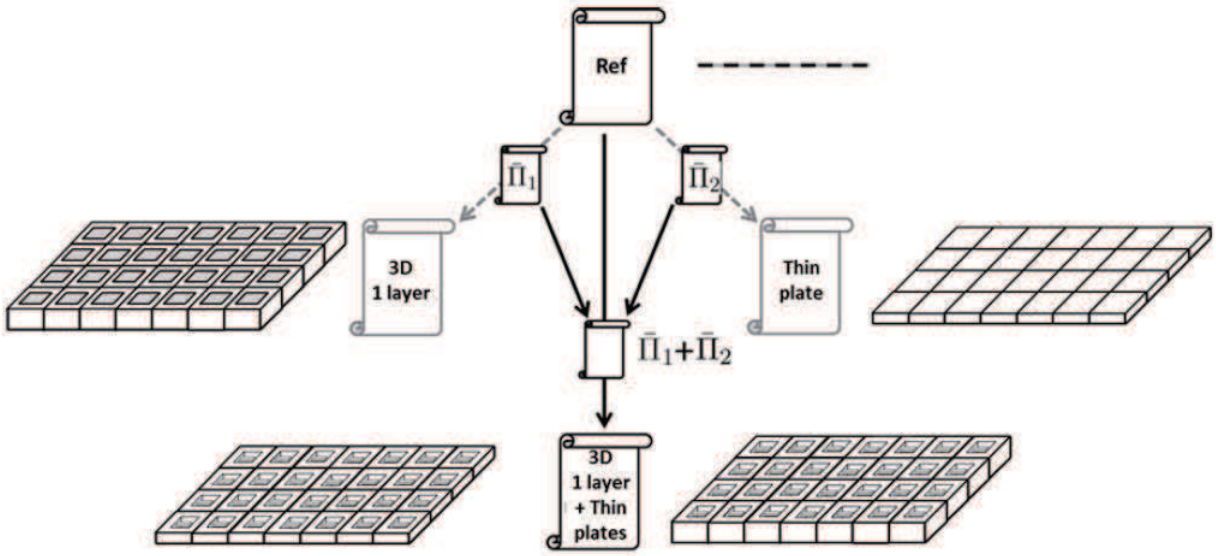


Figure 3: An extension of the reference proof (top) to the 3-dimensional setting (left) and to the thinness setting (right). The combination of these two extensions is depicted on the bottom.

2. The model derivation starts from weak formulations where test functions are chosen according to the asymptotic analysis to be carried out. An asymptotic two-scale is derived by using Step 1.

3. Elimination of micro-scale fields of the two scale model yields the reduced asymptotic model.

Principle of model derivation by extension-combination. In order to carry on a systematic approach for the derivation of multi-scale models that allows to cover a variety of physical features and geometries, we develop a method called *"by extension-combination"*. Figure 3 illustrates the idea behind this method through an example. This method relies on three key principles.

1. Firstly, we introduce a *reference model*, also called *skeleton model*, together with its derivation. This derivation is called the *reference proof*. The reference model is the periodic homogenization model of a scalar second-order elliptic equation posed in a one-dimensional domain, with Dirichlet boundary conditions. Its derivation is based on the technique of the two-scale transform introduced in [3], and reused in [17]. Here, we follow the model derivation

approach of [47] which relies on algebraic reasoning only. Although the reference model covers a very simple case, its proof is expressed in a sufficiently general way. A number of basic algebraic *properties* are formulated as *transformation rules*, they are considered as the building blocks of the proofs. The full derivation of the model is formulated as a sequence of applications of these rules. The proof of some properties is also performed by a sequence of applications of mathematical rules when the others are admitted e.g. the Green rule.

2. Then, an *elementary extension* (also called *elementary generalization*) is obtained by an application of an elementary transformation to the reference proof. Such elementary transformation covers a particular feature. More generally, many elementary transformations can be applied simultaneously to the reference proof, where each transformation covers a distinct feature. We notice that, in practice, when a single feature is taken into account, only a small change occurs in a relatively long proof. In other words, while considering an elementary extension, most of the existing rules could be reused by operating a small change on them, and, on the other hand, only a small number of new rules has to be manually introduced. From this empirical observation, it follows that the extension of the existing proofs to cover a new feature can be generated almost automatically.

3. Finally, we make possible the combination of two initial extensions to produce a new extension that takes into account the features covered by each initial extension. By iterating this process, many elementary extensions can be combined together. The use of the mechanism of the combination of several existing elementary extensions instead of the development of new extension transformations has the advantage of reducing the development effort by avoiding doing complex changes manually. Thus, the *"by extension-combination"* method is a reasonable one since it facilitates the implementation of the two-scale methods.

Rewriting-based principles used in the extension-combination method. We rely on a theoretical tool from computer science, called *term rewriting*. The reason is that equational reasoning can naturally be described by *rewriting rules*, see [4] for a classical reference. Roughly speaking, an equation $t = u$ can be turned into two rewriting rules $t \to u$ and $u \to t$, where t and u are rewriting terms consisting of function symbols and rewriting variables. The rule $t \to u$ states that every occurrence of t has to be transformed into u. Rules can have conditions and can be combined by specifying strategies that determine how to apply the rules, see e.g. [56, 32, 31, 14, 33].

The mathematical objects, such as geometric domains, variables defined on these domains, functions of many variables, operators (e.g. derivatives, integrals, two-scale transform, etc.), are common in the field of partial differential equations. The precise description of these objects is given by a *grammar*. In other words, mathematical expressions need a precise description since they carry all the information required in the formulation of the multi-scale models and their derivations.

Some of the rewriting rules require the computation of the set of mathematical variables on which an expression depends. For instance, in order to establish the linearity rule $L(\lambda\alpha) \to \lambda L(\alpha)$, where L is a linear operator and λ is a scalar, one needs to compute the variables on which λ depends in order to decide whether it is a scalar. For this purpose, we develop a *variable dependency analyzer*. Within this framework, a proof is a sequence of rewriting rules. In order to carry on the extension of the proofs and their combination (i.e."extension-combination" mechanism), we rely on the *second-order* rewriting rules which are applied to the (first-order) rewriting rules in order to extend them.

Implementation of model derivations and of the composition of extensions. We use the symbolic transformation language symbtrans, proposed in [6], to implement the proofs and their extensions as rewriting strategies. This language supports the rewriting modulo associativity and commutativity of the operations $+, \times, \cup$ and $\cap$. It is implemented with the scientific computing language `Maple`. Since, the rewriting strategies in symbtrans are `Maple` expressions, it is possible to apply the symbtrans strategies to themselves. This allowed us to implement the extension of the proofs (each proof is given as a symbtrans strategy) by means of symbtrans strategies. A proof is decomposed into blocks, each block is a series of applications of rewriting rules and strategies. Each rewriting rule corresponds to a mathematical property e.g. Green rule, linearity of certain operators, properties of the two-scale operators. The blocks can be grounded into a strategy that is applied to an initial expression that corresponds to the input PDE. Under some assumption[3], the combination of two extensions, each of which is a symbtrans strategy, is nothing but their sequential composition. This result can be found in [59] and it is detailed in Chapter 1 of this thesis.

Although, the combination of extensions as a sequential composition was useful for some situations, one could see its limitation. This motivates our next point.

A framework for the combination of extensions. It turns out that it is not easy to study the combination of extensions if these extensions are formulated as strategies, as presented in Chapter 1. To solve this problem, we refine the

[3]Namely, when there is not *conflict* between the extensions, i.e. when they operate on different parts of the initial proof.

notion of extension. Firstly, a rewriting rule is transformed into a more general rule such that they remain mathematically equivalent. Secondly, the second rule is generalized by means of a *parametrization* that consists in the replacement of some terms by rewriting variables. For example, consider the rule s:

$$s := \partial_x(uv) \to v\partial_x u + u\partial_x v$$

that represents the derivative of a product of two functions in the 1-dimensional setting. We want to build the rule s'':

$$s'' := \partial_{x_i}(uv) \to v\partial_{x_i} u + u\partial_{x_i} v$$

which is the counterpart of the rule s in the n-dimensional setting. We proceed in two steps. In a first step, we transform s to s':

$$s' := \partial_{x_1}(uv) \to v\partial_{x_1} u + u\partial_{x_1} v.$$

We notice that s and s' are mathematically equivalent and, in some sense, s' is more general than s. In a second step, we replace the constant 1 by the variable i and we get s''.

In Chapter 2 we establish a framework allowing the definition of the notion of generalization and parametrization and their combination.

2.2 Multiscale model and optimization of a thermoelectromechanical system

Since this work has been partially supported by the NANOHEAT project[4], a modelling and optimization activity has been developped for scaning thermal microscopy. We notice that

Motivations of the Scanning Thermal Microscopy. Modern technology of micro/nanoelectronic components, sensors and MEMS/NEMS (Micro/Nano-Electro-Mechanical-Systems) requires increasingly the control of materials at the sub-micrometer down to the nanometer scale. Additionally, the heat transfer phenomena, including e.g. phonon heat conduction mechanism in micro- and nanostructures, may differ significantly from that on the macroscale. Therefore, micro- and nanometer resolution is required for most of the experiments.

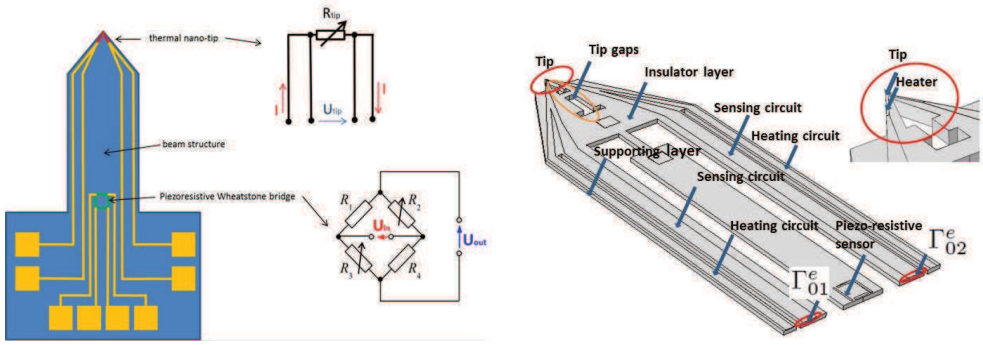
Scanning Thermal Microscopy (SThM) is a versatile scanning probe technique allowing for high resolution mapping of the thermal properties and temperature of various substrates. SThM, as every AFM (Atomic Force Microscopy) related

[4]http://www.nanoheat-project.eu/

technique enables study at micro- and nanoscale which allows designers to a better understanding of heat transport in micro- and nanoelectronic devices.

The invention of the scanning tunneling microscope (STM) [10] and the atomic force microscope (AFM) [9] have allowed sub-micrometer and, at times, atomic scale spatially resolved imaging of surfaces. The spatial resolution of these near-field techniques is only limited by the active area of the sensor (which in the case of STM may only be a few atoms at the end of a metal wire). As described by Dinwiddie and Pylkki in 1994, first scanning thermal microscopy (SThM) probes employed resistance thermometry to measure thermal properties [34]. These probes were fashioned and made from Wollaston process wire consisting of a thin platinum core (ca. 5 μm in diameter) surrounded by a thick silver sheath (ca. 75 μm). Because of its high endurance, Wollaston probe is attractive for microsystem diagnostics , however the active area in the range of a few micrometers does not allow quantitative thermal investigations at the nano-scale. Then, a new thermal probe has been designed in the framework of the NANOHEAT project to achieve quantitative measurement in the range of few tenths nanometers.

The probe design This novel type of nanosensor is equipped with sharp, conductive tip, an integrated deflection sensor, and an actuation system. It is integrated with deflection detection, which will significantly improve the system versatility and will enable new applications. As it is free of the bulk and complicated optical deflection sensors, it can be used in small chambers. The described SThM



(a) Schematic view of NANOHEAT SThm probe

(b) First design of the cantilever

Figure 4: NANOHEAT SThM probe

nanoprobes are designed to operate in two modes: a) as a passive thermosensing element or b) as an active heat flux meter. In the latter case, a larger current is passed through the resistive tip probe. The power that is required to maintain a constant temperature gradient between the tip and the sample corresponds to

the local thermal conductivity of the sample. During active measurements temperature of the tip is increased by $20 - 30$ K above room temperature. In order to perform quantitative measurements of heat transport between the tip and the surface several crucial criteria have to be met:

-low thermal mass of the microtip allowing for AC thermal measurements (e.g. in the range of 10 kHz)

-high mechanical stiffness of the microtip. This ensures high endurance of the thermal sensor, which is brought into contact while surface scanning.

-low stiffness of the SThM cantilever, which is brought in contact with the investigated surface. The low stiffness of the SThM cantilever will enable surface measurements with relatively low load forces. As a consequence the tip wear is reduced and the sample is not modified.

-high thermal resistance of the SThM cantilever and tip's support. The high thermal resistance of the cantilever will reduce the heat transfer from the thermal tip to the cantilever supporting body. The effective thermal mass of the SThM sensor will be reduced, and its influence on the thermal behavior of the investigated structure will be minimized.

Moreover, the heat transferred from the tip to the cantilever base causes parasitic deflection of the sensor. First results of modeling and simulations exhibit significant parasitic, 200 nm deflection of the cantilever due to tip's heating by 11 degrees above the room temperature.

According to the applications, developed SThM nanoprobe will enable surface measurements in contact scanning probe microscopy mode at load force ranging from 10 nN up to 1 microN. The load force will be detected with the resolution of 10 pN in the bandwidth of 100 Hz. The low load forces as well as sub-nanometer vertical spatial resolution in the range will be needed in investigations of graphene and molecular samples, whereas the high force will be applied in investigations of high-k insulators.

Modelling of a NANOHEAT probe. A thin plate model model of the thermoelectromechanical SThM probe [43] has been derived. The device is composed of a thin cantilever equipped with a sharp conductive tip, an integrated deflection sensor, and an actuation system, see Figure 4(b). It might be useful to reduce the simulation time and so to facilitate the probe optimization. The derivation of the model is done following the steps of the reference proof. To this end, the probe is considered to have a periodic and thin structure, and to the end of the derivation, the model can be simplified taking into account the fact that the coefficients are constant instead of periodic which allows for elimination of the microscale variables in the in-plane direction. Evidently, the proof is much more complex than the one for the thin elastic plate model, and help has been found in existing papers, with different techniques, namely [18] for thin periodic elastic plates and [20], [21], [22]

for thin periodic piezoelectric plates with periodic distributed electric circuits. A byproduct of this approach is a model of periodic homogenization of multi-layered thermoelectromechanical systems that can be used, with little or no changes, in other applications in the field of microsystem arrays as for bolometers or arrays of cantilevers with thermal actuation e.g. the millipede from IBM. From the point of view of its implementation in *MEMSALab,* the model includes several special features compared to the reference model and we expect to formulate it using the extension-combination method.

Coupling SIMBAD and COMSOL and applications. The software SIMBAD provides a generic simulation-based design tool for investigating the behaviour of complex modeled systems. A MATLAB link has been set between COMSOL, which is then considered as FEM software in our approach, and SIMBAD so that COMSOL models may be used as an input for a design under SIMBAD. It includes the definition of the optimization problem: the initial value of parameters, the parameter relative ranges, the objective features and the constraints for geometry and objective features. It serves to transmit current parameters between the two software packages. For the application to the NANOHEAT probe, three objective optimization results are reported, namely to decrease the thermo-mechanical tip deflection, to increase the Joule heating effect in the tip and to increase the sensitivity of the piezoresistive sensor. Three SIMBAD toolboxes have been used. The design sensitivity and effects analysis toolbox is used to quantify the impact of design variable modifications on the design objective of interest. It allows the design space to be reduced to the subset of influential variables. The multi-objective performance optimization toolbox is used to obtain an approximation of the Pareto front for the different design objectives. It provides the analyst with a useful indicator on the trade-offs between the objectives of interest. Finally, the model validation and uncertainty quantification is used to quantify the impact of both aleatory and epistemic (lack of knowledge) uncertainties in the design variables and system environment on the design objectives and constraints. A very complete analysis has been carried out to explain the interactions between concurrent phenomena and to conclude to design guidelines.

3 Organization of the thesis

The thesis is organized as follows:

- In Chapter 1 we introduce a framework for computer-aided derivation of multi-scale models. It relies on a combination of an asymptotic method used in the field of partial differential equations with term rewriting techniques.

In this framework, a multi-scale model derivation is characterized by the features taken into account in the asymptotic analysis. Its formulation consists in a derivation of a reference model associated to an elementary reference model, and in a set of transformations to apply to this proof until it takes into account the wanted features. We apply the method to generate a family of homogenized models for second order elliptic equations with periodic coefficients that could be posed in multi-dimensional domains, with possibly multi-domains and/or thin domains.

- In Chapter 2 we address the problem of the combination of the extensions of the proofs related to the multi-scale model derivations. For this purpose, we develop further extension mechanisms that refine the ones introduced in Chapter 1. We elaborate necessary conditions under which these mechanisms can be correctly combined giving rise to rich extensions. We apply these extension mechanisms to many examples, namely to the derivation of the linear operator associated to the microscopic problem in the reference proof. Thus the results of this Chapter significantly improve the results of Chapter 1 since it is not possible, at least in a straightforward way, to provide necessary conditions so that the extension mechanisms established in Chapter 1 can be combined.

- The model of thin multilayer periodic thermoelectromechanical system is derived in Chapter 3. It follows strictly the reference proof excepted a change that has been introduced for the sake of simplification: in some step we prefer to use the two-scale convergence of Nguetseng and Allaire instead of this based on the two-scale transform. All necessary properties and proof are updated.

- The last chapter focuses on the optimization results obtained by coupling `SIMBAD` to `COMSOL` through `MATLAB`. The complete analysis is detailed including the sensitivity analysis, the reduction of the number of active optimization variables and the multi-criteria optimization. General conclusions are drawn in view of helping future SThM probe designers.

Chapter 1

A Rewriting Framework For Computer-Aided Derivation Of Multi-Scale Models

Abstract. *In this Chapter we introduce the first part of a framework for computer-aided derivation of multi-scale models. It relies on a combination of an asymptotic method used in the field of partial differential equations with term rewriting techniques coming from computer science. In our approach, a multi-scale model derivation is characterized by the features taken into account in the asymptotic analysis. Its formulation consists in a derivation of a reference model associated to an elementary nominal model, and in a set of transformations to apply to this proof until it takes into account the wanted features. In addition to the reference model proof, the framework includes first order rewriting principles designed for asymptotic model derivations, second order rewriting principles dedicated to elementary extensions of model derivations and their combinations. The latter point is only briefly sketched and will be detailed in another work. We report implementation results regarding three simple extensions of the reference proof. The results of this Chapter were the subject of the publication [59].*

1.1 Introduction

In this Chapter we introduce a method called *"by extension-combination"*. It consists of three principles.

1. A *reference model* is introduced together with its derivation. It covers a very simple case but its proof is expressed in a sufficiently general form.

2. Then, *elementary extensions* (also called generalizations) are built by elementary transformations of the reference derivation, each of them covering a different feature.

3. Finally, elementary transformations are combined resulting in a complex transformation.

The latter is in turn applied to the reference proof to generate a complex model including all features of the elementary extensions.

The present Chapter focuses on the two first steps when the last one, i.e. combination of transformations, will be detailed in Chapter 2.

We select as the *reference problem* that of the periodic homogenization of a scalar second order elliptic equation posed in a one-dimension domain and with Dirichlet boundary conditions. Its derivation is based on the use of the two-scale transform operator introduced in [3], and reused in [17]. We quote that homogenization of various problems using this transformation was performed according to different techniques in [45, 48, 47, 23, 27, 29]. Here, we follow [47], so a number of basic *properties* coming from this paper are stated and considered as the building blocks of the proofs. The complete derivation of the model is organized into seven *lemmas*, it is performed by a sequence of applications of these *properties*. Their extension to another problem requires generalization of some of the properties, which is assumed to be made independently. It may also require changes in the path of the proof, and even adding new lemmas. Regarding the level of detail in the representation of mathematical objects, on the one hand it has enough precision to cover a fairly wide range of models and on the other hand the calculations are reasonably sized. Moreover, the way the generalizations are made is important so that they could be formulated in a single framework.

The computational framework used to express the method is based on the theory of rewriting. The required mathematical concepts are common in the field of partial differential equations: geometric domains, variables defined on these domains, functions of several variables, operators (e.g. derivatives, integrals, two-scale transform, etc.). The proofs of Lemmas are designed to be realizable by rewriting. Precisely, each *property* is expressed as a rewrite rule that can be conditional, so that it can be applied or not according to a given logical formula. A step in a lemma proof is realized by a strategy that expresses how the rule applies. The complete proof of a lemma is then a sequence of such strategies. Ones we use have been developed in a previous work [6] that is implemented in `Maple`. Here we provide its formalization. To allow the successful application of rewriting strategies to an expression that contains associative and/or commutative operations, such

as $+, *, \cup, \cap$, etc, we use the concept of rewriting modulo an equational theory [4, §11]. Without such concept one needs to duplicate the rewriting rules.

Rewriting operates on expressions whose level of abstraction accurately reflects the mathematical framework. Concrete description of geometric domains, functions or operators are not provided. Their description follows a grammar that has been defined in order that they carry enough information allowing for the design of the rewriting rules and the strategies. In some conditions of rewriting rules, the set of variables on which an expression depends is required. This is for example the case for the linearity property of the integral. Rather than introducing a typing system, which would be cumbersome and restrictive, we introduced a specific functionality in the form of a λ-term (i.e. a program). The language of strategy allows this use. Put together all these concepts can express a lemma proof as a strategy, i.e. a first order strategy, and therefore provide a framework of symbolic computation. The concept of generalization of a proof is introduced as second order rewrite strategies, made with second order rewriting rules, operating on first order strategies. They can transform first order rewrite rules and strategies and, where appropriate, remove or add new ones. This framework has been implemented in the software Maple. We present its application to the complete proof of the reference problem and also to the generalizations of the first lemma, by applying second order strategies, to multi-dimensional geometrical domains, multi-dimensional thin domains and multi-domains.

1.1.1 Organization of the Chapter

This Chapter is organized as follows. The complete method, of extension-combination, is sketched through an example in Section 1.2. Section 1.3 is devoted to all mathematical aspects. This includes all definitions and properties, the lemmas and their proof. The principles of rewrite rules and strategies are formulated in Section 1.4. Section 1.5 is devoted to the theoretical framework that allows to derive a model and its generalizations. Implementation results are described in Section 1.7.

1.2 Illustration of the method of extension-composition

The extension-combination method is illustrated on a model of the mechanical behavior of an array of thin elastic periodic cantilevers supported by an elastic base. It has been established in [47] and later studied in [41], [46] and [42]. The derivation in [47] only partially fits with the reference derivation of this Chapter. The difference is that it is done in two steps, first a thin elastic plate model is obtained, using a different technique, by only assuming small thickness of the

whole structure. Second, the periodicity assumption is combined with a special ratio between the thicknesses of the base and the cantilevers. Through a technique of periodic homogenization for strongly heterogeneous media fitting well with the scheme of the reference proof, this yields the final model.

The same model can be obtained by a one-step proof transforming the three-dimensional nominal model into an homogenized two-dimensional model. Such derivation combines the same features as the two-step proof but is consistent with the reference proof. It requires three orders of magnitude listed in decreasing order: for the period, the base thickness and the cantilever thickness. This forms part of an ongoing work.

The goal of the extension-combination method, as mentioned in page 7, is to build such one-step derivation as a transformation of the reference derivation by a combination of elementary transformations. Figure 3 represents the derivations and the transformations to be applied to derivations as big and little parchments respectively. The reference proof is denoted by *Ref.* The transformation $\overline{\Pi}_1$ yields a derivation of a three-dimensional homogenized model of a periodic single-layered elastic media. The periodic cell is pierced by a large hole. The transformation $\overline{\Pi}_2$ is for the derivation of a periodic thin elastic plate model i.e. a model where the thickness is another small parameter. Then, there are many possible combinations, all denoted by $\overline{\Pi}_1+\overline{\Pi}_2$ for the sake of simplicity, of the two transformations so that the final model inherits their features. The bottom left and right sketches represent two final homogenized models. The first is for a thick periodic layer made with a pierced periodic cell whose hole is partly occupied by a clamped thin moving plate. The second is similar except that the whole structure is thin instead of beeing thick; it corresponds precisely to the model established in [47]. The framework developed in the rest of this Chapter is for expressing model derivations, as those represented by big parchments, and transformations of model derivations as $\overline{\Pi}_1$ and $\overline{\Pi}_2$. Formulating combinations of transformations of model derivations, such as $\overline{\Pi}_1 + \overline{\Pi}_2$, is another big part of the solution will be presented in Chapter 2.

1.3 Skeleton of two-scale modeling

We recall the framework of the two-scale convergence as presented in [47], and the proof of the *reference model* whose implementation and extension under the form of algorithms of symbolic computation are discussed in Section 1.7. The presentation is divided into three subsections. The first one is devoted to basic definitions and properties, stated as *Propositions*. The latter are admitted without proof because they are assumed to be prerequisites, or building blocks, in the proofs. They are used as elementary steps in the two other sections detailing

the proof of the convergence of the two-scale transform of a derivative, and the homogenized model derivation. The main statements of these two subsections are also stated as *Propositions* and their proofs are split into numbered blocks called lemmas. Each lemma is decomposed into steps refering to the definitions and propositions. All components of the *reference model* derivation, namely the definitions, the propositions, the lemmas and the proof steps are designed so that to be easily implemented and also to be generalized for more complex models. We quote that a number of elementary properties are used in the proof but are not explicitely stated nor cited.

1.3.1 Notations, Definitions and Propositions

Note that the functional framework used in this section is not as precise as it should be for a usual mathematical work. The reason is that the functional analysis is not covered by our symbolic computation. So, precise mathematical statements and justifications are not in the focus of this work.

In the sequel, $A \subset \mathbb{R}^n$ is a bounded open set, with measure $|A|$, having a "sufficiently" regular boundary ∂A and with unit outward normal denoted by $n_{\partial A}$. We shall use the set $L^1(A)$ of integrable functions and the set $L^p(A)$, for any $p > 0$, of functions f such that $f^p \in L^1(A)$, with norm $||v||_{L^p(A)} = (\int_A |v|^p \, dx)^{1/p}$. The Sobolev space $H^1(A)$ is the set of functions $f \in L^2(A)$ whose gradient $\nabla f \in L^2(A)^n$. The set of p times differentiable functions on A is denoted by $\mathcal{C}^p(A)$, where p can be any integer or ∞. Its subset $\mathcal{C}_0^p(A)$ is composed of functions whose partial derivatives are vanishing on the boundary ∂A of A until the order p. For any integers p and q, $\mathcal{C}^q(A) \subset L^p(A)$. When $A = (0, a_1) \times ... \times (0, a_n)$ is a cuboid (or rectangular parallelepiped) we say that a function v defined in $\mathbb{R}^n$ is A-periodic if for any $\ell \in \mathbb{Z}^n$, $v(y + \sum_{i=1}^n \ell_i a_i e_i) = v(y)$ where e_i is the i^{th} vector of the canonical basis of $\mathbb{R}^n$. The set of A-periodic functions which are $\mathcal{C}^\infty$ is denoted by $\mathcal{C}_\sharp^\infty(A)$ and those which are in $H^1(A)$ is denoted by $H_\sharp^1(A)$. The operator tr (we say *trace*) can be defined as the restriction operator from functions defined on the closure of A to functions defined on its boundary ∂A. Finally, we say that a sequence $(u^\varepsilon)_{\varepsilon>0} \in L^2(A)$ converges strongly in $L^2(A)$ towards $u^0 \in L^2(A)$ when ε tends to zero if $\lim_{\varepsilon\to 0} ||u^\varepsilon - u^0||_{L^2(A)} = 0$. The convergence is said to be weak if $\lim_{\varepsilon\to 0} \int_A (u^\varepsilon - u^0)v \, dx = 0$ for all $v \in L^2(A)$. We write $u^\varepsilon = u^0 + O_s(\varepsilon)$ (respectively $O_w(\varepsilon)$), where $O_s(\varepsilon)$ (respectively $O_w(\varepsilon)$) represents a sequence tending to zero strongly (respectively weakly) in $L^2(A)$. Moreover, the simple notation $O(\varepsilon)$ refers to a sequence of numbers which simply tends to zero. We do not detail the related usual computation rules.

Proposition 1 ***[Interpretation of a weak equality]*** *For $u \in L^2(A)$ and for any $v \in \mathcal{C}_0^\infty(A)$,*

$$\text{if } \int_A u(x)\ v(x)\ dx = 0 \text{ then } u = 0$$

in the sense of $L^2(A)$ functions.

Proposition 2 ***[Interpretation of a periodic boundary condition]*** *For $u \in H^1(A)$ and for any $v \in \mathcal{C}_\sharp^\infty(A)$,*

$$\text{if } \int_{\partial A} u(x)\ v(x)\ n_{\partial A}(x)\ dx = 0 \text{ then } u \in H_\sharp^1(A)\,.$$

Proposition 3 ***[Weak convergence of product]*** *For sequence $u_n \to u$ strongly, $v_n \to v$ weakly, then the product $u_n v_n \to uv$ weakly.*

This proposition is followed in mathematical proof but not in the programme. The reference proof proposed in this chapter is a simulation of the programme, so this proposition is not refered explictly.
In the remainder of this section, only the dimension $n = 1$ is considered, the general definitions being used for the generalizations discussed in Section 1.7.

Notation 4 ***[Physical and microscopic Domains]*** *We consider an interval $\Omega = \bigcup_{c=1}^{N(\varepsilon)} \Omega_c^{1,\varepsilon} \subset \mathbb{R}$ divided into $N(\varepsilon)$ periodic cells (or intervals) $\Omega_c^{1,\varepsilon}$, of size $\varepsilon > 0$, indexed by c, and with center x_c. The translation and magnification $(\Omega_c^{1,\varepsilon} - x_c)/\varepsilon$ is called the unit cell and is denoted by Ω^1. The variables in Ω and in Ω^1 are denoted by x^ε and x^1.*

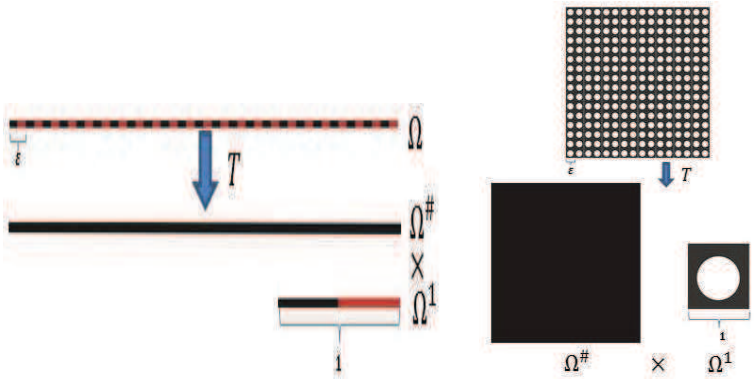
The two-scale transform T is an operator mapping functions defined in the physical domain Ω to functions defined in the two-scale domain $\Omega^\sharp \times \Omega^1$ where for the *reference model* $\Omega^\sharp = \Omega$. In the following, we shall denote by Γ, $\Gamma^\sharp$ and Γ^1 the boundaries of Ω, $\Omega^\sharp$ and Ω^1.

An example of the configuration of physical domain, macroscopic domain and microscopic domain is given in the following.

Definition 5 ***[Two-Scale Transform]*** *The two-scale transform T is the linear operator defined by*

$$(Tu)(x_c, x^1) = u(x_c + \varepsilon x^1) \tag{1.1}$$

and then by extension $T(u)(x^\sharp, x^1) = u(x_c + \varepsilon x^1)$ for all $x^\sharp \in \Omega_c^{1,\varepsilon}$ and each c in $1, .., N(\varepsilon)$.



(a) 1D (b) 2D

Figure 1.1: Physical domian, macroscopic domain and microscopic domain

Notation 6 ***[Measure of Domains]*** $\kappa^0 = \frac{1}{|\Omega|}$ *and* $\kappa^1 = \frac{1}{|\Omega^\sharp \times \Omega^1|}$.

The operator T enjoys the following properties.

Proposition 7 ***[Product Rule]*** *For two functions* u, v *defined in* Ω,

$$T(uv) = (Tu)(Tv). \tag{1.2}$$

Proposition 8 ***[Derivative Rule]*** *If* u *and its derivative are defined in* Ω *then*

$$T\left(\frac{du}{dx}\right) = \frac{1}{\varepsilon}\frac{\partial(Tu)}{\partial x^1}. \tag{1.3}$$

Proposition 9 ***[Integral Rule]*** *If a function* $u \in L^1(\Omega)$ *then* $Tu \in L^1(\Omega^\sharp \times \Omega^1)$ *and*

$$\kappa^0 \int_\Omega u \, dx = \kappa^1 \int_{\Omega^\sharp \times \Omega^1} (Tu) \, dx^\sharp dx^1. \tag{1.4}$$

The next two properties are corollaries of the previous ones.

Proposition 10 ***[Inner Product Rule]*** *For two functions* u, $v \in L^2(\Omega)$,

$$\kappa^0 \int_\Omega u \, v \, dx = \kappa^1 \int_{\Omega^\sharp \times \Omega^1} (Tu) \, (Tv) \, dx^\sharp dx^1. \tag{1.5}$$

Proposition 11 ***[Norm Rule]*** *For a function* $u \in L^2(\Omega)$,

$$\kappa^0 \|u\|^2_{L^2(\Omega)} = \kappa^1 \|Tu\|^2_{L^2(\Omega^\sharp \times \Omega^1)}. \tag{1.6}$$

Definition 12 ***[Two-Scale Convergence]*** *A sequence $u^\varepsilon \in L^2(\Omega)$ is said to be two-scale strongly (respect. weakly) convergent in $L^2(\Omega^\sharp \times \Omega^1)$ to a limit $u^0(x^\sharp, x^1)$ if Tu^ε is strongly (respect. weakly) convergent towards u^0 in $L^2(\Omega^\sharp \times \Omega^1)$.*

Definition 13 ***[Adjoint or Dual of T]*** *As T is a linear operator from $L^2(\Omega)$ to $L^2(\Omega^\sharp \times \Omega^1)$, its adjoint T^* is a linear operator from $L^2(\Omega^\sharp \times \Omega^1)$ to $L^2(\Omega)$ defined by*

$$\kappa^0 \int_\Omega T^* v \; u \; dx = \kappa^1 \int_{\Omega^\sharp \times \Omega^1} v \; Tu \; dx^\sharp dx^1. \tag{1.7}$$

The expression of T^* can be explicited, it maps regular functions in $\Omega^\sharp \times \Omega^1$ to piecewise-constant functions in Ω. The next definition introduces an operator used as a smooth approximation of T^*.

Definition 14 ***[Regularization of T^*]*** *The operator B is the linear continuous operator defined from $L^2(\Omega^\sharp \times \Omega^1)$ to $L^2(\Omega)$ by*

$$Bv = v(x, \frac{x}{\varepsilon}). \tag{1.8}$$

The nullity condition of a function $v(x^\sharp, x^1)$ on the boundary $\partial\Omega^\sharp \times \Omega^1$ is transferred to the range Bv as follows.

Proposition 15 ***[Boundary Conditions of Bv]*** *If $v \in \mathcal{C}_0^\infty(\Omega^\sharp; \mathcal{C}^\infty(\Omega^1))$ then $Bv \in \mathcal{C}_0^\infty(\Omega)$.*

Proposition 16 ***[Derivation Rule for B]*** *If v and its partial derivatives are defined on $\Omega^\sharp \times \Omega^1$ and they are smooth enough, then*

$$\frac{d(Bv)}{dx} = B(\frac{\partial v}{\partial x^\sharp}) + \varepsilon^{-1} B(\frac{\partial v}{\partial x^1}). \tag{1.9}$$

The next proposition states that the operator B is actually an approximation of the operator T^* for Ω^1-periodic functions. This property is only used for the test functions so that v could be regular enough.

Proposition 17 ***[Approximation between T^* and B]*** *If $v(x^\sharp, x^1)$ is continuous, continuously differentiable in $x^\sharp$ and Ω^1-periodic in x^1 then*

$$T^* v = Bv - \varepsilon B(x^1 \frac{\partial v}{\partial x^\sharp}) + \varepsilon O_s(\varepsilon). \tag{1.10}$$

Conversely,

$$Bv = T^*(v) + \varepsilon T^*(x^1 \frac{\partial v}{\partial x^\sharp}) + \varepsilon O_s(\varepsilon). \tag{1.11}$$

The proof of this proposition is detailed in Appendix 3 of reference [47].

Remark 18 *Operators T, T^* and B depend on the small parameter ε, but we do not write it explictly just for simplification of notations.*

Next, the formula of integration by parts is stated in a form compatible with the Green formula used in some extensions. The boundary Γ is composed of the two end points of the interval Ω, and the unit outward normal n_Γ defined on Γ is equal to -1 and $+1$ at the left- and right-endpoints respectively.

Proposition 19 ***[Green Rule]*** *If $u,\ v \in H^1(\Omega)$ then the traces of u and v on Γ are well defined and*

$$\int_\Omega u\frac{dv}{dx}\ dx = \int_\Gamma tr(u)\ tr(v)\ n_\Gamma\ ds(x) - \int_\Omega v\frac{du}{dx}\ dx. \tag{1.12}$$

The last proposition is stated as a building block of the homogenized model derivation.

Proposition 20 ***[The linear operator associated to the Microscopic problem]*** *For $\mu \in \mathbb{R}$, there exist $\theta^\mu \in H^1_\sharp(\Omega^1)$ solutions to the linear weak formulation*

$$\int_{\Omega^1} a^0\frac{\partial\theta^\mu}{\partial x^1}\frac{\partial w}{\partial x^1}\ dx^1 = -\mu\int_{\Omega^1} a^0\frac{\partial w}{\partial x^1}\ dx^1 \text{ for all } w \in \mathcal{C}^\infty_\sharp(\Omega^1), \tag{1.13}$$

and $\frac{\partial\theta^\mu}{\partial x^1}$ is unique. Since the mapping $\mu \mapsto \dfrac{\partial\theta^\mu}{\partial x^1}$ from $\mathbb{R}$ to $L^2(\Omega^1)$ is linear then

$$\frac{\partial\theta^\mu}{\partial x^1} = \mu\frac{\partial\theta^1}{\partial x^1}. \tag{1.14}$$

Moreover, this relation can be extended to any $\mu \in L^2(\Omega^\sharp)$.

1.3.2 Two-Scale Approximation of a Derivative

Here we detail the *reference computation* of the weak two-scale limit $\eta = \lim_{\varepsilon\to 0} T(\frac{du^\varepsilon}{dx})$ in $L^2(\Omega^\sharp \times \Omega^1)$ when

$$\|u^\varepsilon\|_{L^2(\Omega)} \text{ and } \left\|\frac{du^\varepsilon}{dx}\right\|_{L^2(\Omega)} \leq C, \tag{1.15}$$

C being a constant independent of ε. To simplify the proof, we further assume that there exist $u^0,\ u^1 \in L^2(\Omega^\sharp \times \Omega^1)$ such that

$$T(u^\varepsilon) = u^0 + \varepsilon u^1 + \varepsilon O_w(\varepsilon),$$

i.e.

$$\int_{\Omega^\sharp\times\Omega^1}(T(u^\varepsilon)-u^0-\varepsilon u^1)v\ dx^\sharp dx^1=\varepsilon O(\varepsilon)\text{ for all }v\in L^2(\Omega^\sharp\times\Omega^1). \tag{1.16}$$

We quote that Assumption (1.16) is not necessary, it is introduced to simplify the proof since it avoids some non-equational steps. The statement proved in the remaining of the subsection is the following.

Proposition 21 ***[Two-scale Limit of a Derivative]*** *If u^ε is a sequence bounded as in (1.15) and satisfying (1.16), then u^0 is independent of x^1,*

$$\tilde{u}^1=u^1-x^1\partial_{x^\sharp}u^0 \tag{1.17}$$

defined in $\Omega^\sharp\times\Omega^1$ is Ω^1-periodic and

$$\eta=\frac{\partial u^0}{\partial x^\sharp}+\frac{\partial\tilde{u}^1}{\partial x^1}. \tag{1.18}$$

Moreover, if $u^\varepsilon=0$ on Γ then $u^0=0$ on $\Gamma^\sharp$.

The proof is split into four Lemmas corresponding to the first four blocks discussed in Section 1.7, the other three being detailed in subsection 1.3.3.

Lemma 22 ***[First Block: Constraint on u^0]*** *u^0 is independent of x^1.*

Proof. We introduce

$$\Psi=\varepsilon\kappa^0\int_\Omega\frac{du^\varepsilon}{dx}Bv\ dx$$

with $v\in\mathcal{C}_0^\infty(\Omega^\sharp;\mathcal{C}_0^\infty(\Omega^1))$. From the Cauchy-Schwartz inequality and (1.15), $\lim_{\varepsilon\to0}\Psi=0$.

- **Step 1.** The Green formula (1.12) and Proposition 15 $\Longrightarrow$

$$\Psi=-\varepsilon\kappa^0\int_\Omega u^\varepsilon\frac{d(Bv)}{dx}\ dx.$$

- **Step 2.** Proposition 16 $\Longrightarrow$

$$\Psi=\kappa^0\int_\Omega u^\varepsilon B(\frac{\partial v}{\partial x^1})\ dx+O(\varepsilon).$$

- **Step 3.** Proposition 17 $\Longrightarrow$

$$\Psi=\kappa^0\int_\Omega u^\varepsilon T^*(\frac{\partial v}{\partial x^1})\ \ dx+O(\varepsilon).$$

- **Step 4.** Definition 13 $\Longrightarrow$

$$\Psi = \kappa^1 \int_{\Omega^\sharp \times \Omega^1} T(u^\varepsilon) \frac{\partial v}{\partial x^1}\, dx + O(\varepsilon).$$

- **Step 5.** Assumption (1.16) and passing to the limit when $\varepsilon \to 0$ $\Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp \times \Omega^1} u^0 \frac{\partial v}{\partial x^1}\, dx = 0.$$

- **Step 6.** The Green formula (1.12) and $v = 0$ on $\Omega^\sharp \times \Gamma^1$ $\Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^0}{\partial x^1}\, v\, dx = 0.$$

- **Step 7.** Proposition 1 $\Longrightarrow$

$$\frac{\partial u^0}{\partial x^1} = 0.$$

■

Lemma 23 ***[Second Block: Two-Scale Limit of the Derivative]*** $\eta = \frac{\partial u^1}{\partial x^1}$.

Proof. We choose $v \in \mathcal{C}_0^\infty(\Omega^\sharp; \mathcal{C}_0^\infty(\Omega^1))$ in

$$\Psi = \kappa^1 \int_{\Omega^\sharp \times \Omega^1} T(\frac{du^\varepsilon}{dx}) v\, dx^\sharp dx^1. \tag{1.19}$$

- **Step 1.** Definition 13 $\Longrightarrow$

$$\Psi = \kappa^0 \int_\Omega \frac{du^\varepsilon}{dx} T^* v\, dx.$$

- **Step 2.** Proposition 17 (to approximate T^* by B), the Green formula (1.12), the linearity of integrals, and again Proposition 17 (to approximate B by T^*) $\Longrightarrow$

$$\Psi = -\kappa^0 \int_\Omega u^\varepsilon T^*(\frac{\partial v}{\partial x^\sharp})\, dx - \frac{\kappa^0}{\varepsilon} \int_\Omega u^\varepsilon T^*(\frac{\partial v}{\partial x^1})\, dx - \kappa^0 \int_\Omega u^\varepsilon T^*(\frac{\partial^2 v}{\partial x^1 \partial x^\sharp} x^1)\, dx + O(\varepsilon).$$

- **Step 3.** Definition 13 $\Longrightarrow$

$$\begin{aligned} \Psi \;=\; & -\kappa^1 \int_{\Omega^\sharp \times \Omega^1} T(u^\varepsilon) \frac{\partial v}{\partial x^\sharp}\, dx^\sharp dx^1 - \frac{\kappa^1}{\varepsilon} \int_{\Omega^\sharp \times \Omega^1} T(u^\varepsilon) \frac{\partial v}{\partial x^1}\, dx^\sharp dx^1 \\ & -\kappa^1 \int_{\Omega^\sharp \times \Omega^1} T(u^\varepsilon) x^1 \frac{\partial^2 v}{\partial x^1 \partial x^\sharp}\, dx^\sharp dx^1 + O(\varepsilon). \end{aligned}$$

- **Step 4.** Assumption (1.16) $\Longrightarrow$

$$\begin{aligned}\Psi &= -\kappa^1 \int_{\Omega^\sharp\times\Omega^1} u^0 \frac{\partial v}{\partial x^\sharp}\, dx^\sharp dx^1 - \frac{\kappa^1}{\varepsilon}\int_{\Omega^\sharp\times\Omega^1} u^0 \frac{\partial v}{\partial x^1}\, dx^\sharp dx^1 - \kappa^1 \int_{\Omega^\sharp\times\Omega^1} u^1 \frac{\partial v}{\partial x^1}\, dx^\sharp dx^1 \\ &\quad -\kappa^1 \int_{\Omega^\sharp\times\Omega^1} u^0 \frac{\partial^2 v}{\partial x^1 \partial x^\sharp} x^1 + O(\varepsilon).\end{aligned}$$

- **Step 5.** The Green formula (1.12), Lemma 22, and passing to the limit when $\varepsilon \to 0$ $\Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp\times\Omega^1} \eta\, v\, dx^\sharp dx^1 = \kappa^1 \int_{\Omega^\sharp\times\Omega^1} \frac{\partial u^0}{\partial x^\sharp} v\, dx^\sharp dx^1 + \kappa^1 \int_{\Omega^\sharp\times\Omega^1} \frac{\partial u^1}{\partial x^1} v\, dx^\sharp dx^1.$$

- **Step 6.** Proposition 1 $\Longrightarrow$

$$\eta = \frac{\partial u^0}{\partial x^\sharp} + \frac{\partial u^1}{\partial x^1}.$$

■

Lemma 24 ***[Third Block: Microscopic Boundary Condition]*** *$\tilde{u}^1$ is Ω^1-periodic.*

Proof. In (1.19), we choose $v \in \mathcal{C}_0^\infty(\Omega^\sharp; \mathcal{C}_\sharp^\infty(\Omega^1))$.

- **Step 1.** The steps 1-5 of the second block $\Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp\times\Omega^1} \eta v\, dx^\sharp dx^1 - \kappa^1 \int_{\Omega^\sharp\times\Gamma^1} (u^1 - x^1 \frac{\partial u^0}{\partial x^\sharp}) v\, n_{\Gamma^1}\, dx^\sharp dx^1 - \kappa^1 \int_{\Omega^\sharp\times\Omega^1} (\frac{\partial u^0}{\partial x^\sharp} + \frac{\partial u^1}{\partial x^1}) v\, dx^\sharp dx^1 = 0$$

- **Step 2.** Lemma 23 $\Longrightarrow$

$$\int_{\Omega^\sharp\times\Gamma^1} (u^1 - x^1 \frac{\partial u^0}{\partial x^\sharp}) v\, n_{\Gamma^1}\, dx^\sharp ds(x^1) = 0. \tag{1.20}$$

- **Step 3.** Definition (1.17) of $\tilde{u}^1$ and Proposition 2 $\Longrightarrow$

$$\tilde{u}^1 \text{ is } \Omega^1\text{-periodic.} \tag{1.21}$$

■

Lemma 25 ***[Fourth Block: Macroscopic Boundary Condition]*** *u^0 vanishes on $\Gamma^\sharp$.*

Proof. We choose $v \in \mathcal{C}_0^\infty(\Omega^\sharp)$,

- **Step 1.** The steps 1-5 of the second block and $u^\varepsilon = 0$ on $\Gamma \Longrightarrow$

$$\int_{\Gamma^\sharp \times \Omega^1} u^0 v \; n_{\Gamma^\sharp} \; ds(x^\sharp) dx^1 = 0.$$

- **Step 2.** Proposition 1 $\Longrightarrow$

$$u^0 = 0 \text{ on } \Gamma^\sharp.$$

■

1.3.3 Homogenized Model Derivation

Here we provide the *reference proof* of the homogenized model derivation. It uses Proposition 21 as an intermediary result. Let u^ε, the solution of a linear boundary value problem posed in Ω,

$$\left\{ \begin{array}{l} -\dfrac{d}{dx}(a^\varepsilon(x)\dfrac{du^\varepsilon(x)}{dx}) = f \text{ in } \Omega \\ u^\varepsilon = 0 \text{ on } \Gamma, \end{array} \right. \tag{1.22}$$

where the right-hand side $f \in L^2(\Omega)$, the coefficient $a^\varepsilon \in \mathcal{C}^\infty(\Omega)$ is $\varepsilon\Omega^1$-periodic, and there exist two positive constants α and β independent ε such that

$$0 < \alpha \leq a^\varepsilon(x) \leq \beta. \tag{1.23}$$

The weak formulation is obtained by multiplication of the differential equation by a test function $v \in \mathcal{C}_0^\infty(\Omega)$ and application of the Green formula,

$$\kappa^0 \int_\Omega a^\varepsilon(x) \frac{du^\varepsilon}{dx} \frac{dv}{dx} \; dx = \kappa^0 \int_\Omega f(x) v(x) \; dx. \tag{1.24}$$

It is known that its unique solution u^ε is bounded as in (1.15). Moreover, we assume that for some functions $a^0(x^1)$ and $f^0(x^\sharp)$,

$$T(a^\varepsilon) = a^0 \text{ and } T(f) = f^0(x^\sharp) + O_w(\varepsilon). \tag{1.25}$$

The next proposition states the homogenized model and is the main result of the *reference proof*. For θ^1 a solution to the microscopic problem (1.13) with $\mu = 1$, the homogenized coefficient and right-hand side are defined by

$$a^H = \int_{\Omega^1} a^0 \left(1 + \frac{\partial \theta^1}{\partial x^1}\right)^2 \; dx^1 \text{ and } f^H = \int_{\Omega^1} f^0 \; dx^1. \tag{1.26}$$

Proposition 26 ***[Homogenized Model]*** *The limit u^0 is solution to the weak formulation*

$$\int_{\Omega^\sharp} a^H \frac{du^0}{dx^\sharp}\frac{dv^0}{dx^\sharp}\ dx^\sharp = \int_{\Omega^\sharp} f^H v^0\ dx^\sharp \tag{1.27}$$

for all $v^0 \in \mathcal{C}_0^\infty(\Omega^\sharp)$.

The proof is split into three lemmas.

Lemma 27 ***[Fifth Block: Two-Scale Model]*** *The couple $(u^0, \widetilde{u}^1)$ is solution to the two-scale weak formulation*

$$\int_{\Omega^\sharp\times\Omega^1} a^0\left(\frac{\partial u^0}{\partial x^\sharp}+\frac{\partial \widetilde{u}^1}{\partial x^1}\right)\left(\frac{\partial v^0}{\partial x^\sharp}+\frac{\partial v^1}{\partial x^1}\right)\ dx^\sharp dx^1 = \int_{\Omega^\sharp\times\Omega^1} f^0 v^0\ dx^\sharp dx^1 \tag{1.28}$$

for any $v^0 \in \mathcal{C}_0^\infty(\Omega^\sharp)$ and $v^1 \in \mathcal{C}_0^\infty(\Omega^\sharp, C_\sharp^\infty(\Omega^1))$.

Proof. We choose the test functions $v^0 \in \mathcal{C}_0^\infty(\Omega^\sharp)$, $v^1 \in \mathcal{C}_0^\infty(\Omega^\sharp, C_\sharp^\infty(\Omega^1))$.

- **Step 1** Posing $v = B(v^0 + \varepsilon v^1)$ in (1.24) and Proposition 15 $\Longrightarrow$

$$Bv \in \mathcal{C}_0^\infty(\Omega) \text{ and } \kappa^0 \int_\Omega a^\varepsilon \frac{du^\varepsilon}{dx}\frac{dB(v^0+\varepsilon v^1)}{dx}\ dx = \kappa^0 \int_\Omega f\ B(v^0+\varepsilon v^1)\ dx.$$

- **Step 2** Propositions 16 and 17 $\Longrightarrow$

$$\kappa^0 \int_\Omega a^\varepsilon \frac{du^\varepsilon}{dx} T^*\left(\frac{\partial v^0}{\partial x^\sharp}+\frac{\partial v^1}{\partial x^1}\right) dx = \kappa^0 \int_\Omega f\ T^*(v^0)dx + O(\varepsilon).$$

- **Step 3** Definition 13 and Proposition 7 $\Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp\times\Omega^1} T(a^\varepsilon) T(\frac{du^\varepsilon}{dx})\left(\frac{\partial v^0}{\partial x^\sharp}+\frac{\partial v^1}{\partial x^1}\right)\ dx^\sharp dx^1 = \kappa^1 \int_{\Omega^\sharp\times\Omega^1} T(f)\ v^0\ dx^\sharp dx^1 + O(\varepsilon). \tag{1.29}$$

- **Step 4** Definitions (1.25), Lemma 21, and passing to the limit when $\varepsilon \to 0$ $\Longrightarrow$

$$\int_{\Omega^\sharp\times\Omega^1} a^0\left(\frac{\partial u^0}{\partial x^\sharp}+\frac{\partial \widetilde{u}^1}{\partial x^1}\right)\left(\frac{\partial v^0}{\partial x^\sharp}+\frac{\partial v^1}{\partial x^1}\right)\ dx^\sharp dx^1 = \int_{\Omega^\sharp\times\Omega^1} f^0 v^0\ dx^\sharp dx^1$$

which is the expected result.

■

Lemma 28 ***[Sixth Block: Microscopic Problem]*** *$\widetilde{u}^1$ is solution to (1.13) with $\mu = \dfrac{\partial u^0}{\partial x^\sharp}$ and*

$$\frac{\partial \widetilde{u}^1}{\partial x^1} = \frac{\partial u^0}{\partial x^\sharp}\frac{\partial \theta^1}{\partial x^1}.$$

Proof. We choose $v^0 = 0$ and $v^1(x^\sharp, x^1) = w(x^1)\varphi(x^\sharp)$ in (1.28) with $\varphi \in \mathcal{C}^\infty(\Omega^\sharp)$ and $w^1 \in \mathcal{C}^\infty_\sharp(\Omega^1)$.

- **Step 1** Proposition 1, Lemma 22, and the linearity of the integral $\Longrightarrow$

$$\int_{\Omega^1} a^0 \frac{\partial \widetilde{u}^1}{\partial x^1}\frac{\partial w^1}{\partial x^1}\, dx^1 = -\frac{\partial u^0}{\partial x^\sharp}\int_{\Omega^1} a^0 \frac{\partial w^1}{\partial x^1}\, dx^1. \tag{1.30}$$

- **Step 2** Proposition 20 with $\mu = \dfrac{\partial u^0}{\partial x^\sharp}$ $\Longrightarrow$

$$\frac{\partial \widetilde{u}^1}{\partial x^1} = \frac{\partial u^0}{\partial x^\sharp}\frac{\partial \theta^1}{\partial x^1}$$

  as announced.

■

Lemma 29 ***[Seventh Block: Macroscopic Problem]*** *u^0 is solution to (1.27).*

Proof. We choose $v^0 \in \mathcal{C}^\infty_0(\Omega^\sharp)$ and $v^1 = \dfrac{\partial v^0}{\partial x^\sharp}\dfrac{\partial \theta^1}{\partial x^1} \in \mathcal{C}^\infty_0(\Omega^\sharp, C^\infty_\sharp(\Omega^1))$ in (1.28).

- **Step 1** Lemma 28 $\Longrightarrow$

$$\int_{\Omega^\sharp\times\Omega^1} a^0 \left(\frac{\partial u^0}{\partial x^\sharp} + \frac{\partial \theta^1}{\partial x^1}\frac{\partial u^0}{\partial x^\sharp}\right)\left(\frac{\partial v^0}{\partial x^\sharp} + \frac{\partial \theta^1}{\partial x^1}\frac{\partial v^0}{\partial x^\sharp}\right)\, dx^\sharp dx^1 = \int_{\Omega^\sharp\times\Omega^1} f^0 v^0\, dx^\sharp dx^1. \tag{1.31}$$

- **Step 2** Factorizing and definitions (1.26) $\Longrightarrow$

$$\int_{\Omega^\sharp} a^H \frac{\partial u^0}{\partial x^\sharp}\frac{\partial v^0}{\partial x^\sharp}\, dx^\sharp = \int_{\Omega^\sharp} f^H v^0\, dx^\sharp.$$

■

1.4 Rewriting strategies

In this section we recall the rudiments of rewriting, namely, the definitions of terms over a signature, of substitution and of rewriting rules. We introduce a strategy language: its syntax and semantics in terms of partial functions. This language will allow us to express most of the useful rewriting strategies.

1.4.1 Term, substitution and rewriting rule.

We start with an example of rewriting rule. We define a set of rewriting variables $\mathcal{X} = \{x, y\}$ and a set of function symbols $\Sigma = \{f, g, a, b, c\}$. A term is a combination of elements of $\mathcal{X} \cup \Sigma$, for instance $f(x)$ or $f(a)$. The rewriting rule $f(x) \rightsquigarrow g(x)$ applied to a term $f(a)$ is a two-step operation. First, it consists in matching the left term $f(x)$ with the input term $f(a)$ by matching the two occurences of the function symbol f, and by matching the rewriting variable x with the function symbol a. Then, the result $g(a)$ of the rewriting operation is obtained by replacing the rewriting variable x occuring in the right hand side $g(x)$ by the subterm a that have been associated to x. In case where a substitution is not possible, as in the application of $f(b) \to g(x)$ to $f(a)$, we say that the rewriting rule fails.

Definition 30 *Let Σ be a countable set of function symbols, each symbol $f \in \Sigma$ is associated with a non-negative integer n, its* arity *$ar(f)$ i.e. the number of arguments of f. Let $\mathcal{X}$ be a countable set of variables such that $\Sigma \cap \mathcal{X} = \emptyset$. The set of terms, denoted by $\mathcal{T}(\Sigma, \mathcal{X})$, is inductively defined by*

- *$\mathcal{X} \subseteq \mathcal{T}(\Sigma, \mathcal{X})$ (i.e. every rewriting variable is a term),*
- *for all $f \in \Sigma$ of arity n, and all $t_1, \ldots, t_n \in \mathcal{T}(\Sigma, \mathcal{X})$, the expression $f(t_1, \ldots, t_n) \in \mathcal{T}(\Sigma, \mathcal{X})$ (i.e. the application of function symbols to terms gives rise to terms).*

We denote by Σ_n the subset of Σ of the function symbols of arity n. For instance in the example f and g belong to Σ_1 while a and b belong to Σ_0. Two other common examples of terms are the expressions $Integral(\Omega, f(x), x)$ and $diff(f(x), x)$ which represent the expressions $\int_\Omega f(x)\,dx$ and $\dfrac{df(x)}{dx}$. Notice that $Integral \in \Sigma_3$, $diff \in \Sigma_2$, $f \in \Sigma_1$ and $x, \Omega \in \Sigma_0$. For the sake of simplicity we often keep the symbolic mathematical notation to express the rewriting rules. In the following we see a term as an oriented, ranked and rooted tree as it is usual in symbolic computation. We recall that in a ranked tree the child order is important. For instance the tree associated to the term $Integral(\Omega, f(x), x)$ has $Integral$ as its root which has three children in the order Ω, f, x and f has one child x.

Definition 31 *A* substitution *is a function $\sigma : \mathcal{X} \to \mathcal{T}(\Sigma, \mathcal{X})$ such that $\sigma(x) \neq x$ for $x \in \mathcal{X}$. The set of variables that σ does not map to themselves is called the* domain *of σ, i.e. $Dom(\sigma) = \{x \in \mathcal{X} \mid \sigma(x) \neq x\}$. If $Dom(\sigma) = \{x_1, \cdots, x_n\}$ then we might write σ as $\sigma = \{x_1 \mapsto t_1, \ldots, x_n \mapsto t_n\}$ for some terms $t_1, .., t_n$. Any substitution σ can be extended to a mapping $\mathcal{T}(\Sigma, \mathcal{X}) \to \mathcal{T}(\Sigma, \mathcal{X})$ as follows: for $x \in \mathcal{X}$, $\hat{\sigma}(x) = \sigma(x)$, and for any non-variable term $s = f(s_1, \cdots, s_n)$, we define $\hat{\sigma}(s) = f(\hat{\sigma}(s_1), \cdots, \hat{\sigma}(s_n))$. To simplify the notation we do not distinguish between a substitution $\sigma : \mathcal{X} \to \mathcal{T}(\Sigma, \mathcal{X})$ and its extension $\hat{\sigma} : \mathcal{T}(\Sigma, \mathcal{X}) \to \mathcal{T}(\Sigma, \mathcal{X})$.*

The application *of a substitution σ to a term t, denoted by $\sigma(t)$, simultaneously replaces all occurrences of variables in t by their σ-images.*

For instance, the maping σ defined by $\sigma(x) = a$ is a substitution and its extension $\hat{\sigma}$ maps $f(x)$ and $g(x)$ into $f(a)$ and $g(a)$.

A *rewriting rule*, is a pair (l, r) where l and r are terms in $\mathcal{T}(\Sigma, \mathcal{X})$; it will also be denoted by $l \rightsquigarrow r$. We observe that for any two terms s, t, there exists at most one substitution σ such that $\sigma(s) = t$. We mention that a rewriting rule stands for the rule application at the top position. It is more useful to be able to apply a rule at arbitrary position, and more generally to specify the way rules are applied. For this purpose we next present a strategy language that allows to built strategies out of basic constructors. To this end, we introduce strategy constructor symbols $;, \rightsquigarrow, \oplus, \mu, etc$ that do not belong to $\Sigma \cup \mathcal{X}$. Informally, the constructor ";" stands for the composition, " $\oplus$ " for the left choice, *Some* for the application of a strategy to the immediate subterms of the input term, $\eta(x)$ for the fail as identity constructor, $Child(j, s)$ applies the strategy s to the j^{th} immediate subterm, X is a fixed-point variable, and μ is the fixed-point or the iterator constructor, its purpose is to define recursive strategies. For example, the strategy $\mu X.(s; X)$ stands for $s; s; \ldots$, that is, it is the iteration of the application of s until a fixed-point is reached. The precise semantics of these constructors is given in Definition 33.

Definition 32 ***(Strategy)*** *Let $\mathcal{F}$ be a finite set of fixed-point variables. A strategy is inductively defined by the following grammar:*

$$s ::= l \rightsquigarrow r \mid s; s \mid s \oplus s \mid \eta(s) \mid Some(s) \mid Child(j, s) \mid X \mid \mu X.s \quad (1.32)$$

where $j \in \mathbb{N}$ and $X \in \mathcal{F}$. The set of strategies defined from a set of rewriting rules in $\mathcal{T}(\Sigma, \mathcal{X}) \times \mathcal{T}(\Sigma, \mathcal{X})$ is denoted by $\mathcal{S}_{\mathcal{T}}$.

We denote by $\mathbb{F}$ the failing result of a strategy and $\mathcal{T}^*(\Sigma, \mathcal{X}) = \mathcal{T}(\Sigma, \mathcal{X}) \cup \mathbb{F}$.

Definition 33 ***(Semantics of a strategy)*** *The semantics of a strategy is a function* $[\![.]\!] : \mathcal{S}_{\mathcal{T}(\Sigma,\mathcal{X})} \to (\mathcal{T}^*(\Sigma,\mathcal{X}) \to \mathcal{T}^*(\Sigma,\mathcal{X}))$ *defined by its application to each grammar component:*

$$[\![s]\!](\mathbb{F}) = \mathbb{F}$$

$$[\![l \rightsquigarrow r]\!](t) = \begin{cases} \sigma(r) & \text{if } \sigma(l) = t \\ \mathbb{F} & \text{otherwise} \end{cases}$$

$$[\![s_1; s_2]\!](t) = [\![s_2]\!]([\![s_1]\!](t))$$

$$[\![s_1 \oplus s_2]\!](t) = \begin{cases} [\![s_1]\!](t) & \text{if } [\![s_1]\!](t) \neq \mathbb{F} \\ [\![s_2]\!](t) & \text{otherwise} \end{cases}$$

$$[\![\eta(s)]\!](t) = \begin{cases} t & \text{if } [\![s]\!](t) = \mathbb{F} \\ [\![s]\!](t) & \text{otherwise} \end{cases}$$

$$[\![Some(s)]\!](t) = \begin{cases} \mathbb{F} & \text{if } ar(t) = 0 \\ f(\eta(s)(t_1), \ldots, \eta(s)(t_n)) & \text{if } t = f(t_1, \ldots, t_n) \text{ and } \exists i \in [1..n] \text{ s.t. } [\![s]\!](t_i) \neq \\ \mathbb{F} & \text{otherwise} \end{cases}$$

$$[\![Child(j, s)]\!](t) = \begin{cases} \mathbb{F} & \text{if } ar(t) = 0, \text{ or } t = f(t_1, \ldots, t_n) \text{ and } j > n \\ f(t_1, \ldots, t_{j-1}, [\![s]\!](t_j), t_{j+1}, \ldots, t_n) & \text{if } t = f(t_1, \ldots, t_n) \text{ and } j \leq n. \end{cases}$$

The semantics of the fixed-point constructor is more subtle. One would write:

$$[\![\mu X.s]\!] = [\![s[X/\mu X.s]]\!] \tag{1.33}$$

but this equation cannot be directly used to define $[\![\mu X.s]\!]$, since the right-hand side contains as a subphrase the phrase whose denotation we are trying to define. Notice that the equation (1.33) amounts to saying that $[\![\mu X.s]\!]$ should be the least fixed-point of the operator F:

$$F(X) = \lambda X^{(\mathcal{T}^*(\Sigma,\mathcal{X}) \to \mathcal{T}^*(\Sigma,\mathcal{X}))}\, [\![s]\!]^{(\mathcal{T}^*(\Sigma,\mathcal{X}) \to \mathcal{T}^*(\Sigma,\mathcal{X}))}.$$

Let $D = \mathcal{T}^*(\Sigma,\mathcal{X}) \to \mathcal{T}^*(\Sigma,\mathcal{X})$ and define $\sqsubseteq$ a partial order on D as follows:

$$w \sqsubseteq w' \text{ iff } graph(w) \subseteq graph(w').$$

Let $\perp$ be the function of empty graph, and let

$$F_0 = \perp$$
$$F_n = F(F_{n-1}).$$

One can show, using Knaster-Tarsky fixed-point theorem [55], that F_∞ is the least fixed-point of the operator F, that is

$$F(w) = w \implies F_\infty \sqsubseteq w.$$

Such fixed point equations arise very often in giving denotational semantics to languages with recursive features, for instance the semantics of the loop “while" of the programming languages [53, §9, §10].

Example 34 *Out of the basic constructors of strategies given in Definition 32, we built up some useful strategies. The strategy $OuterMost(s)$ applies the strategy s to an input term t in a top down way starting from the root, it stops when it succeeds. That is, if the strategy s succeeds on some subterm t' of t, then it is not applied to the proper subterms of t'. The strategy $TopDown(s)$ behaves exactly like $OuterMost(s)$ apart that if the strategy s succeeds on some subterm t' of t, then it is also applied to the proper subterms of t'. The strategy $InnerMost(s)$ (resp. $BottomUp(s)$) behaves like $InnerMost(s)$ (resp. $BottomUp(s)$) but in the opposite direction, i.e. it traverses a term t starting from the leafs. The strategy $Normalizer(s)$ iterates the application of s until a fixed-point is reached. The formal definition of these strategies follows:*

$$\begin{aligned} OuterMost(s) &:= \mu X.(s \oplus Some(OuterMost(X))),\\ TopDown(s) &:= \mu X.(s; Some(TopDown(X))),\\ InnerMost(s) &:= \mu X.(Some(InnerMost(X)) \oplus s),\\ BottomUp(s) &:= \mu X.(Some(BottomUp(X)); s),\\ Normalizer(s) &:= \mu X.(s; X). \end{aligned}$$

Example 35 *Let the variable set $\mathcal{X} = \{y, z, t, w\}$ and the partition $\Sigma = \Sigma_0 \cup \Sigma_1 \cup \Sigma_2$ of the set of function symbols with respect to their arity with $\Sigma_0 = \{x, x^1, x^2, \partial\Omega, \Omega, \varepsilon\}$, $\Sigma_1 = \{u, v, n, O, B\}$, $\Sigma_2 = \{derivative\}$, $\Sigma_3 = \{Integral\}$. We present the strategy that rewrites the expression*

$$\Psi = \int_{\partial\Omega} u(x)\ n(x)\ B(v(x^1, x^2))\ dx - \int_{\Omega} u(x)\ \frac{d}{dx}(B(v(x^1, x^2)))\ dx + O(\varepsilon),$$

taking into account that $B(v)$ vanishes on the boundary $\partial\Omega$. This term is written under mathematical form for simplicity, but in practice it is written from the above defined symbol of functions. Remark that the expression $B(v(x^1, x^2))$ is a function of the variable x but this does not appear explicitly in this formulation. Such a case cannot appear when the grammar for terms introduced in the next section is used. We need the two rewriting rules

$$\begin{aligned} r_1 &:= \int_{\partial\Omega} w\ dt \rightsquigarrow \int_{\partial\Omega} w\ dt,\\ r_2 &:= B(v(z, y)) \rightsquigarrow 0, \end{aligned}$$

and the strategy OuterMost already defined. Notice that the rule r_1 has no effect but to detect the presence of the integral over the boundary. Finally, the desired strategy, denoted by F, is:

$$F := OuterMost(r_1; OuterMost(r_2)),$$

and the result is

$$[\![F]\!](\Psi) = \int_{\partial\Omega} u(x)\ n(x)\ B(0)\ dx - \int_{\Omega} u(x)\ \frac{d}{dx}(B(v(x^1, x^2)))\ dx + O(\varepsilon).$$

1.4.2 Rewriting modulo equational theories

So far the semantics of strategies does not take into account the properties of some function symbols, e.g. associativity and commutativity equalities of "+". In particular the application of the rule $a + b \rightsquigarrow f(a, b)$ to the term $(a + c) + b$ fails. More generally we next consider the rewriting modulo an equational theory, i.e. a theory that is axiomatized by a set of equalities.
For the sake of illustration, we consider the commutativity and associativity theory of $+$, $E = \{x + y = y + x, (x + y) + z = x + (y + z)\}$ and the rewrite rule $f(x+y) \rightsquigarrow f(x)+f(y)$ applying the linearity rule of a function f. Its application to the term $f((a + b) + c)$ modulo E yields the set of terms $\{f(a+b)+f(c)$, $f(a)+f(b+c)$, $f(b)+f(a+c)\}$. In the following, we define part of the semantics of a strategy modulo a theory, we use the notation $\mathcal{P}(\mathcal{T}(\Sigma, \mathcal{X}))$ to denote the set of subsets of $\mathcal{T}(\Sigma, \mathcal{X})$.

Definition 36 ***(Semantics of a strategy modulo)*** *Let be E be a finitary equational theory, the semantics of a strategy modulo E is a function $[\![.]\!]^E : \mathcal{S}_{\mathcal{T}(\Sigma,\mathcal{X})} \rightarrow (\mathcal{P}(\mathcal{T}^*(\Sigma, \mathcal{X})) \rightarrow \mathcal{P}(\mathcal{T}^*(\Sigma, \mathcal{X})))$ that is defined by*

$$[\![s]\!]^E(\{t_1, \ldots, t_n\}) = \cup_{i=1}^{n} [\![s]\!]^E(t_i)$$
$$[\![l \rightsquigarrow r]\!]^E(t_1) = \cup_j \{\sigma_j(r)\} \text{ if } E \implies \sigma_j(l) = t,$$
$$[\![s_1; s_2]\!]^E(t) = [\![s_2]\!]^E([\![s_1]\!]^E(t))$$
$$[\![s_1 \oplus s_2]\!]^E(t) = \begin{cases} [\![s_1]\!]^E(t) & \text{if } [\![s_1]\!](t) \neq \{\mathbb{F}\} \\ [\![s_2]\!]^E(t) & \text{otherwise} \end{cases}$$
$$[\![\eta(s)]\!]^E(t) = \begin{cases} \{t\} & \text{if } [\![s]\!]^E(t) = \{\mathbb{F}\} \\ [\![s]\!]^E(t) & \text{otherwise.} \end{cases}$$

The semantics of *Some* and *Child* is more complex and we do not detail it here. The semantics of the fixed-point operator is similar to the one given in the rewriting modulo an empty theory.

1.4.3 Conditional rewriting

Rewriting with conditional rules, also known as conditional rewriting, extends the basic rewriting with the notion of condition. A conditional rewrite rule is a triplet:

$$(l, r, c)$$

where c is a constraint expressed in some logic. The semantics of the rule application is given by

$$[\![(l,r,c)]\!]^E(t) = \begin{cases} \cup_j\{\sigma_j(r)\} & \text{if the formula } \sigma_j(c) \text{ can be derived from } E, \\ \mathbb{F} & \text{otherwise.} \end{cases}$$

The set of strategies defined over rewriting rules $(l, r, c) \in \mathcal{T} \times \mathcal{T} \times \mathcal{T}_c$ is denoted by $\mathcal{S}_{\mathcal{T},\mathcal{T}_c}$.

1.4.4 Rewriting with memory

Some definitions or computations require storing the history of the transformations of some terms. To carry on, we introduce a particular function symbol $\mathbb{M} \in \Sigma_2$ of arity two to represent the memory. Intuitively the term $\mathbb{M}(t_1, t_2)$ represents the term t_1, besides the additional information that t_2 was transformed to t_1 at an early stage. From this consideration if follows that any strategy applied to $\mathbb{M}(t_1, t_2)$ should only be applied to t_1. Formally, we define the semantics of strategy application taking into account the memory as a partial function: $[\![.]\!]_{\mathbb{M}} : \mathcal{S}_{\mathcal{T}(\Sigma,\mathcal{X})} \to (\mathcal{T}^*(\Sigma, \mathcal{X}) \to \mathcal{T}^*(\Sigma, \mathcal{X}))$ so that:

$[\![s]\!]_{\mathbb{M}}(t) = \mathbb{M}([\![s]\!]_{\mathbb{M}}(t_1), t_2)$ if $t = \mathbb{M}(t_1, t_2)$, and behaves like $[\![.]\!]$, otherwise. That is,

$[\![s]\!]_{\mathbb{M}}(\mathbb{F}) = \mathbb{F}$

$$[\![l \rightsquigarrow r]\!]_{\mathbb{M}}(t) = \begin{cases} \sigma(r) & \text{if } \sigma(l) = t \\ \mathbb{F} & \text{otherwise} \end{cases}$$

$[\![s_1; s_2]\!]_{\mathbb{M}}(t) = [\![s_2]\!]_{\mathbb{M}}([\![s_1]\!]_{\mathbb{M}}(t))$

$$[\![s_1 \oplus s_2]\!]_{\mathbb{M}}(t) = \begin{cases} [\![s_1]\!]_{\mathbb{M}}(t) & \text{if } [\![s_1]\!]_{\mathbb{M}}(t) \neq \mathbb{F} \\ [\![s_2]\!]_{\mathbb{M}}(t) & \text{otherwise} \end{cases}$$

etc.

1.5 A Symbolic Computation Framework for Model Derivation

In this section we propose a framework for the two-scale model proofs. As in Example 35, the latter are formulated as rewriting strategies. We notice that the

following framework differs from that used in Example 35 in that it allows for the complete representation of the data. It does not rely on external structures such as hash tables. To this end, we define the syntax of the mathematical expressions by means of a grammar $\mathcal{G}$.

1.5.1 A Grammar for Mathematical Expressions

The grammar includes four rules to built terms for mathematical functions $\mathcal{F}$, regions $\mathcal{R}$, mathematical variables $\mathcal{V}$, and boundary conditions $\mathcal{C}$. It involves Σ_{Reg}, Σ_{Var}, Σ_{Fun}, Σ_{Oper}, and Σ_{Cons} which are sets of names of regions, variables, functions, operators, and constants so subsets of Σ_0. Empty expressions in Σ_{Reg} and Σ_{Fun} are denoted by $\perp_{\mathcal{R}}$ and $\perp_{\mathcal{F}}$. The set of usual algebraic operations $\Sigma_{Op} = \{+, -, \times, /, \hat{}\}$ is a subset of Σ_2. The elements of $\Sigma_{Type} = \{Unknown, Test, Known, \perp_{Type}\} \subset \Sigma_0$, $\perp_{Type}$ denoting the empty expression, are to specify the nature of a function, namely an unknown function (as u^{ε}, u^0, u^1 in the proof), a test function (as v, v^0, v^1) in a weak formulation or another known function (as a^{ε}, f^{ε}, a^0, f^0 or n_{Γ^1}). The boundary conditions satisfied by a function are specified by the elements of $\Sigma_{BC} = \{d, n, pd, apd, t\} \subset \Sigma_0$ to express that it satisfies Dirichlet, Neuman, periodic, anti-periodic or transmission conditions. The grammar also involve the symbols of functions `Reg`, `Fun`, `IndexedFun`, `IndexedReg`, `IndexedVar`, `Oper`, `Var`, and `BC` that define regions, mathematical functions, indexed functions or regions or variables, operators, mathematical variables and boundary conditions. The grammar reads as

$$
\begin{aligned}
\mathcal{F} ::= {} & \circledast\,(\mathcal{F}, \mathcal{F}) \;\mid\; d \;\mid\; \mathcal{V} \;\mid \\
& \texttt{Fun}(f, [\mathcal{V}, \ldots, \mathcal{V}], [\mathcal{C}, \ldots, \mathcal{C}], K) \;\mid \\
& \texttt{IndexedFun}(\mathcal{F}, \mathcal{V}) \;\mid \\
& \texttt{Oper}(A, [\mathcal{F}, \ldots, \mathcal{F}], [\mathcal{V}, \ldots, \mathcal{V}], [\mathcal{V}, \ldots, \mathcal{V}], [d, \ldots, d]) \;\mid \\
& \perp_{\mathcal{F}} \;\mid\; \mathbb{M}(\mathcal{F}, \mathcal{F}), \\
\mathcal{R} ::= {} & \texttt{Reg}(\Omega, [d, \ldots, d], \{\mathcal{R}, \ldots, \mathcal{R}\}, \mathcal{R}, \mathcal{F}) \;\mid \\
& \texttt{IndexedReg}(\mathcal{F}, \mathcal{V}) \;\mid \\
& \perp_{\mathcal{R}} \;\mid\; \mathbb{M}(\mathcal{R}, \mathcal{R}), \\
\mathcal{V} ::= {} & \texttt{Var}(x, \mathcal{R}) \;\mid\; \texttt{IndexedVar}(\mathcal{V}, \mathcal{V}) \;\mid\; \mathbb{M}(\mathcal{V}, \mathcal{V}), \\
\mathcal{C} ::= {} & \texttt{BC}(c, \mathcal{R}, \mathcal{F}) \;\mid\; \mathbb{M}(\mathcal{C}, \mathcal{C}),
\end{aligned}
$$

where the symbols Ω, d, $\circledast$, f, K, A, x and c hold for any function symbols in Σ_{Reg}, Σ_{Cons}, Σ_{Op}, Σ_{Fun}, Σ_{Type}, Σ_{Oper}, Σ_{Var}, and Σ_{BC}. The arguments of a region term are its region name, the list of its space directions (e.g. [1,3] for a plane in the variables (x_1, x_3)), the (possibly empty) set of subregions, the boundary and the outward unit normal. Those of a function term are its function name, the

list of the mathematical variables that range over its domain, its list of boundary conditions, and its nature. Those for an indexed region or variable or function term are its function or variable term and its index (which should be discrete). For an operator term these are its name, the list of its arguments, the list of mathematical variable terms that it depends, the list of mathematical variable terms of its co-domain (useful e.g. for T when the image cannot be deduced from the initial set), and a list of parameters. Finally, the arguments of a boundary condition term are its type, the boundary where it applies and an imposed function if there is one. For example, the imposed function is set to 0 for an homogeneous Dirichlet condition and there is no imposed function in a periodicity condition. We shall denote by $\mathcal{T}_{\mathcal{R}}(\Sigma,\emptyset)$, $\mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset)$, $\mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset)$, and $\mathcal{T}_{\mathcal{C}}(\Sigma,\emptyset)$ the set of terms generated by the grammar starting from the non-terminal $\mathcal{R}$, $\mathcal{F}$, $\mathcal{V}$, and $\mathcal{C}$. The set of all terms generated by the grammar (i.e. starting from $\mathcal{R}$, $\mathcal{F}$, $\mathcal{V}$, or $\mathcal{C}$) is denoted by $\mathcal{T}_{\mathcal{G}}(\Sigma,\emptyset)$. Finally, we also define the set of terms $\mathcal{T}_{\mathcal{G}}(\Sigma,\mathcal{X})$ where each non-terminal $\mathcal{R}$, $\mathcal{F}$, $\mathcal{V}$, and $\mathcal{C}$ can be replaced by a rewriting variable in $\mathcal{X}$. Equivalently, it can be generated by the extension of $\mathcal{G}$ obtained by adding " | x" with $x \in \mathcal{X}$ in the definition of each non-terminal term. Or, by adding $N ::= x$, with $x \in \mathcal{X}$ for each non-terminal N.

Example 37 *Throughout this Chapter, an underlined symbol represents a short-cut whose name corresponds to the term name. For instance,*

$$\underline{\Omega} = \texttt{Reg}(\Omega,[2],\emptyset,\underline{\Gamma},\underline{n}),\ \textit{where}\ \underline{\Gamma} = \texttt{Reg}(\Gamma,[],\emptyset,\perp_{\mathcal{R}},\perp_{\mathcal{F}}),$$
$$\underline{n} = \texttt{Fun}(n,[\underline{x}'],[],\mathit{Known}),\ \underline{x}' = \texttt{Var}(x,\underline{\Omega}')\ \textit{and}\ \underline{\Omega}' = \texttt{Reg}(\Omega,[2],\emptyset,\underline{\Gamma},\perp_{\mathcal{F}})$$

represents a region-term a one-dimensional domain named Ω, oriented in the direction x_2, with boundary $\underline{\Gamma}$ and with outward unit normal $\underline{n}$. The shortcut $\underline{\Gamma}$ is also for a region term representing the boundary named Γ.

Example 38 *An unknown function $u(x)$ defined on $\underline{\Omega}$ satisfying homogeneous Dirichlet boundary condition $u(x) = 0$ on $\underline{\Gamma}$ is represented by the function-term,*

$$\underline{u}(\underline{x}) = \texttt{Fun}(u,[\underline{x}],\texttt{BC}(d,\underline{\Gamma},0),\texttt{Unknown})\ \textit{where}\quad \underline{x} = \texttt{Var}(x,\underline{\Omega}).$$

1.5.2 Short-cut Terms

For the sake of conciseness, we introduce shortcut terms that are constantly used in the end of the Chapter: $\underline{\Omega} \in \mathcal{T}_{\mathcal{R}}(\Sigma,\mathcal{X})$, $\underline{x} \in \mathcal{T}_{\mathcal{V}}(\Sigma,\mathcal{X})$ defined in $\underline{\Omega}$, $\underline{I} \in \mathcal{T}_{\mathcal{R}}(\Sigma,\mathcal{X})$ used for (discrete) indices, $\underline{i} \in \mathcal{T}_{\mathcal{V}}(\Sigma,\mathcal{X})$ used as an index defined in $\underline{I}$, $\underline{u} \in \mathcal{T}_{\mathcal{F}}(\Sigma,\mathcal{X})$ or $\underline{u}(\underline{x}) \in \mathcal{T}_{\mathcal{F}}(\Sigma,\mathcal{X})$ to express that it depends on the variable $\underline{x}$ and $\underline{u}_{\underline{i}}$ the indexed-term of the function $\underline{u}$ indexed by $\underline{i}$. Similar definitions can be given for the other notations used in the proof as $\underline{\Omega}^\sharp$, $\underline{x}^\sharp$, $\underline{\Omega}^1$, $\underline{x}^1$, $\underline{\Omega}'$, $\underline{x}'$, $\underline{v}(\underline{x}^\sharp,\underline{x}^1)$ etc. The operators

necessary for the proof are the integral, the derivative, the two-scale transform T, its adjoint T^*, and B. In addition, for some extensions of the reference proof we shall use the discrete sum.
Instead of writing operator-terms as defined in the grammar, we prefer to use the usual mathematical expressions. The table below establishes the correspondance between the two formulations.

$$\begin{aligned}
\int \underline{u}\, d\underline{x} &\equiv \mathtt{Oper}(\mathtt{Integral}, \underline{u}, [\underline{x}], [], []),\\
\frac{\partial \underline{u}}{\partial \underline{x}} &\equiv \mathtt{Oper}(\mathtt{Partial}, \underline{u}, [\underline{x}], [\underline{x}], []),\\
tr(\underline{u}, \underline{x})(\underline{x'}) &\equiv \mathtt{Oper}(\mathrm{Restriction}, \underline{u}, [\underline{x}], [\underline{x'}], []),\\
T(\underline{u}, \underline{x})(\underline{x}^\sharp, \underline{x}^1) &\equiv \mathtt{Oper}(T, \underline{u}, [\underline{x}], [\underline{x}^\sharp, \underline{x}^1], [\varepsilon]),\\
T^*(\underline{v}, [\underline{x}^\sharp, \underline{x}^1])(\underline{x}) &\equiv \mathtt{Oper}(T^*, \underline{v}, [\underline{x}^\sharp, \underline{x}^1], [\underline{x}], [\varepsilon]),\\
B(\underline{v}, [\underline{x}^\sharp, \underline{x}^1])(\underline{x}) &\equiv \mathtt{Oper}(B, \underline{v}, [\underline{x}^\sharp, \underline{x}^1], [\underline{x}], [\varepsilon]),\\
\sum_{\underline{i}} \underline{u_i} &\equiv \mathtt{Oper}(\mathtt{Sum}, \underline{u_i}, [\underline{i}], [], []).
\end{aligned}$$

The multiplication and exponentiation involving two terms f and g are written fg and f^g as usual in mathematics. All these conventions have been introduced for terms in $\mathcal{T}(\Sigma, \emptyset)$. For terms in $\mathcal{T}(\Sigma, X)$ as those encoutered in rewriting rules, the rewriting variables can replace any of the above short cut terms.

Example 39 *The rewriting rule associated to the Green rule (1.12) reads*

$$\int \frac{\partial u}{\partial \underline{x}} v \; d\underline{x} \rightsquigarrow -\int u \frac{\partial v}{\partial \underline{x}} \; d\underline{x} + \int tr(u)\; tr(v)\; n \; d\underline{x'}.$$

with the short-cuts $\underline{\Gamma} = \mathtt{Reg}(\Gamma, d1, \emptyset, \perp_{\mathcal{R}}, \perp_{\mathcal{F}})$, $\underline{\Omega} = \mathtt{Reg}(\Omega, d2, \emptyset, \underline{\Gamma}, n)$, $\underline{x} = \mathtt{Var}(x, \underline{\Omega})$ *and* $\underline{x'} = \mathtt{Var}(x, \underline{\Gamma})$. *The other symbols* u, v, x, Ω, Γ, $d1$, $d2$, n *are rewriting variables, and for instance*

$$\frac{\partial u}{\partial x} \equiv \mathtt{Oper}(\mathtt{Partial}, u, x, [], []).$$

Applying this rule according to an appropriate strategy, say the top down strategy, to a term in $\mathcal{T}(\Sigma, \emptyset)$ *like*

$$\Psi = \int \frac{\partial \underline{f}(\underline{z})}{\partial \underline{z}} \underline{g}(\underline{z}) \; d\underline{z},$$

for a given variable term $\underline{z}$ *and function terms* $\underline{f}$, $\underline{g}$. *As expected, the result is*

$$-\int \underline{f}\, \frac{\partial \underline{g}}{\partial \underline{z}} \; d\underline{z} + \int \underline{f}\; \underline{g}\; \underline{n}\; d\underline{z'}$$

with evident notations for $\underline{n}$ *and* $\underline{z'}$.

1.5.3 A Variable Dependency Analyzer

The *variable dependency analyzer* Θ is related to *effect systems* in computer science [51]. It is a function from $\mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset)$ to the set $\mathcal{P}(\mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset))$ of the parts of $\mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset)$. When applied to a term $t \in \mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset)$, it returns the set of mathematical variables on which t depends. The analyzer Θ is used in the condition part of some rewriting rules and is inductively defined by

$$
\begin{array}{l}
\Theta(d) = \emptyset \text{ for } d \in \Sigma_{Cons},\\
\Theta(\underline{x}) = \{\underline{x}\} \text{ for } \underline{x} \in \mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset),\\
\Theta(\circledast(\underline{u},\underline{v})) = \Theta(\underline{u}) \cup \Theta(\underline{v}) \text{ for } \underline{u},\underline{v} \in \mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset) \text{ and } \circledast \in \Sigma_{Op},\\
\Theta(\bot_{\mathcal{F}}) = \emptyset,\\
\Theta(\underline{u}(\underline{x^1},..,\underline{x^n})) = \{\underline{x^1},..,\underline{x^n}\} \text{ for } \underline{u} \in \mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset) \text{ and } \underline{x^1},..,\underline{x^n} \in \mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset),\\
\Theta(\underline{u_{\underline{i}}}) = \Theta(\underline{u}) \text{ for } \underline{u} \in \mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset) \text{ and } \underline{i} \in \mathcal{T}_{\mathcal{V}}(\Sigma,\emptyset),\\
\Theta([\underline{u^1},\ldots,\underline{u^n}]) = \Theta(\underline{u^1}) \cup \cdots \cup \Theta(\underline{u^n}) \text{ for } \underline{u^1},\ldots,\underline{u^n} \in \mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset).
\end{array}
$$

The definition of Θ on the operator-terms is done case by case,

$$
\begin{array}{l}
\Theta(\int \underline{u}\, d\underline{x}) = \Theta(\underline{u}) \setminus \Theta(\underline{x}),\\
\Theta(\dfrac{\partial \underline{u}}{\partial \underline{x}}) = \begin{cases} \Theta(\underline{u}) \text{ if } \Theta(\underline{x}) \subseteq \Theta(u),\\ \emptyset \text{ otherwise,} \end{cases}\\
\Theta(tr(\underline{u},\underline{x})(\underline{x'})) = \Theta(\underline{x'}),\\
\Theta(T(\underline{u},\underline{x})(\underline{x}^\sharp,\underline{x}^1)) = (\Theta(\underline{u}) \setminus \Theta(\underline{x})) \cup \Theta([\underline{x}^\sharp,\underline{x}^1]) \text{ if } \Theta(\underline{x}) \cap \Theta(\underline{u}) \neq \emptyset,\\
\Theta(T^*(\underline{v},[\underline{x}^\sharp,\underline{x}^1])(\underline{x})) = (\Theta(\underline{v}) \setminus \Theta([\underline{x}^\sharp,\underline{x}^1])) \cup \Theta(\underline{x}) \text{ if } \Theta([\underline{x}^\sharp,\underline{x}^1]) \cap \Theta(\underline{v}) \neq \emptyset,\\
\Theta(B(\underline{v},[\underline{x}^\sharp,\underline{x}^1])(\underline{x}))) = (\Theta(\underline{v}) \setminus \Theta([\underline{x}^\sharp,\underline{x}^1])) \cup \Theta(\underline{x}) \text{ if } \Theta([\underline{x}^\sharp,\underline{x}^1]) \cap \Theta(\underline{v}) \neq \emptyset,\\
\Theta(\sum\limits_{\underline{i}} \underline{u_{\underline{i}}}) = \bigcup\limits_{\underline{i}} \Theta(\underline{u_{\underline{i}}}).
\end{array}
$$

We observe that these definitions are not very general, but they are sufficient for the applications of this Chapter. To complete the definition of Θ, it remains to define it on memory terms,

$$\Theta(\mathbb{M}(\underline{u},\underline{v})) = \Theta(\underline{u}).$$

Example 40 *For*

$$\Psi = \int_{\underline{\Omega}^\sharp} [\int_{\underline{\Omega}^1} T(\underline{u}(\underline{x}),\underline{x})(\underline{x}^\sharp,\underline{x}^1) \frac{\partial \underline{v}(\underline{x}^\sharp,\underline{x}^1)}{\partial \underline{x}^1} d\underline{x}^1] d\underline{x}^\sharp \in \mathcal{T}_{\mathcal{F}}(\Sigma,\emptyset),$$

the set $\Theta(\Psi)$ *of mathematical variables on which* Ψ *depends is hence inductively computed as follows:* $\Theta(\underline{u}(\underline{x})) = \{\underline{x}\}$, $\Theta(T(\underline{u}(\underline{x}),\underline{x})(\underline{x}^\sharp,\underline{x}^1)) = \{\underline{x}^\sharp,\underline{x}^1\}$, $\Theta(\underline{v}(\underline{x}^\sharp,\underline{x}^1)) = \{\underline{x}^\sharp,\underline{x}^1\}$, $\Theta(\frac{\partial \underline{v}(\underline{x}^\sharp,\underline{x}^1)}{\partial \underline{x}^1}) = \{\underline{x}^\sharp,\underline{x}^1\}$, $\Theta(T(\underline{u}(\underline{x}),\underline{x})\ (\underline{x}^\sharp,\underline{x}^1)\ \frac{\partial \underline{v}(\underline{x}^\sharp,\underline{x}^1)}{\partial \underline{x}^1}) = \{\underline{x}^\sharp,\underline{x}^1\}$, $\Theta(\int_{\underline{\Omega}^1} T(\underline{u}(\underline{x}),\underline{x})(\underline{x}^\sharp,\underline{x}^1)\ \frac{\partial \underline{v}(\underline{x}^\sharp,\underline{x}^1)}{\partial \underline{x}^1} d\underline{x}^1) = \{\underline{x}^\sharp\}$, *and* $\Theta(\Psi) = \emptyset$, *that is,* Ψ *is a constant function.*

1.5.4 Formulation of the Symbolic Framework for Model Derivation

Now we are ready to define the framework for two-scale model derivation by rewriting. To do so, the rewriting rules are restricted to left and right terms $(l, r) \in \mathcal{T}_{\mathcal{G}}(\Sigma, \mathcal{X}) \times \mathcal{T}_{\mathcal{G}}(\Sigma, \mathcal{X})$. Their conditions c are formulas generated by a grammar, not explicited here, combining terms in $\mathcal{T}_{\mathcal{G}}(\Sigma, \mathcal{X})$ with the usual logical operators in $\Lambda = \{\vee, \wedge,], \in\}$. It also involves operations with the dependency analyzer Θ. The set of terms generated by this grammar is denoted by $\mathcal{T}_{\mathcal{L}}(\Sigma, \mathcal{X}, \mathcal{G}, \Theta, \Lambda)$.

It remains to argue that, given a strategy s in $\mathcal{S}_{\mathcal{T}_{\mathcal{G}}(\Sigma,\mathcal{X}),\mathcal{T}_{\mathcal{L}}(\Sigma,\mathcal{X},\mathcal{G},\Theta,\Lambda)}$, the set of terms $\mathcal{T}_{\mathcal{G}}(\Sigma, \emptyset)$ is closed under the application of s. It is sufficient to show that for each rewriting r rule in s, the application of r to any term $t \in \mathcal{T}_{\mathcal{G}}(\Sigma, \emptyset)$ at any position yields a term in $\mathcal{T}_{\mathcal{G}}(\Sigma, \emptyset)$. As an example, $\mathcal{T}_{\mathcal{G}}(\Sigma, \emptyset)$ is not closed under the application of the rule $x \rightsquigarrow \underline{\Omega}$, where x is a variable. But it is closed under the application of the linearity rule $\int_z f+g\,dx \rightsquigarrow \int_z f\,dx+\int_z g\,dx$ at any position, where f, g, x, z are rewriting variables. The argument is, since $\int_z f+g\,dx \in \mathcal{T}_{\mathcal{F}}(\Sigma, \emptyset)$, then $f+g \in \mathcal{T}_{\mathcal{F}}(\Sigma, \emptyset)$, and hence $f, g \in \mathcal{T}_{\mathcal{F}}(\Sigma, \emptyset)$. Thus, $\int_z f\,dx+\int_z g\,dx \in \mathcal{T}_{\mathcal{F}}(\Sigma, \emptyset)$. That is, a term in $\mathcal{T}_{\mathcal{F}}(\Sigma, \emptyset)$ is replaced by a another term in $\mathcal{T}_{\mathcal{F}}(\Sigma, \emptyset)$. A more general setting that deals with the closure of regular languages under specific rewriting strategies can be found in [35].
A model derivation is divided into several intermediary lemmas. Each of them is intended to produce a new property that can be expressed as one or few rewriting rules to be applied in another part of the derivation. Since dynamical creation of rules is not allowed, a strategy is covering one lemma only and is operating with a fixed set of rewriting rules. The conversion of a result of a strategy to a new set of rewriting rules is done by an elementary external operation that is not a limitation for generalizations of proofs. The following definition summarizes the framework of symbolic computation developed in this Chapter.

Definition 41 *The components of the quintuplet* $\Xi = \langle \Sigma, \mathcal{X}, E, \mathcal{G}, \Theta \rangle$ *provide a framework for symbolic computation to derive multi-scale models. A two-scale model derivation is expressed as a strategy* $\pi \in \mathcal{S}_{\mathcal{T}_{\mathcal{G}}(\Sigma,\mathcal{X}),\mathcal{T}_{\mathcal{L}}(\Sigma,\mathcal{X},\mathcal{G},\Theta,\Lambda)}$ *for which the semantics* $[\![\pi]\!]^E$ *is applicable to an initial expression* $\Psi \in \mathcal{T}(\Sigma, \emptyset)$.

In the end of this section we argue that this framework is in the same time relatively simple, it covers the *reference model* derivation and it allows for the extensions presented in the next section.

The grammar of terms is designed to cover all mathematical expressions occuring in the proof of the *reference model* as well as of their generalizations. A term that follows the grammar includes locally all useful information. This avoids the use of external tables and facilitates design of rewriting rules, in particular to take into account the context of subterms to be transformed. It allows also for local definitions, for instance a same name of variable x can be used in different parts of a same term with different meaning, which is useful for instance in integrals. A limitation regarding generalizations presented in the next section, is that the grammar must cover by anticipation all needed features.

Each step in the proof consists in replacing parts of an expression according to a known mathematical property. This is well done, possibly recursively, using rewriting rules together with strategies allowing for precise localization. Some steps need simplifications and often use the second linearity rule of a linear operator, $A(\lambda u) = \lambda Au$ when λ is a scalar (or is independent of the variables in the initial set of A). So variable dependency of each subterm should be determined, this is precisely what Θ, the *variable dependency analyzer*, is producing. The other simplifications do not require the use of Θ. In addition to the grammar $\mathcal{G}$, the analyzer Θ must be upgraded in view of each new extension.

In all symbolic computation based on the grammar $\mathcal{G}$, it is implicitely assumed that the derivatives, the integrals and the traces (i.e. restriction of a function to the boundary) are well defined since the regularity of functions is not encoded.

Due to the algebraic nature of the mathematical proofs, this framework has been formulated by considering these proofs as a calculus rather than formal proofs that can be formalized and checked with a proof assistant [8, 57]. Indeed, this is far simpler and allows, from a very small set of tools, for building significant mathematical derivation. To cover broader proofs, the framework must be changed by extending the grammar and the variable dependency analyzer only. Yet, the language Tom [5] does not provide a complete environment for the implementation of our framework since it does not support the transformation of rewriting rules, despite it provides a rich strategy language and a module for the specification of the grammar.

1.6 Transformation of Strategies as Second Order Strategies

For a given rewriting strategy representing a model proof, one would like to transform it to obtain a derivation of more complex models. Transforming a strategy $\pi \in \mathcal{S}_{\mathcal{T}(\Sigma,\mathcal{X})}$ is achieved by applying strategies to the strategy π itself. For this purpose, we consider two levels of strategies: the first order ones $\mathcal{S}_{\mathcal{T}(\Sigma,\mathcal{X})}$ as defined in Definition 32, and the strategies of second order in such a way that second order strategies can be applied to first order ones. That is, the second order strategies are considered as terms in a set $\mathcal{T}(\overline{\Sigma},\overline{\mathcal{X}})$ of terms where $\overline{\Sigma}$ and $\overline{\mathcal{X}}$ remain to be defined. Given a set of strategies $\mathcal{S}_{\mathcal{T}(\Sigma,\mathcal{X})}$ that comes with a set of fixed-point variables $\mathcal{F}$, we pose $\overline{\Sigma} \supset \Sigma \cup \{\rightsquigarrow, ;, \oplus, Some, Child, \eta, \mu\} \cup \mathcal{F}$. Let $\overline{\mathcal{X}}$ be a set of second order rewriting variables such that $\overline{\mathcal{X}} \cap (\mathcal{X} \cup \overline{\Sigma}) = \emptyset$. Notice that first order rewriting variables and fixed-point variables are considered as constants in $\mathcal{T}(\overline{\Sigma},\overline{\mathcal{X}})$, i.e. function symbols in $\overline{\Sigma}_0$. Notice also that the arity of the function symbols $\rightsquigarrow, ;, \oplus, Child, \mu$ is two, and the arity of $Some$ and η is one. In particular, the rule $l \rightsquigarrow r$ can be viewed as the term $\rightsquigarrow (l, r)$ with the symbol $\rightsquigarrow$ at the root, and the strategy $\mu X.s$ viewed as the term $\mu(X, s)$. This allows us to define second order strategies $\overline{\mathcal{S}}_{\mathcal{T}(\overline{\Sigma},\overline{\mathcal{X}})}$ by the grammar

$$\bar{s} ::= l \bar{\rightsquigarrow} r \mid \bar{s} \bar{;} \bar{s} \mid \bar{s} \bar{\oplus} \bar{s} \mid \bar{\eta}(\bar{s}) \mid \overline{Some}(\bar{s}) \mid \overline{Child}(j, \bar{s}) \mid X \mid \bar{\mu} X.\bar{s} \quad (1.34)$$

Again we assume that the symbols $\bar{\rightsquigarrow}, \bar{;}, \overline{\oplus}, \ldots$ of the second order strategies do no belong to $\overline{\Sigma}$. The semantics of the strategies in $\overline{\mathcal{S}}_{\mathcal{T}(\overline{\Sigma},\overline{\mathcal{X}})}$ are similar to the semantics of first order strategies. In addition, we assume that second order strategies transform first order strategies, to which they are applied, into first order strategies. Composing several second order strategies and applying such composition to a given first order strategy s provide successive transformations of s.

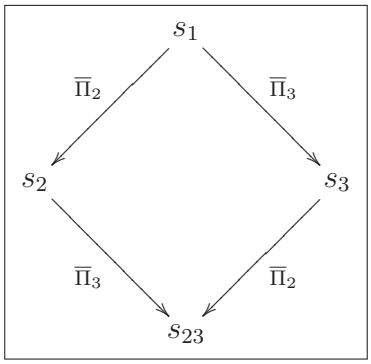


Figure 1.2: An example of the composition of transformations of strategies.

In the following example we illustrate the extension of an elementary strategy which is a rewriting rule.

Example 42 *For the set* $\mathcal{X} = \{i, j, x, x^\sharp, x^1, u, \varepsilon\}$ *we define* s_1, s_2, s_3, *and* s_{23} *four rewriting rules,*

$$s_1 := T(\frac{\partial u}{\partial x}, x)(x^\sharp, x^1) \rightsquigarrow \frac{1}{\varepsilon}\frac{\partial T(u,x)(x^\sharp, x^1)}{\partial x^1} \text{ for } x \in \Omega \text{ and } (x^\sharp, x^1) \in \Omega^\sharp \times \Omega^1,$$
$$s_2 := T(\frac{\partial u}{\partial x_i}, x)(x^\sharp, x^1) \rightsquigarrow \frac{1}{\varepsilon}\frac{\partial T(u,x)(x^\sharp, x^1)}{\partial x_i^1} \text{ for } x \in \Omega \text{ and } (x^\sharp, x^1) \in \Omega^\sharp \times \Omega^1,$$
$$s_3 := T(\frac{\partial u}{\partial x}, x)(x^\sharp, x^1) \rightsquigarrow \frac{1}{\varepsilon}\frac{\partial T(u,x)(x^\sharp, x^1)}{\partial x^1} \text{ for } x \in \Omega_j \text{ and } (x^\sharp, x^1) \in \Omega_j^\sharp \times \Omega_j^1,$$
$$s_{23} := T(\frac{\partial u}{\partial x_i}, x)(x^\sharp, x^1) \rightsquigarrow \frac{1}{\varepsilon}\frac{\partial T(u,x)(x^\sharp, x^1)}{\partial x_i^1} \text{ for } x \in \Omega_j \text{ and } (x^\sharp, x^1) \in \Omega_j^\sharp \times \Omega_j^1.$$

The rule s_1 *is encountered in the reference proof,* s_2 *is a (trivial) generalization of* s_1 *in the sense that it applies to multi-dimensional regions* Ω^1 *referenced by a set of variables* $(x_i^1)_i$, *and* s_3 *is a second (trivial) generalization of* s_1 *on the number of sub-regions* $(\Omega_j)_j$, $(\Omega_j^\sharp)_j$ *and* $(\Omega_j^1)_j$ *in* Ω, $\Omega^\sharp$ *and* Ω^1. *The rule* s_{23} *is a generalization combining the two previous generalizations. First, we aim at transforming the strategy* s_1 *into the strategy* s_2 *or the strategy* s_3. *To this end, we introduce two second order strategies with* $\overline{\mathcal{X}} = \{v, z\}$ *and* $\overline{\Sigma} \supset \{i,\ j,\ \Omega,\ \Omega^\sharp,\ \Omega^1,\ Partial, IndexedFun, IndexedVar, IndexedReg\}$,

$$\bar{\Pi}_1 := \overline{TopDown}(\frac{\partial v}{\partial z} \bar{\rightsquigarrow} \frac{\partial v}{\partial z_i})$$
$$\bar{\Pi}_2 := \overline{TopDown}(\Omega \bar{\rightsquigarrow} \Omega_j); \overline{TopDown}(\Omega^\sharp \bar{\rightsquigarrow} \Omega_j^\sharp); \overline{TopDown}(\Omega^1 \bar{\rightsquigarrow} \Omega_j^1)$$

Notice that $\bar{\Pi}_1$ *(resp.* $\bar{\Pi}_2$*) applies the rule* $\frac{\partial v}{\partial z} \bar{\rightsquigarrow} \frac{\partial v}{\partial z_i}$ *(resp.* $\Omega \bar{\rightsquigarrow} \Omega_j$, $\Omega^\sharp \bar{\rightsquigarrow} \Omega_j^\sharp$, *and* $\Omega^1 \bar{\rightsquigarrow} \Omega_j^1$*) at all of the positions* [5] *of the input first order strategy so that*

$$\bar{\Pi}_1(s_1) = s_2 \text{ and } \bar{\Pi}_2(s_1) = s_3.$$

Once $\bar{\Pi}_1$ *and* $\bar{\Pi}_2$ *have been defined, they can be composed to produce* s_{23} :

$$\bar{\Pi}_2\bar{\Pi}_1(s_1) = s_{23} \text{ or } \bar{\Pi}_1\bar{\Pi}_2(s_1) = s_{23}.$$

The diagram of Figure 1 illustrates the application of $\bar{\Pi}_1$, $\bar{\Pi}_2$ *and of their compositions.*

[5] Notice the difference with $\overline{OuterMost}$ which could not apply these rules at any position.

The next example shows how an extension can not only change rewriting rules but also to add new ones.

Example 43 *To operate simplifications in the reference model, we use the strategy*

$$s_1 := OuterMost(\frac{\partial x}{\partial x} \rightsquigarrow 1).$$

In the generalization to multi-dimensional regions, it is replaced by two strategies involving the Kronecker symbol δ, usually defined as $\delta(i,j) = 1$ if $i = j$ and $\delta(i,j) = 0$ otherwise,

$$\begin{aligned} s_2 &: = OuterMost\left(\frac{\partial x_i}{\partial y_j} \rightsquigarrow \delta(i,j),\ x = y\right), \\ s_3 &: = OuterMost\left(\delta(i,j) \rightsquigarrow 1,\ i = j\right), \\ s_4 &: = OuterMost\left(\delta(i,j) \rightsquigarrow 0,\ i \neq j\right). \end{aligned}$$

The second order strategy that transforms s_1 into the strategy $Normalizer(s_2 \oplus s_3 \oplus s_4)$ is

$$\bar{\Pi} := \overline{OuterMost}(s_1 \bar{\rightsquigarrow} s_2 \oplus s_3 \oplus s_4).$$

1.7 Implementation and Experiments

The framework presented in Section 1.5.4 has been implemented in Maple®. The implementation includes the language *Symbtrans* of strategies already presented in [6]. The derivation of the reference model presented in Section 1.3 has been fully implemented. It starts from an input term which is the weak formulation (1.24) of the physical problem,

$$\int \underline{a} \frac{\partial \underline{u}}{\partial \underline{x}} \frac{\partial \underline{v}}{\partial \underline{x}} \, d\underline{x} = \int \underline{f} \; \underline{v} \, d\underline{x}, \tag{1.35}$$

where $\underline{a} = \mathtt{Fun}(a, [\underline{\Omega}], [\,], Known)$, $\underline{u} = \mathtt{Fun}(u, [\underline{\Omega}], [\underline{Dirichlet}], Unknown)$, $\underline{v} = \mathtt{Fun}(u, [\underline{\Omega}], [\underline{Dirichlet}], Test)$, $\underline{\Omega} = \mathtt{Reg}(\Omega, [1], \emptyset, \underline{\Gamma}, n_\Omega)$, $\underline{\Gamma} = \mathtt{Reg}(\Gamma, [\,], \emptyset, \perp_{\mathcal{R}}, \perp_{\mathcal{F}})$, $\underline{Dirichlet} = \mathtt{BC}(Dirichlet, \underline{\Gamma}, 0)$ and where the short-cuts of the operators are those of Section 1.5.2. The information regarding the two-scale transformation is provided through the test functions. For instance, in the first block the proof starts with the expression

$$\Psi = \int \frac{\partial \underline{u}}{\partial \underline{x}} B(\underline{v}(\underline{x^\sharp}, \underline{x^1})(\underline{x}) \, d\underline{x},$$

where the test function $B(\underline{v}(\underline{x^\sharp}, \underline{x^1})(\underline{x})$ is also an input, with $\underline{v} = \mathtt{Fun}(a, [\underline{x^\sharp}, \underline{x^1}], [\underline{Dirichlet\sharp}], Test)$, $\underline{x^\sharp} = \mathtt{Var}(x^\sharp, \underline{\Omega^\sharp})$, $\underline{x^1} = \mathtt{Var}(x^1, \underline{\Omega^1})$, $\underline{\Omega^\sharp} = \mathtt{Reg}(\Omega^\sharp, [1], \emptyset, \underline{\Gamma^\sharp}, n_{\Omega^\sharp})$, $\underline{\Gamma^\sharp} = \mathtt{Reg}(\Gamma^\sharp, [\,], \emptyset, \perp_{\mathcal{R}}, \perp_{\mathcal{F}})$, $\underline{\Omega^1} = \mathtt{Reg}(\Omega^1, [1], \emptyset, \underline{\Gamma^1}, n_{\Omega^1})$, $\underline{\Gamma^1} = \mathtt{Reg}(\Gamma^1, [\,], \emptyset, \perp_{\mathcal{R}}, \perp_{\mathcal{F}})$, and $\underline{Dirichlet\sharp} = \mathtt{BC}(Dirichlet\sharp, \underline{\Gamma^\sharp}, 0)$.

The proof is divided into five strategies corresponding to the five blocks of the proof, each ending by some results transformed into rewriting rules used in the following blocks. The rewriting rules used in the strategies are FO-rules and can be classified into the three categories.

- *Usual mathematical rules:* that represent the properties of the derivation and integration operators, such as the linearity, the chain rule, the Green rule, etc,
- *Specialized rules:* for the properties of the two-scale calculus, as those of the two-scale transform, the approximation of B by the adjoint T^* etc,
- *Auxiliary tools:* for transformations of expressions format that are not related to operator properties such as the rule which transforms $\psi_1 = \psi_2$ into $\psi_1 - \psi_2 = 0$.

	Usual Rules	Specialized Rules	Aux. Tools
Skeleton	53	14	28

Table 1.1: The number of first order rules used in the reference model.

The Table 1.1 summarizes the number of first order (FO) rules, used in the reference model, by categories.

The reference model has been extended to cover three different kinds of configurations. To proceed to an extension, the new model derivation is established in a form that is as close as possible of the *reference proof.* The grammar and the dependency analyzer should be completed. Then, the initial data is determined, and second order (SO) strategies yielding the generalized model derivation are found and optimized. As it has been already mentioned, $\mathcal{G}$ and Θ have already been designed to cover the three extensions.

The first generalization is to cover multi-dimensional regions, i.e. $\Omega \subset \mathbb{R}^n$ with $n \geq 1$. When $n = 2$, the initial term is

$$\sum_{\underline{i}=1}^{n} \sum_{\underline{j}=1}^{n} \int \underline{a}_{\underline{ij}} \frac{\partial \underline{u}}{\partial \underline{x}_{\underline{i}}} \frac{\partial \underline{v}}{\partial \underline{x}_{\underline{j}}} \, d\underline{x} = \int \underline{f} \; \underline{v} \; d\underline{x},$$

where $\underline{\Omega} = \texttt{Reg}(\Omega, [1,2], \emptyset, \underline{\Gamma}, n_\Omega)$, $\underline{a}_{\underline{ij}} = \texttt{Indexed}(\texttt{Indexed}(\underline{a}, \underline{j}), \underline{i})$, $\underline{i} = \texttt{Var}(i, \underline{I})$, and $\underline{I} = \texttt{Reg}(I, [1,2], \emptyset, \perp_{\mathcal{R}}, \perp_{\mathcal{F}})$ and the choice of the test function is trivially deduced. Then, the model derivation is very similar to this of the *reference model*, see [47], so much so it is obtained simply by applying the SO strategy $\bar{\Pi}_1$defined in Example 42. This extension has been tested on the four first blocks.

The second generalization transforms the *reference model* into a model with several adjacent one-dimensional regions (or intervals) $(\Omega_k)_{k=1,..,m}$ so that Ω is still an interval i.e. $\Omega \subset \mathbb{R}$. For $m = 2$, the initial term is the same as (1.35) but with $\underline{\Omega} = \texttt{Reg}(\Omega, [1],\ \{\underline{\Omega_1}, \underline{\Omega_2}\},\ \underline{\Gamma}, n_\Omega)$, $\underline{\Omega_1} = \texttt{Reg}(\Omega_1, [1],\ \emptyset,\ \underline{\Gamma_1}, n_{\Omega_1})$, and $\underline{\Omega_2} = \texttt{Reg}(\Omega_2, [1],\ \emptyset,\ \underline{\Gamma_2}, n_{\Omega_2})$. The two-scale geometries, all variables, all kind of functions and also the operators B and T are defined subregion by subregion. All definitions and properties apply for each subregion, and the proof steps are the same after spliting the integrals over the complete region Ω into integrals over the subregions. The only major change is in the fourth step where the equality $u_1^0 = u_2^0$ at the interface between Ω_1 and Ω_2 which is encoded as transmission conditions in the boundary conditions of u_1^0 and u_2^0.

The third extension transforms the multi-dimensional model obtained from the first generalization to a model related to thin cylindrical regions, in the sense that the dimension of Ω is in the order of ε in some directions $i \in I^\natural$ and of the order 1 in the others $i \in I^\sharp$ e.g. $\Omega = (0,1) \times (0,\varepsilon)$ where $I^\natural = \{2\}$ and $I^\sharp = \{1\}$. The boundary Γ is split in two parts, the lateral part Γ_{lat} and the other parts Γ_{other} where the Dirichlet boundary conditions are replaced by homogeneous Neuman boundary conditions i.e. $\frac{du^\varepsilon}{dx} = 0$. In this special case the integrals of the initial term are over a region whose size is of the order of ε so it is required to multiply each side of the equality by the factor $1/\varepsilon$ to work with expressions of the order of 1. Moreover, the macroscopic region differs from Ω, it is equal to $\Omega^\sharp = (0,1)$ when the microscopic region remains unchanged. In general, the definition of the adjoint T^* is unchanged but $(Bv)(x) = v((x_i)_{i\in I^\sharp}, (x - x_c^\sharp)/\varepsilon)$ where $x_c^\sharp$ is the center of the c^{th} cell in $\Omega^\sharp$. It follows that the approximations (1.10, 1.11) are between T^* and εB with $\sum_{i\in I^\sharp} x_i^1 \frac{\partial v}{\partial x_i^\sharp}$ instead of $\sum_{i=1}^n x_i^1 \frac{\partial v}{\partial x_i^\sharp}$. With these main changes in the definitions and the preliminary properties, the proof steps may be kept unchanged.

	Usual Rules	Specialized Rules	Aux. Tools
Multi-Dimension	6	0	4
Thin-Region	2	0	0
Multi-Region	3	0	0

Table 1.2: The number of first order rules used in the three extensions.

The mathematical formulation of the second and third extensions has been derived. This allows for the determination of the necessary SO-strategies, but they have not been implemented nor tested. To summarize the results about the principle of extension of strategies, we show its benefit through some statistics. In particular the main concerned is the reusability and the extensibility of existing strategies. The Table 1.2 shows an estimate of the number of new FO-rules for the three extensions in each category and for the first four blocks.

	Usual Rules	Specialized Rules	Aux. Tools
Multi-Dimension	9	2	3
Thin-Region	0	0	0
Multi-Region	1	0	0

Table 1.3: The number of second order strategies used in the extension of proofs.

Input model	Resulting model	% Modi. FO-rules	% Modi. FO-strategies
Reference	Multi-Dim.	16.6%	5%
Multi-Dim.	Thin	0	0
Thin	Multi-Reg.	0	2.5%

Table 1.4: The ratio of modified FO-rules and FO-strategies.

The Table 1.3 shows the number of SO-strategies used in each extension. Finally, the Table 1.4 shows the ratio of the modified FO-rules and the ratio of the modified FO-strategies. The reusability ratio is high since most of the FO-strategies defined in the skeleton model are reused. Besides very little number of SO-strategies is used in the extensions. This systematic way of the generation of proofs is a promising path that will be further validated within more complex configurations for which the proofs can not be obtained by hand. In the future, we plan to introduce dedicated tools to aid in the design of composition of several extensions.

Chapter 2

Extension Mechanisms and Their Combination For Multi-Scale Model Derivations

Abstract *In this Chapter we address the problem of the combination of the extensions of the proofs related to the multi-scale model derivations. For this purpose, we develop further extension mechanisms which turn to be more rudimentary than the ones introduced in Chapter 1. The simplicity of these new mechanisms allows us to elaborate necessary conditions under which these mechanisms can be correctly combined giving rise to rich extensions. We illustrate the application of these extension mechanisms to many examples, namely to the derivation of the linear operator associated to the microscopic problem in the reference proof. Thus the results of this Chapter significantly improve the results of Chapter 1 since it is not possible, at least in a straightforward way, to provide necessary conditions so that the extension mechanisms established in Chapter 1 can be combined.*

2.1 Introduction

We follow the approach presented in Chapter 1 that consists in formalizing the multi-scale proofs by means of symbolic transformations. In particular, the mathematical properties, lemmas and theorems are represented as rewriting rules; and the proofs are represented as rewriting strategies.

In this Chapter we address the problem of the generation of complex models by *reusing* the proofs and tools used for the generation of simpler models. More precisely, we address the problem of the *combination* of the extensions. This problem can be formulated as follows: Given a reference proof, an extension E_1 (viewed as a transformation) of the reference proof to some general setting (e.g.

multi-dimensional setting), an extension E_2 of the reference proof to an another general setting (e.g. thinness setting), we would like to construct an extension E' so that the application of E' to the reference proof yields a proof that covers both the two settings.

It turned out that it is not easy to study the combination of extensions if these extensions are formulated as second-order strategies, as presented in Chapter 1. To solve this problem, we refine the notion of extension by proposing two extension mechanisms:

1. Firstly, we follow the approach of Chapter 1 that consists in extending first-order rules by means of second-order rules. Since, obviously, not every second-order rule is *adequate* for this extension, we provide some *syntactic* requirements under which second-order rules can extend first-order ones. These syntactic requirements deal with the notions of:

   (a) a second-order rule s_2 being *subsumed* by a second-order rule s_1. This can be understood as s_1 being *more general* than s_2, and

   (b) the *mathematical equivalence* between second-order rules. For instance, we would like to formulate the idea that the two expressions $\sum_{i=1}^{i=1} \alpha_i$ and α are mathematically equivalent.

   However, it is not clear how to build these second-order rules nor how to combine them. This leads to the second point.

2. Secondly, we establish a second extension mechanism that consists in defining rudimentary components, called *added terms*, allowing, on the hand, to express the kind of extensions that we want to make, and, on the other hand, they can be combined to build more complex components. These components will be inserted at certain positions of a FO-term and a FO-rule. The careful choice of the added terms as well as the way they are combined ensure the correctness of the extension.

As a concrete application, we apply the second extension mechanism to extend one step of the two-scale model derivation of the stationary heat equation (Eq. (1.22)) to the multi-dimensional and the vector-valued settings as well as their combination. We plan to implement these extensions mechanisms with the symbolic transformation language if proposed in [6]. It is worth mentioning that if was successfully used to encode many examples of the multi-scale derivations e.g. [58, 59, 6].

2.1.1 Organization of the Chapter

The Chapter is organized as follows: Section 2.2 introduces computer science tools and concepts which will be used to formulate the extension mechanisms for the multi-scale model derivations. Namely, the notion of term rewriting will be introduced. In section 2.3 we introduce the notion of second-order rewriting rules that operate on (first-order) rewriting rules and we define a grammar for the mathematical expressions. In section 2.4 we introduce the first extension mechanism that consists in the extension of (first-order) rules by means of second-order rules that fulfill some conditions. In section 2.5 we introduce the second extension mechanism, called the *outward growth*, for the extension of mathematical expressions. In order to construct complex extensions by means of outward growths, we define the operation of *combination* of outward growths and its properties. In section 2.6 we formulate the outward growth mechanism as second-order rewriting rules. Such outward growths are called *second-order outward growth*. We define the operation of *combination* of second-order outward growths as well as its properties. In section 2.7 we introduce the mechanism of *parametrization* that can be composed with the mechanism of outward growth. In section 2.8 we apply the mechanism of the outward growth to extend one step in the two-scale model derivation of the stationary heat equation. In section 2.9 we conclude the Chapter with several remarques and perspectives, namely we will discuss the formulation of the outward growths and the parametrization and their combination by means of strategies.

2.2 Term rewriting

In this section we introduce some computer science concepts and tools which will be used to formulate the extension mechanisms for the multi-scale model derivations. In particular, we shall introduce the notion of term rewriting. Before we formally introducing it, we firstly give the main ideas behind it.

The set of rewriting terms, denoted by $\mathcal{T}(\mathcal{F}, \mathcal{X})$, is built up as a combination of function symbols in a set $\mathcal{F}$ and rewriting variables in a set $\mathcal{X}$. Besides, each function symbol in $\mathcal{F}$ comes with a *fixed arity*. The arity of a function symbol can be viewed as the number of its "arguments". Therefore, the function symbols $\mathcal{F}$ can be written as a union $\mathcal{F} = \mathcal{F}_0 \cup \mathcal{F}_1 \ldots \cup \mathcal{F}_n$ of function symbols, where $\mathcal{F}_i$ is a set of function symbols of arity i. In particular, function symbols of zero arity, i.e. those in $\mathcal{F}_0$, are called *constants*. We emphasize that function symbols should not to be confused with mathematical functions, and on the other hand, rewriting variables should not be confused with mathematical variables. For example, let $\mathcal{X} = \emptyset$ and $\mathcal{F} = \mathcal{F}_0 \cup \mathcal{F}_1 \cup \mathcal{F}_2$ where $\mathcal{F}_0 = \{x, \Omega\}$, $\mathcal{F}_1 = f$ and $\mathcal{F}_3 = \texttt{Integral}$. Then, $\texttt{Integral}(\Omega, f(x), x)$ is a term in $\mathcal{T}(\mathcal{F}, \mathcal{X})$. It corresponds to the mathematical

expression $\int_\Omega f(x)\,dx$. Notice that both x and Ω are function symbols of arity zero, i.e. they are constants in the rewriting sense while x is a variable in the mathematical sense. To make clear this distinction, the mathematical variables will be denoted by the letters $x, y, z, \ldots$ however the rewriting variables will be denoted by the capital letters $X, Y, Z, \ldots$

A rewriting rule is a pair

$$(l, r) \in \mathcal{T}(\mathcal{F}, \mathcal{X}) \times \mathcal{T}(\mathcal{F}, \mathcal{X})$$

of terms. It transforms a term l to the term r. We shall write $l \to r$ instead of (l, r). For example the equation $\sin(\alpha)^2 = 1 - \cos(\alpha)^2$ can be turned into two rewriting rules:

$$\sin(X)^2 \to 1 - \cos(X)^2, \text{ and}$$
$$1 - \cos(X)^2 \to \sin(X)^2,$$

where sin, cos, 1, and '$-$' $\in \mathcal{F}$ and $X \in \mathcal{X}$.

The grammars of mathematical objects such as regions, functions and variables are discussed. By the grammar, all mathematical information required i.e. the dimension of the region, the domain of the variables and the variables of the functions, for the derivation are saved, in fact, this grammar gives the base for the mathematical derivation.

2.2.1 Terms, positions, substitutions, rewriting rule, term rewriting

In what follows, let $\mathcal{F}$ be a set of function symbols, each symbol having a fixed arity and let $\mathcal{X}$ be a set of variables.

Definition 44 (Terms) *The syntax of the terms in $\mathcal{T}(\mathcal{F}, \mathcal{X})$ is defined by the following grammar:*

$$t \ ::= \ X \ \mid \ f(t, \ldots, t)$$

where $X \in \mathcal{X}$, $f \in \mathcal{F}$.

Definition 45 (Positions [4]) *Let t be a term in $\mathcal{T}(\mathcal{F}, \mathcal{X})$.*

1. *The set of positions of the term t, denoted by $\mathcal{P}os(t)$, is a set of strings[6] of positive integers such that:*

[6] A string is an element of $\mathbb{N}^\omega = \{\epsilon\} \cup \mathbb{N} \cup (\mathbb{N} \times \mathbb{N}) \cup (\mathbb{N} \times \mathbb{N} \times \mathbb{N}) \cup \cdots$. Given two strings $p = p_1 p_2 \ldots p_n$ and $q = q_1 q_2 \ldots q_m$, the *concatenation* of p and q, denoted by $p \cdot q$ or simply pq, is the string $p_1 p_2 \ldots p_n q_1 q_2 \ldots q_m$. Notice that $(\mathbb{N}^\omega, \cdot)$ is a monoid with ϵ as the identity element.

- *If* $t = X \in \mathcal{X}$, *then* $\mathcal{P}os(t) = \{\epsilon\}$, *where* ϵ *denotes the empty string.*
- *If* $t = f(t_1, ..., t_n)$ *then*

$$\mathcal{P}os(t) = \{\epsilon\} \cup \bigcup_{i=1}^{n} \{ip \mid p \in \mathcal{P}os(t_i)\}.$$

We denote the set of the positions of a subterm r *in a term* t *by* $\mathcal{P}os(t, r)$. *The position* ϵ *is called the root position of term* t, *and the function or variable symbol at this position is called root symbol of* t.

2. *The prefix order defined as*

$$p \leq q \text{ iff there exists } p' \text{ such that } pp' = q \tag{2.1}$$

is a partial order on positions. We say that the position p, q *are parallel* $(p \parallel q)$ *iff* p *and* q *are incomparable with respect to* $\leq$. *The position* p *is above* q *if* $p \leq q$. *The position* p *is strictly above* q, *written* $p < q$ *iff there exists* p' *such that* $p' \neq \epsilon$ *and* $pp' = q$.

We define a binary relation $\sqsubset$ *on the positions as follows:*

$$p \sqsubset q \quad \text{iff} \quad \big(p < q \text{ or } p \parallel q\big) \tag{2.2}$$

Similarly, we define a binary relation $\sqsubseteq$ *on the positions as follows:*

$$p \sqsubseteq q \quad \text{iff} \quad \big(p \leq q \text{ or } p \parallel q\big) \tag{2.3}$$

3. *For* $p \in \mathcal{P}os(t)$, *the subterm of* t *at position* p, *denoted by* $t|_p$, *is defined by*

$$\begin{aligned} t|_\epsilon &= t, \\ f(t_1, ..., t_n)|_{iq} &= t_i|_q. \end{aligned}$$

Note that, for $p = iq, p \in \mathcal{P}os(s)$ *implies that* t *is of the form* $t = f(t_1, ..., t_n)$ *with* $i \leq n$.

The replacement of a term u *by a term* s *in* t, *denoted by* $t[u := s]$, *is defined by*

$$t[u := s] = \big(((t[s]|_{p_1})[s]|_{p_2}) \ldots\big)[s]|_{p_n} \quad \text{where } \{p_1, \ldots, p_n\} = \{p \in \mathcal{P}os(t) \text{ s.t. } t|_p = u\}$$

4. *For* $p \in \mathcal{P}os(t)$, *we denote by* $t[s]_p$ *the term that is obtained from* t *by replacing the subterm at position* p *by* s, *i.e.*

$$\begin{aligned} t[s]_\epsilon &= s, \\ f(t_1, ..., t_n)[s]|_{iq} &= f\Big(t_1, ..., t_i[s]_q, ..., t_n\Big) \end{aligned}$$

5. *By* $\mathcal{V}ar\,(t)$ *we denote the set of variables occurring in* t*, i.e.*

$$\mathcal{V}ar\,(t) = \{x \in \mathcal{X} \mid \exists p \in \mathcal{P}os\,(t) : t|_p = x\}$$

We call $p \in \mathcal{P}os\,(t)$ *a variable position if* $t|_p$ *is a variable.*

Example 46 *Let* t *be the term*

$$t = \texttt{Oper}(\texttt{Integral}, \texttt{Fun}(u, \texttt{Var}(x, \texttt{Reg}(\Omega, 1))), \texttt{Var}(x, \texttt{Reg}(\Omega, 1)), \emptyset) \tag{2.4}$$

where $\mathcal{V}ar(t) = \emptyset$*. It represents the norm of a function* u *in* $L^2\,(\Omega)$*. Its tree structure as well as the positions of all its subterms are depicted in Figure 2.1.*

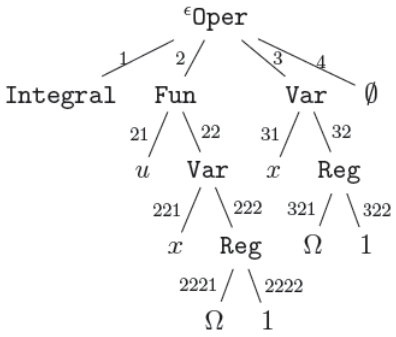


Figure 2.1: The tree structure of the term t defined in Eq. (2.4) and the positions of its subterms.

The set of all the positions of t *can be computed as follows. Let* $t = f\,(t_1, t_2, t_3, t_4)$*, where* $t_1 = t|_1$*,* $t_2 = t|_2$*,* $t_3 = t|_3$ *,* $t_4 = t|_4$*,* $t_{22} = t|_{22} = t_2|_2 = (t|_2|_2)$ *and* $t_{221} = t_2|_{21} = t_{22}|_1 = ((t|_2)\,|_2)\,|_1$*.*

Firstly, notice that $\mathcal{P}os\,(t_{21}) = \mathcal{P}os\,(t_{221}) = \mathcal{P}os\,(t_{2221}) = \mathcal{P}os\,(t_{2222}) = \{\epsilon\}$*. Hence, the set of positions* $\mathcal{P}os\,(t_2)$*, in the second branch of* t*, can be computed as follows:*

$$\begin{aligned}
\mathcal{P}os\,(t_{22}) &= \{\epsilon\} \cup \{1p \mid p \in \mathcal{P}os\,(t_{221})\} \cup \{2p \mid p \in \mathcal{P}os\,(t_{222})\} \\
&= \{\epsilon, 1, 2, 21, 22\}\,. \\
\mathcal{P}os\,(t_{222}) &= \{\epsilon\} \cup \{1p \mid p \in \mathcal{P}os\,(t_{2221})\} \cup \{2p \mid p \in \mathcal{P}os\,(t_{2222})\} \\
&= \{\epsilon, 1, 2\}\,, \\
\mathcal{P}os\,(t_2) &= \{\epsilon\} \cup \{1p \mid p \in \mathcal{P}os\,(t_{21})\} \cup \{2p \mid p \in \mathcal{P}os\,(t_{22})\} \\
&= \{\epsilon, 1, 2, 21, 22, 221, 222\}\,.
\end{aligned}$$

Secondly, notice that $\mathcal{P}os(t_{31}) = \mathcal{P}os(t_{321}) = \mathcal{P}os(t_{322}) = \{\epsilon\}$. *Hence the set of positions* $\mathcal{P}os(t_3)$ *in the third branch of* t *can be computed as follows:*

$$\begin{aligned}\mathcal{P}os(t_{32}) &= \{\epsilon\} \cup \{1p \mid p \in \mathcal{P}os(t_{321})\} \cup \{2p \mid p \in \mathcal{P}os(t_{322})\} \\ &= \{\epsilon, 1, 2\} \\ \mathcal{P}os(t_3) &= \{\epsilon\} \cup \{1p \mid p \in \mathcal{P}os(t_{31})\} \cup \{2p \mid p \in \mathcal{P}os(t_{32})\} \\ &= \{\epsilon, 1, 2, 21, 22\}.\end{aligned}$$

Finally, since $\mathcal{P}os(t_1) = \mathcal{P}os(t_4) = \{\epsilon\}$, *the set of positions* $\mathcal{P}os(t)$ *of the term* t *is given by:*

$$\begin{aligned}\mathcal{P}os(t) &= \{\epsilon\} \cup \{1p \mid p \in \mathcal{P}os(t_1)\} \cup \{2p \mid p \in \mathcal{P}os(t_2)\} \cup \{3p \mid p \in \mathcal{P}os(t_3)\} \cup \{4p \mid p \in \mathcal{P}os(t_4)\} \\ &= \{\epsilon\} \cup \{1\} \cup \{2, 21, 22, 221, 222, 2221, 2222\} \cup \{3, 31, 32, 321, 322\} \cup \{4\}.\end{aligned}$$

The claims in the following Proposition are not hard to prove.

Proposition 47 (See [4, Chapter 1]) *Let* s, t, r *be terms and* p, q *be strings. The following hold.*

1. *If* $pq \in \mathcal{P}os(s)$, *then* $s|_{pq} = (s|_p)|_q$.
2. *If* $p \in \mathcal{P}os(s)$ *and* $q \in \mathcal{P}os(t)$, *then*

$$\begin{aligned}\left(s[t]_p\right)|_{pq} &= t|_q, \\ \left(s[t]_p\right)[r]_{pq} &= s\left[t[r]_q\right]_p.\end{aligned}$$

3. *If* $pq \in \mathcal{P}os(s)$, *then*

$$\begin{aligned}\left(s[t]_{pq}\right)|_p &= (s|_p)[t]_q, \\ \left(s[t]_{pq}\right)[r]_p &= s[r]_p.\end{aligned}$$

4. *If* p *and* q *are parallel positions in* s (*i.e.* $p \parallel q$), *then*

$$\begin{aligned}\left(s[t]_p\right)|_q &= s|_q, \\ \left(s[t]_p\right)[r]_q &= \left(s[r]_q\right)[t]_p.\end{aligned}$$

Proof. See Annex 2.10.1. ■

Definition 48 (Substitution) *A $\mathcal{T}(\mathcal{F},\mathcal{X})$-substitution, or a substitution for short, is a function $\sigma : \mathcal{X} \to \mathcal{T}(\mathcal{F},\mathcal{X})$ such that $\sigma(X) \neq X$ for only finitely many Xs. The (finite) set of variables that σ does not map to themselves is called the domain of σ:*

$$\mathcal{D}om(\sigma) \stackrel{def}{=} \{X \in \mathcal{X} \mid \sigma(X) \neq X\}.$$

If $\mathcal{D}om(\sigma) = \{X_1, ..., X_n\}$ then we write σ as:

$$\sigma = \{X_1 \mapsto \sigma(X_1), ..., X_n \mapsto \sigma(X_n)\}.$$

The range of σ is $\mathcal{R}an(\sigma) := \{\sigma(X) \mid X \in \mathcal{D}om(\sigma)\}$, and the variable range of σ consists of the variables occurring in $\mathcal{R}an(\sigma)$:

$$\mathcal{VR}an(\sigma) \stackrel{def}{=} \bigcup_{X \in \mathcal{D}om(\sigma)} \mathcal{V}ar(\sigma(X)).$$

A substitution $\sigma : \mathcal{X} \to \mathcal{T}(\mathcal{F},\mathcal{X}))$ uniquely extends to an endomorphism $\widehat{\sigma} : \mathcal{T}(\mathcal{F},\mathcal{X}) \to \mathcal{T}(\mathcal{F},\mathcal{X})$ defined by:

1. *$\widehat{\sigma}(X) = \sigma(X)$ for all $X \in \mathcal{D}om(\sigma)$,*
2. *$\widehat{\sigma}(X) = X$ for all $X \notin \mathcal{D}om(\sigma)$,*
3. *$\widehat{\sigma}(f(t_1, \ldots, t_n)) = f(\widehat{\sigma}(t_1), \ldots, \widehat{\sigma}(t_n))$ for $f \in \mathcal{F}$.*

In what follows we do not distinguish between a substitution and its extension. The set of all $\mathcal{T}(\mathcal{F},\mathcal{X})-$substitutions will be denoted by $\mathcal{S}ub(\mathcal{T}(\mathcal{F},\mathcal{X}))$ or simply $\mathcal{S}ub$. The composition $\sigma\gamma$ of two substitutions σ and γ is defined by

$$\sigma\gamma(X) \stackrel{def}{=} \sigma(\gamma(X)).$$

for all $X \in \mathcal{D}om(\gamma)$.

Now we are ready to define the notions of rewriting rule and rewriting system.

Definition 49 (Rewriting rule, term rewriting system) *A* rewriting rule *over a signature $\mathcal{F}$ is a pair $(l, r) \in \mathcal{T}(\mathcal{F},\mathcal{X}) \times \mathcal{T}(\mathcal{F},\mathcal{X})$, denoted by $l \to r$, such that*

$$\mathcal{V}ar(r) \subseteq \mathcal{V}ar(l). \tag{2.5}$$

Usually, $l \neq x$ with $x \in \mathcal{X}$. Besides, l is called the left-hand side of the rewriting rule and r the right-hand side.

A term rewriting system (TRS) is a set of rewriting rules.

We next define the notion rewriting relation yielded by a rewriting system $\mathcal{R}$. Intuitively, a term t rewrites into a term u if there exists a rewriting rule of $\mathcal{R}$ that can be applied to position of t and yields the term u. The formal definition follows.

Definition 50 (Term rewriting) *Given a rewriting system $\mathcal{R}$, we say that $t \in \mathcal{T}(\mathcal{F}, \mathcal{X})$* rewrites into *a term $u \in \mathcal{T}(\mathcal{F}, \mathcal{X})$ w.r.t. $\mathcal{R}$, denoted by $t \longrightarrow_{\mathcal{R}} u$, iff there exist*

(i) a position $p \in \mathcal{P}\text{os}(t)$,

(ii) a rewrite rule $l \to r \in \mathcal{R}$, and

(iii) a substitution σ with $\mathcal{D}om(\sigma) = \mathcal{V}ar(l)$ such that

$$t_{|p} = \sigma(l) \text{ and } u = t\,[\sigma(r)]_p.$$

We can use the notation $t \overset{l \to r, \sigma, p}{\longrightarrow} u$ to make explicit the corresponding rewriting rule, position and substitution respectively. We denote by $\longrightarrow^*{}_{\mathcal{R}}$ the reflexive transitive closure of the relation $\longrightarrow_{\mathcal{R}}$.

2.2.2 Term unification

We introduce a well known algorithmic process, called *unification*. It has been widely used in logic and automated reasoning for solving equations over symbolic terms. It will be used in Section 2.6 in the extension of first-order rules.

Definition 51 *A term u is subsumed by a term t if there is a substitution σ s.t. $\sigma(t) = u$. A substitution σ is subsumed by a substitution γ, where $\mathcal{D}om(\sigma) = \mathcal{D}om(\gamma)$, iff for every variable $X \in \mathcal{D}om(\sigma)$, the term $\sigma(X)$ is subsumed by the term $\gamma(X)$.*

Definition 52 (Unification problem, unifier, complete and minimal set of unifiers) *Let t_i, u_i be terms where $i = 1, \ldots, n$.*

- *A unification problem E is a set of oriented equations:*

$$E = \{t_1 \doteq u_1, \ldots, t_n \doteq u_n\}.$$

- *A unifier of E is a substitution σ which is a solution of E, i.e. $\sigma(l_i) = \sigma(t_i)$ for all $i \in \{1, \ldots, n\}$. If E admits a solution, then it is called solvable.*

- *For a given unification problem E, a (possibly infinite) set $S = \{\sigma_1, \sigma_2, \ldots\}$ of unifiers of E is complete iff each solution of E is subsumed by some unifier $\sigma_i \in S$. The set S is minimal if none of its substitutions subsumes another one.*

The existence of a complete and minimal solution of a unification problem is ensured by the following proposition:

Proposition 53 (See [4]) *Each solvable unification problem E has a complete and minimal singleton solution set $\{\sigma\}$. The solution σ is called the most general unifier of E, and it is denoted by* $\texttt{mgu}(E)$.

A unification algorithm. We mention that there is a simple algorithm, see for instance [4], that computes the most general unifier of a unification problem E by transforming the equations of E into a set of equations of the form $\{X_1 \doteq u_1, \ldots, X_m \doteq u_m\}$ where X_i are distinct variables and u_i are terms so that none of them contains a variable among $\{X_1, \ldots, X_m\}$. We reproduce next the unification algorithm which is specified as a set of reduction rules.

Algorithm 1: Unification

input : A unification problem $E = \{t_1 \doteq u_1, \ldots, t_n \doteq u_n\}$, where t_i, u_i are terms.

output: The most general unifier of E if it exists, see Definition 52 and Proposition 53.

1

$$E \cup \{t \doteq t\} \rightsquigarrow E \qquad \textbf{(delete)}$$

$$E \cup \{f(t_1, \ldots, t_n) \doteq f(u_1, \ldots, u_n)\} \rightsquigarrow E \cup \{t_1 \doteq u_1, \ldots, t_n \doteq u_n\} \qquad \textbf{(decompose)}$$

$$E \cup \{f(t_1, \ldots, t_n) \doteq g(u_1, \ldots, u_m)\} \rightsquigarrow \texttt{fail} \quad \text{if } g \neq f \qquad \textbf{(conflict)}$$

$$E \cup \{f(t_1, \ldots, t_n) \doteq X\} \rightsquigarrow E \cup \{X \doteq f(t_1, \ldots, t_n)\} \qquad \textbf{(swap)}$$

$$E \cup \{x \doteq t\} \rightsquigarrow E[X := t] \cup \{X \doteq t\} \quad \text{if } X \notin \mathcal{V}ar(t) \text{ and } X \in \mathcal{V}ar(E) \qquad \textbf{(eliminate)}$$

$$E \cup \{X \doteq f(X_1, \ldots, X_n)\} \rightsquigarrow \texttt{fail} \quad \text{if } X \in \mathcal{V}ar(f(X_1, \ldots, X_n)) \qquad \textbf{(recursion)}$$

2.3 Second-order rules, SA-expressions and short-cut terms

In this section we introduce second-order rewriting rules that operate on (first-order) rewriting rules. Then we define a grammar for the mathematical expressions.

2.3.1 Second-order rules

Given a rewriting strategy representing a a model derivation, we would like to transform it in order to obtain a derivation of more complex models. This can be achieved, see e.g. [59], by transforming first-order strategies by second-order strategies. Unlike [59], in this Section we only deal with the particular setting in which only first-order rules are transformed by second-order rules. This particular setting is powerful enough in practice to extend our two-scale models. Hence, we need to consider two levels of rules: the first-order ones as defined in Definition 54, and the second-order one in such a way that second-order rules can be convincingly applied to first-order ones. More precisely a first-order rule $l \to r$ will be considered the first-order term $\to (l, r)$ where "$\to$" is a functional symbol of arity two.

Definition 54 (Second-order rules) *Let $\mathcal{X}^0$ be a set of FO-variables, and $\mathcal{F}^0$ be a set of FO-function symbols. Let $\mathcal{X}^1$ be a set of SO-variables such that the sets $\mathcal{X}^0, \mathcal{F}^0, \mathcal{X}^1$ are pairwise disjoint. Let $\mathcal{SC}onst = \{\to\}$.*

(i) The set of FO-terms is the set of terms $\mathcal{T}(\mathcal{F}^0, \mathcal{X}^0)$.

(ii) A FO-rule is a pair of FO-terms in $\mathcal{T}(\mathcal{F}^0, \mathcal{X}^0) \times \mathcal{T}(\mathcal{F}^0, \mathcal{X}^0)$.

(iii) The set of SO-terms is the set of terms $\mathcal{T}(\mathcal{F}^0 \cup \mathcal{X}^0 \cup \mathcal{SC}onst, \mathcal{X}^1)$.

(iv) A SO-rule is a pair of SO-terms in $\mathcal{T}(\mathcal{F}^0 \cup \mathcal{X}^0 \cup \mathcal{SC}onst, \mathcal{X}^1) \times \mathcal{T}(\mathcal{F}^0 \cup \mathcal{X}^0 \cup \mathcal{SC}onst, \mathcal{X}^1)$. A SO-rule will be denoted by $l \rightrightarrows r$.

Item *(iii)* of Definition 54 states that the variables of the first order become constants in the second order, and the FO-rule constructor " $\to$ " becomes SO-function symbols. That is, the FO-rules become SO-terms. Item *(iv)* of the same definition states that SO-rules operate on SO-terms, in particular they operate on FO-rules. FO-variables will be denoted by the letter $X, Y, Z, \ldots$ and SO-variables will be denoted by $\alpha, \beta, \ldots$. The semantics of the SO-rules (i.e. rule application at the top) is defined in the same way as the one of FO-rules.

2.3.2 A grammar for SA-expressions, short-cut terms

We propose a more precise way to represent the mathematical expressions and the data used in the formulation of the proofs and their extensions. Such mathematical expressions as well as the data coming with are henceforth called *specific application expressions*, or SA-expressions for short. More precisely, instead of representing the SA-expressions by terms in $\mathcal{T}(\mathcal{F}, \mathcal{X})$, see Definition 44, we represent them by the sub set of terms in $\mathcal{T}(\mathcal{F}, \mathcal{X})$ that follow the grammar $\mathcal{F}$ defined afterwards.

Let
$\mathcal{M}ath\mathcal{V}ar = \{x, y, \ldots\}$ be the set of mathematical variable names,
$\mathcal{M}ath\mathcal{D}isc\mathcal{V}ar = \{i, j, \ldots\}$ be the set of discrete mathematical variable names,
$\mathcal{M}ath\mathcal{D}isc\mathcal{D}om = \{I, J, \ldots\}$ be the set of discrete mathematical variable domain names,
$\mathcal{M}ath\mathcal{F}un = \{f, g, \ldots\}$ be the set of mathematical function names,
$\mathcal{M}ath\mathcal{F}un\mathcal{K}ind = \{known, unknown, test\}$,
$\mathcal{M}ath\mathcal{R}eg = \{\Omega, \Gamma, \ldots\}$ be the set of region names,
$\mathcal{M}ath\mathcal{O}per = \{$`Deriv, Integral, Sum`$, \ldots\}$ be the set of mathematical operator names,
$\mathcal{M}ath\mathcal{D}im = \{d_1, d_2, \ldots\} \cup \mathbb{N}$ be the set of symbolic/numeric dimensions,
and
$\odot = \{+, \times, -\}$. The syntax of SA-expressions is defined by the following grammar:

$$\mathcal{F} ::= \mathcal{V} \mid \mathcal{F} \odot \mathcal{F} \mid \mathcal{F}^n \mid \texttt{Fun}(f, [\mathcal{V}, \cdots, \mathcal{V}], k) \mid \texttt{Indexed}(\mathcal{F}, \mathcal{V}) \mid \texttt{Oper}(o, \mathcal{F}, [\mathcal{F}, \cdots, \mathcal{F}])$$
$$\mathcal{V} ::= \texttt{Var}(x, \mathcal{R}) \mid \texttt{Indexed}(\mathcal{F}, \mathcal{V}) \mid \texttt{Index}(i, \texttt{Set}(I, \{l, d\}))$$
$$\mathcal{R} ::= \texttt{Reg}(\Omega, d)$$

where $n \in \mathbb{N}$, $f \in \mathcal{M}ath\mathcal{F}un$, $k \in \mathcal{M}ath\mathcal{F}un\mathcal{K}ind$, $o \in \mathcal{M}ath\mathcal{O}per$, $x \in \mathcal{M}ath\mathcal{V}ar$, $i \in \mathcal{M}ath\mathcal{D}isc\mathcal{V}ar$ $I \in \mathcal{M}ath\mathcal{D}isc\mathcal{D}om$, $\Omega \in \mathcal{M}ath\mathcal{R}eg$, and $l, d \in \mathcal{M}ath\mathcal{D}im$.

For simplicity and to improve the readability, we use the short-cut expressions instead of complete SA-expressions, leading to more concise expressions. An example of the short-cut terms is given bellow.

$$\underline{\Omega} \equiv \texttt{Reg}(\Omega, d), \tag{2.6}$$
$$\underline{x} \equiv \texttt{Var}(x, \underline{\Omega}),$$
$$\underline{y} \equiv \texttt{Var}(y, \underline{\Omega}),$$
$$\underline{i} \equiv \texttt{Index}(i, \texttt{Set}(I, \{1, d\})),$$
$$\underline{j} \equiv \texttt{Index}(i, \texttt{Set}(I, \{1, d\})),$$
$$\underline{u}(\underline{x}) \equiv \texttt{Fun}(u, [\underline{x}], \texttt{unknown}),$$
$$\underline{u}(\underline{x}, \underline{y}) \equiv \texttt{Fun}(u, [\underline{x}, \underline{y}], \texttt{unknown}),$$
$$\underline{v}(\underline{x}) \equiv \texttt{Fun}(v, [\underline{x}], \texttt{test}),$$
$$\underline{u}_{\underline{i}}(\underline{x}) \equiv \texttt{Indexed}(\underline{u}(\underline{x}), \underline{i}),$$
$$\underline{u}_{\underline{i}\underline{j}}(\underline{x}) \equiv \texttt{Indexed}\left(\texttt{Indexed}\left(\underline{u}(\underline{x}), \underline{i}\right), \underline{j}\right), \tag{2.7}$$
$$\frac{\partial \underline{u}(\underline{x})}{\partial \underline{x}} \equiv \texttt{Oper}(\texttt{Deriv}, \underline{u}(\underline{x}), [\underline{x}]), \tag{2.8}$$
$$\frac{\partial \underline{u}_{\underline{i}}(\underline{x})}{\partial \underline{x}_{\underline{j}}} \equiv \texttt{Oper}(\texttt{Deriv}, \underline{u}_{\underline{i}}(\underline{x}), [\underline{x}_{\underline{j}}]), \tag{2.9}$$
$$\int \underline{u}(\underline{x})\, d\underline{x} \equiv \texttt{Oper}(\texttt{Integral}, \underline{u}(\underline{x}), [\underline{x}]),$$
$$\int \underline{u}(\underline{x}, \underline{y})\, d\underline{x} \equiv \texttt{Oper}(\texttt{Integral}, \underline{u}(\underline{x}, \underline{y}), [\underline{x}]), \tag{2.10}$$
$$\sum_{\underline{i}} \underline{u}_{\underline{i}}(\underline{x}) \equiv \texttt{Oper}\left(\texttt{Sum}, \underline{u}_{\underline{i}}(\underline{x}), [\underline{i}]\right), \tag{2.11}$$
$$\sum_{\underline{i}} \underline{u}_{\underline{i}\underline{j}}(\underline{x}) \equiv \texttt{Oper}\left(\texttt{Sum}, \underline{u}_{\underline{i}\underline{j}}(\underline{x}), [\underline{i}]\right). \tag{2.12}$$

The tree structures of the short-cut terms $\partial_{\underline{x}} \underline{u}(\underline{x})$, $\partial \underline{u}_{\underline{i}} \underline{x}_{\underline{j}}$, $\int \underline{u}(\underline{x})\, d\underline{x}$, $\sum_{\underline{i}} \underline{u}(\underline{x})$ and $\underline{u}(\underline{x})^2$ are depicted in Figure 2.2.

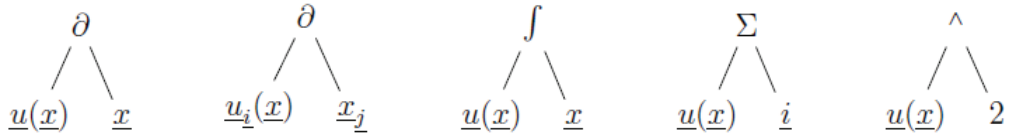


Figure 2.2: Tree structures of the short-cut terms $\partial_{\underline{x}} \underline{u}(\underline{x})$, $\partial \underline{u}_{\underline{i}} \underline{x}_{\underline{j}}$, $\int \underline{u}(\underline{x})\, d\underline{x}$, $\sum_{\underline{i}} \underline{u}(\underline{x})$ and $\underline{u}(\underline{x})^2$.

The following example shows a rewriting rule that uses short-cut terms of SA-expressions.

Example 55 *The rewrite rule which transforms any function u into its L^2-norm is defined by*

$$s := \underline{u}(\underline{x}) \to \int (\underline{u}(\underline{x}))^2 d\underline{x}.$$

By replacing the short-cut terms with their related full SA-expressions, we get the rewriting rule:

$s := \mathtt{Fun}(U, [\mathtt{Var}(X, \Omega)], K) \to \mathtt{Oper}(\mathtt{Integral}, \mathtt{Fun}(U, [\mathtt{Var}(X, \Omega)], K)\mathtt{\hat{}}2, \mathtt{Var}(X, \Omega))$

where $U, X, K, \Omega \in \mathcal{X}^0$ are rewriting variables.

2.4 Extension of first-order rules by second-order rules

In this section we introduce the first mechanism allowing the extension of FO-rules. It consists in the extension of FO-rules by means of SO-rules that enjoy certain properties. More precisely, we provide a set of requirements that the SO-rules must fulfill so that they can extend FO-rules.

2.4.1 Parametrization of second-order rules

A SO-rewriting rule is called *parametrized* if its right-hand side part contains FO-variables which are not in its left-hand side part. The idea behind parametrization is to build The formal definition of parametrized SO-rules follow.

Definition 56 (Parametrized SO-rule) *Let $S = l \rightrightarrows r$ be a SO-rule. The set of parameters of S, denoted by $\mathcal{V}^0(S)$, is the set of FO-variables defined by:*

$$\mathcal{V}^0(S) = \mathcal{V}ar^0(r) \setminus \mathcal{V}ar^0(l)$$

The SO-rule S is called parametrized *iff $\mathcal{V}^0(S)$ is non-empty.*

Example 57 *Consider the equation*

$$\underline{H^1}(\underline{u}(\underline{x})) = \int (\frac{d\underline{u}(\underline{x})}{d\underline{x}})^2 d\underline{x} \tag{2.13}$$

that represents the H^1 norm of the function $\underline{u}(\underline{x})$, where

$$\begin{cases} \underline{H^1}(\underline{u}(\underline{x})) & \equiv \mathtt{Oper}(H^1, \underline{u}(\underline{x}), \underline{x}), \text{ and} \\ \underline{x} & \equiv \mathtt{Var}(x, \mathtt{Reg}(\Omega, 1)) \end{cases}$$

are SA-expressions and u, x, Ω are function symbols in $\mathcal{F}^0$. The equation (2.13) can be turned into the FO-rule s:

$$s := \underline{H^1}(\underline{u}(\underline{x})) \to \int (\frac{d\underline{u}(\underline{x})}{d\underline{x}})^2 d\underline{x}$$

where

$$\begin{cases} \underline{x} \equiv & \texttt{Var}(x, \texttt{Reg}(\Omega, 1)), \quad \textit{and} \\ & u, x, \Omega \in \mathcal{X}^0 \end{cases}$$

Let S be the SO-rule:

$$S := \left(\underline{H^1}(\underline{u}(\underline{x})) \to \int \frac{d\underline{u}(\underline{x})}{d\underline{x}} d\underline{x}\right) \rightrightarrows \left(\underline{H^1}(\underline{u}(\underline{x}')) \to \int \sum_{\underline{i}} \frac{\partial \underline{u}(\underline{x}')}{\partial \underline{x}'_{\underline{i}}} d\underline{x}'\right)$$

where

$$\begin{cases} \underline{x} \equiv & \texttt{Var}(x, \texttt{Reg}(\Omega, 1)), \\ \underline{x}' \equiv & \texttt{Var}(x, \texttt{Reg}(\Omega, d)), \\ & u, x, \Omega, d \in \mathcal{X}^0. \end{cases}$$

The SO-rule S transforms the FO-rule s into its n-dimensional counterpart. If we denote by l_S (resp. r_S) the left-hand side (resp. right-hand side) of S, then we have that

$$\begin{cases} \mathcal{V}ar^0(\ell_S) = \{u, x, \Omega\}, \ \textit{and} \\ \mathcal{V}ar^0(r_S) = \{u, x, \Omega, d\}. \end{cases}$$

Therefore,

$$\mathcal{V}^0(S) = \mathcal{V}ar^0(r_S) \setminus \mathcal{V}ar^0(\ell_S) = \{d\} \in \mathcal{X}^0.$$

Since $\mathcal{V}^0(S)$ is non-empty, then according to Definition 56, the SO-rule S is parametrized.

The application of the SO-rule S to the FO-rule s, denoted by $S(s)$, yields the FO-rule:

$$S(s) := \underline{H^1}(\underline{u}(\underline{x}')) \to \int \sum_{\underline{i}} \frac{\partial \underline{u}(\underline{x}')}{\partial \underline{x}'_{\underline{i}}} d\underline{x}'$$

where

$$\begin{cases} \underline{x}' = & \texttt{Var}(x, \texttt{Reg}(\Omega, d)), \ \textit{and} \\ & u, x, \Omega, d \in \mathcal{X}^0. \end{cases}$$

The FO-rule $S(s)$ is a generalization of the FO-rule s to the n-dimensional setting.

In the following, the concept of generalization of FO-rules by means of SO-rules is defined.

2.4.2 Mathematical equivalence between first-order rules

The notion of the *mathematical equivalence* between FO-rules, is a crucial ingredient in the formulation of the extension mechanisms by SO-rules. For instance $\sum_{i=1}^{i=1} \beta$ and β are mathematically equivalent, where β is an SA-expression. The notion of mathematical equivalence is formulated in Definition 58 bellow by means of an *equational system* $\mathcal{R}$, i.e. a set of equations. Two FO-rules are mathematically equivalent if they are syntactically equal [7] modulo the system $\mathcal{R}$.

Definition 58 (Mathematical equivalence) *Let s_1 and s_2 be two FO-rules. Let $\mathcal{R}$ an equational system composed. The rules s_1 and s_2 are mathematically equivalent with respect to $\mathcal{R}$, written $s_1 \simeq_{\mathcal{R}} s_2$, iff they are syntactically equal modulo $\mathcal{R}$.*

Definition 59 ($\mathcal{R}$-semantic conservation SO-rule) *Let $\mathcal{R}$ be an equational system. A SO-rule S is $\mathcal{R}$-semantic conservation iff for all FO-rule s, we have that $S(s) \simeq_{\mathcal{R}} s$.*

Example 60 *Let S_0 be the SO-rule:*

$$S_0 := \left(\underline{H^1}(\underline{u}(\underline{x})) \to \int (\frac{d\underline{u}(\underline{x})}{d\underline{x}})^2 \; d\underline{x}\right) \rightrightarrows \left(\underline{H^1}(\underline{u}(\underline{x})) \to \int \sum_{\underline{i}} (\frac{\partial \underline{u}(\underline{x})}{\partial \underline{x}_{\underline{i}}})^2 \; d\underline{x}\right)$$

where

$$\begin{cases} \underline{x} = & \texttt{Var}(x, \texttt{Reg}(\Omega, 1)), \\ \underline{i} = & \texttt{Var}(i, \texttt{Reg}(I, 1)), \\ \underline{x}_{\underline{i}} = & \texttt{Indexed}(\underline{x}, \underline{i}), \text{ and} \\ & i, I, u, x, \Omega \in \mathcal{X}^1 \end{cases}$$

Notice that the variable $\underline{i}$ ranges from 1 to 1 in the right-hand side of S_0. Let $\mathcal{R}$ be the equational system:

$$\mathcal{R} = \{ \sum_{\underline{i}} \alpha = \alpha, \\ \texttt{Indexed}\,(\alpha, \texttt{Index}(i, Set(I, \{1, \ldots, 1\}))) = \alpha\} \tag{2.14}$$

The second equation of $\mathcal{R}$ states that an expression α_i is equal to α if i ranges from 1 to 1. We have that S_0 is an $\mathcal{R}$-semantic conservation, since for every FO-rule s, $S_0(s)$ is mathematically equivalent to s modulo $\mathcal{R}$.

[7] The syntactic equality between rewriting rules has always to be done modulo α-equivalence. Two rewriting rules are α-equivalent if they are syntactically identical up to a renaming of their variables. For instance, the rules $f(x) \to g(x)$ and $f(y) \to g(y)$, where x and y are variables, are α-equivalent. Two strategies are α-equivalent if they are syntactically identical up to a renaming of the variables of their rewriting rules. For instance, the strategies $\texttt{BottomUp}(f(x) \to g(x))$ and $\texttt{BottomUp}(f(y) \to g(y))$ are α-equivalent.

2.4.3 Generalization of first-order rules by admissible parameterized second-order strategies

Combining the notions of parametrization and mathematical equivalence, defined respectively in Definitions 56 and 58, we are able to define the notion of generaliztion of FO-rules.

Definition 61 (Generalization of a parametrized SO-rule) *Let S be a parametrized SO-rule and S' be a SO-rule. We say that S generalizes S' if there exists a mapping γ of the first order variables in $\mathcal{V}(S)$ such that*

$$\gamma(S) = S'$$

Example 62 *Consider the parametrized SO-rule S of Example 57 and the SO-rule S_0 of Example 60. We have that S is a generalization of S_0, since for the mapping $\gamma = \{d \to 1\}$, we get $\gamma(S') = S$.*

Definition 63 (Admissible parametrized SO-rule) *Let S be a parametrized SO-rule and S' be an $\mathcal{R}$-semantic conservation SO-rule for an equational system $\mathcal{R}$. We say that S is (S'-$\mathcal{R}$)-admissible iff $\mathcal{S}'$ is $\mathcal{R}$-semantic conservation and S generalizes S'. We shall simply say that S is admissible if it is (S'-$\mathcal{R}$)-admissible for some $\mathcal{R}$-semantic conservation strategy S'.*

Using the concepts introduced so far, we are ready to define the notion of generalization of a FO-rule. We notice that the notion of generalization of a FO-rule has not to be confused with the one of generalization of a parametrized SO-rule given in Definition 61.

Definition 64 (Generalization of a FO-rule) *Let s_0 and s_1 be FO-rules. We say that s_1 is a generalization of s_0 iff there exists an admissible parametrized SO-rule S such that*

$$s_1 = S(s_0).$$

And we say that S generalizes s_0 to s_1.

Example 65 *Let s_0 be the FO-rule:*

$$s_0 := \underline{H^1}(\underline{u}(\underline{x})) \to \int (\frac{d\underline{u}(\underline{x})}{d\underline{x}})^2 d\underline{x},$$

where

$$\begin{cases} \underline{x} = & \mathtt{Var}(x, \mathtt{Reg}(\Omega, 1)) \text{ and} \\ & u, x, \Omega \in \mathcal{X}^0. \end{cases}$$

Let s_1 be the FO-rule :

$$s_1 := \underline{H^1}(\underline{u}(\underline{x})) \to \int \sum_{\underline{i}} (\frac{\partial \underline{u}(\underline{x})}{\partial \underline{x}_{\underline{i}}})^2 d\underline{x},$$

where

$$\begin{cases} \underline{x} = & \mathtt{Var}(x, \mathtt{Reg}(\Omega, d)) \text{ and} \\ & u, x, \Omega, d \in \mathcal{X}^0, \text{ and} \\ & i \in \mathcal{F}^0. \end{cases}$$

We shall find an admissible parametrized SO-rule S' that generalizes s_0 to s_1. We start from the semantic conservation SO-rule S_0:

$$S_0 := \Big(\underline{H^1}(\underline{u}(\underline{x})) \to \int (\frac{d\underline{u}(\underline{x})}{d\underline{x}})^2 \, d\underline{x}\Big) \rightrightarrows \Big(\underline{H^1}(\underline{u}(\underline{x})) \to \int \sum_{\underline{i}} (\frac{\partial \underline{u}(\underline{x})}{\partial \underline{x}_{\underline{i}}})^2 \, d\underline{x}\Big),$$

where

$$\begin{cases} \underline{i} = \mathtt{Var}(i, \mathtt{Reg}(I, 1)), \\ u, x, \Omega \in \mathcal{X}^1, \text{and} \\ I, i \in \mathcal{F}^0. \end{cases}$$

By replacing the constant 1 by the variable $d \in \mathcal{X}^0$ in both $\underline{x}$ and $\underline{i}$ in the right-hand side of S_0, we get the SO-rule S':

$$S' := \Big(\underline{H^1}(\underline{u}(\underline{x})) \to \int (\frac{d\underline{u}(\underline{x})}{d\underline{x}})^2 \, d\underline{x}\Big) \rightrightarrows \Big(\underline{H^1}(\underline{u}(\underline{x})) \to \int \sum_{\underline{i}} (\frac{\partial \underline{u}(\underline{x})}{\partial \underline{x}_{\underline{i}}})^2 \, d\underline{x}\Big),$$

where $\underline{x} = \mathtt{Var}(x, \mathtt{Reg}(\Omega, d))$, $\underline{i} = \mathtt{Var}(i, \mathtt{Reg}(I, d))$, $u, x, \Omega \in \mathcal{X}^1$ and I, $i \in \mathcal{F}^0$. We have that the SO-rule S' is $(S_0 - \mathcal{R})$-admissible, where $\mathcal{R}$ is the equational system given in Eq 2.14. Since $S'(s_0) = s_1$, then s_1 is a generalization of s_0.

2.5 Extension of first-order terms by outward growths

In Section 2.4, we have established the first mechanism for the extension of FO-rules. There, we have defined requirements for SO-rules so that they can correctly extend FO-rules. However, we did not provide a clear process to build such SO-rules. To deal with this issue, we elaborate a second mechanism for the extension of FO-terms (in this section) and of FO-rules (in section 2.6). This second mechanism

is based on the notion of *outward growths* that, roughly speaking, consists in the following: *(i)* firstly, we need to define rudimentary components, called *added terms*, allowing, on one hand, to express the kind of extensions that we want to make, and, on the other hand can be combined to build more complex components. *(ii)* Secondly, these components will be inserted at certain positions of a FO-term and a FO-rule. That is, the positions on which the extension is made.

In fact, these two extension mechanisms are equivalent in the sense that they have the same effect when applied to the same term. Besides, outward growth mechanisms can be used to construct semantic preservation as well as admissible SO-rules.

Definition 66 *Let $\mathcal{F}^{add} = \mathcal{F}^0 \cup \{\bot\}$ where $\bot \notin \mathcal{F}^0$. The set of "added terms", denoted by $\mathcal{T}^{add}$, is defined by $\mathcal{T}^{add} = \mathcal{T}(\mathcal{F}^{add}, \mathcal{X}^0)$.*

Throughout this chapter, we assume that the symbol $\bot$ occurs only once in an added term in $\mathcal{T}^{add}$. The position of $\bot$ in τ is denoted by $q(\tau)$. In what follows we use the arrow '$\rightsquigarrow$' to denote mappings/reductions rules, not to be confused with the rewrite rules. We mention that the notion of added terms is close to the one of *context*.

2.5.1 Unit outward growths to the root and their composition

Definition 67 (Unit outward growth to the root) *The unit outward growth with an added term $\tau \in \mathcal{T}^{add}$, denoted by $\mathcal{G}_\tau$, is a mapping from $\mathcal{T}(\mathcal{F}^0, \mathcal{X}^0)$ to $\mathcal{T}(\mathcal{F}^0, \mathcal{X}^0)$ defined by:*

$$\mathcal{G}_\tau : t \rightsquigarrow \tau[t]_q.$$

The ground outward growth $\mathcal{G}_\tau$ is called parametrized if τ includes variables from $\mathcal{X}^0$.

The application of a unit outward growth $\mathcal{G}_\tau$ to a term t to the root is depicted in Figure **??** bellow.

Example 68 *Let $t = h(c)$ be a term where c is a constant. Let $\tau = \texttt{Indexed}(\bot, \underline{i})$ be an added term. Let $\mathcal{G}_\tau : t \rightsquigarrow \tau[t]_q$ be an outward growth with the added term τ. The application of $\mathcal{G}_\tau$ to t yields the term:*

$$\mathcal{G}_\tau(t) = h_{\underline{i}}.$$

The terms t, τ and $h_{\underline{i}}$ are depicted in Figure 2.4.

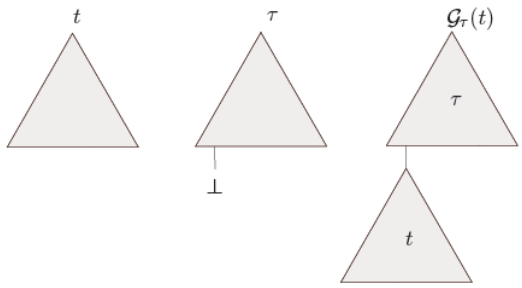


Figure 2.3: Schematic diagram of the application of a unit outward growth $\mathcal{G}_\tau$ (with an added term τ) to a term t to the root.

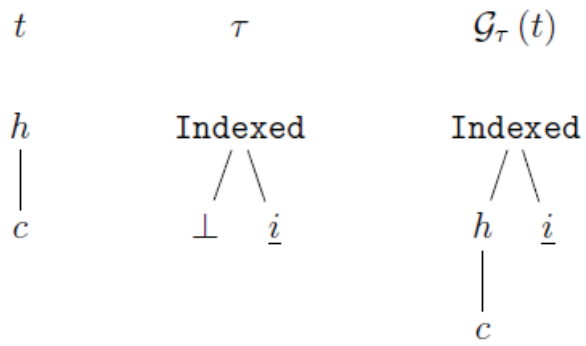


Figure 2.4: Application of the unit outward growth $\mathcal{G}_\tau$ (of added term τ) to the term t to the root.

Definition 69 (Composition of added terms) *The composition for two added terms τ, $\tau' \in \mathcal{T}^{add}$ is defined in the usual sense by*

$$\tau'//\tau = \tau'[\tau]_{q(\tau')} \in \mathcal{T}^{add}$$

Remark 70 *Notice that the composition of added terms is associative but not commutative.*

Example 71 *Let τ and τ' be the added terms*

$$\begin{cases} \tau = \texttt{Indexed}(\bot, i), \text{ and} \\ \tau' = \sum_{\underline{i}}(\bot) \end{cases}$$

Their composition $\tau'//\tau = \sum_{\underline{i}}(\texttt{Indexed}(\bot, \underline{i}))$ is depicted in Figure 2.5.

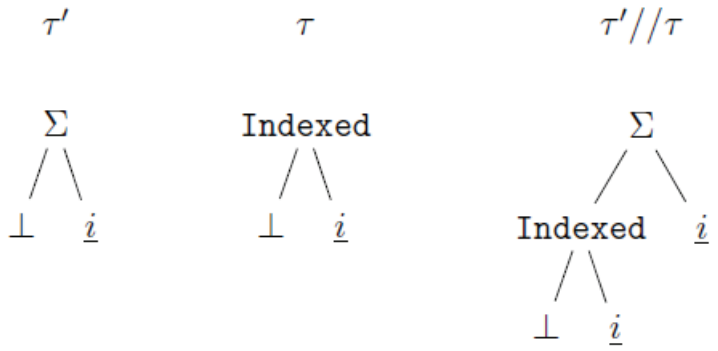


Figure 2.5: Composition of two added terms.

Notice that the composition $\tau//\tau' = \texttt{Indexed}(\sum_{\underline{i}}(\bot), \underline{i})$ *has no significance since it does not allow to build a sound SA-expression.*

Property 72 (Composition of two unit outward growths to the root) *For any* $\tau, \tau' \in \mathcal{T}^{add}$*, the composition* $\mathcal{G}_\tau; \mathcal{G}_{\tau'}$ *of two unit ground outward growths to the root is the unit ground outward growth with added term* $\tau'//\tau$*, i.e.*

$$\mathcal{G}_\tau; \mathcal{G}_{\tau'} = \mathcal{G}_{\tau'//\tau} : t \rightsquigarrow (\tau'//\tau)[t]_{q(\tau'//\tau)}.$$

Since the composition of added terms is not commutative, the composition of outward growth to the root is not commutative as well.

2.5.2 Unit outward growths to a position and their combination

We next generalize the definition of unit outward growths to the root to be applied to any position.

Definition 73 (Unit outward growth to a position) *Let* $\mathcal{G}_\tau$ *be unit ground outward growth and* p *be a position. The unit outward growth* $\mathcal{G}_{\tau,p}$ *to position* p *is a mapping*

$$\mathcal{G}_{\tau,p} : t \rightsquigarrow t[\mathcal{G}_\tau(t_{|p})]_p,$$

which is defined only if $p \in \mathcal{P}os(t)$*.*

If there is no ambiguity, unit outward growths to a position will be simply called unit outward growths.

The application of a unit outward growth $\mathcal{G}_{\tau,p}$ with an added term τ to a term t at the position p is depicted in Figure 2.6.

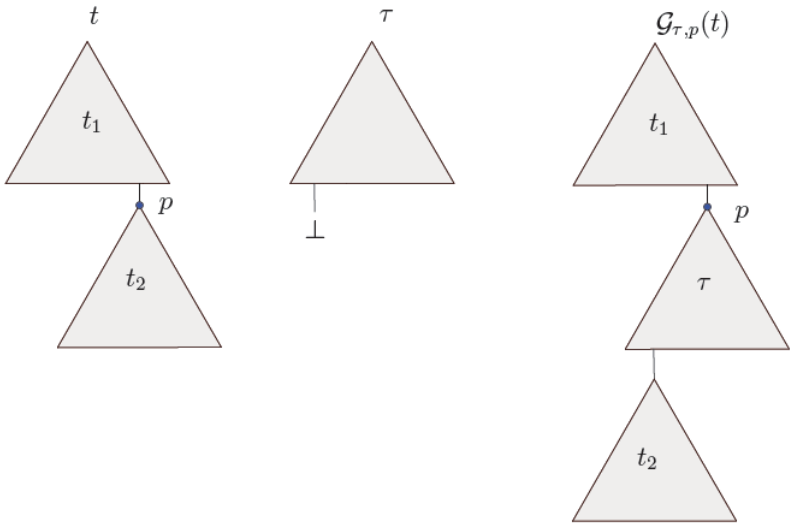


Figure 2.6: Schematic diagram of the application of a unit outward growth $\mathcal{G}_{\tau,p}$ (with an added term τ) to a term t at the position p.

Example 74 *Let $t = \partial_{\underline{x}}\underline{u}(\underline{x})$ be a term and $\tau := \texttt{Indexed}(\perp, \underline{i})$ be an added term. Let p be the position of $\underline{x}$ in t, that is, $p = 2$. The application of the unit outward growth $\mathcal{G}_{\tau,p}$ to t yields:*

$$\begin{aligned}\mathcal{G}_{\tau,p}(t) &= t[\mathcal{G}_{\tau}(t_{|p})]_p \\ &= \partial_{\underline{x}_{\underline{i}}}\underline{u}(\underline{x}).\end{aligned}$$

The terms t, τ and $\mathcal{G}_{\tau,p}(t)$ are depicted in Figure 2.7.

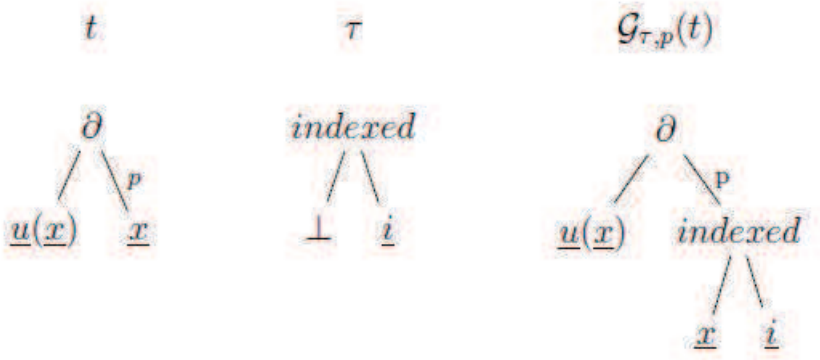


Figure 2.7: Application of the unit outward growth $\mathcal{G}_{\tau}$ (of added term τ) to the term t at the position p.

Property 75 (Composition of two unit outward growths to the same position) *Let $\mathcal{G}_{\tau,p}$ and $\mathcal{G}_{\tau',p}$ be two unit outward growths to the same position p. Their composition, denoted by $\mathcal{G}_{\tau,p};\mathcal{G}_{\tau',p}$, can be expressed as follows:*

$$\mathcal{G}_{\tau,p};\mathcal{G}_{\tau',p} = \mathcal{G}_{\tau'//\tau,p} : t \rightsquigarrow t[\mathcal{G}_{\tau'//\tau}(t_{|p})]_p.$$

Example 76 *Let $t = \int \underline{a}\, d\underline{x}$ be a term and p be the position of $\underline{a}$ in t. Let τ and τ' be the added terms:*

$$\begin{cases} \tau = \texttt{Indexed}(\bot, i), \\ \tau' = \sum_i(\bot). \end{cases}$$

Let $\mathcal{G}_{\tau,p}$ and $\mathcal{G}_{\tau',p}$ be two unit outward growths to the position p. We have

$$\tau'//\tau = \sum_{\underline{i}}(\texttt{Indexed}(\bot, \underline{i})).$$

Therefore

$$\begin{aligned} (\mathcal{G}_{\tau,p};\mathcal{G}_{\tau',p})\,(t) &= \mathcal{G}_{\tau'//\tau,p}(t) \\ &= \int \sum_{\underline{i}} \underline{a}_{\underline{i}}\, d\underline{x}. \end{aligned}$$

We define next the composition of outward growths to different positions.

Definition 77 (Composition of two unit outward growths to different positions) *Let $\mathcal{G}_{\tau,p}$ and $\mathcal{G}_{\tau',p'}$ be two unit outward growths to the position p and p', respectively. Their composition $\mathcal{G}_{\tau,p};\mathcal{G}_{\tau',p'}$ is defined if and only if when $p' \sqsubseteq p$.*

Notice that if the positions p and p' are incomparable, i.e. $p \parallel p'$ then $\mathcal{G}_{\tau,p};\mathcal{G}_{\tau',p'} = \mathcal{G}_{\tau',p'};\mathcal{G}_{\tau,p}$. On the other hand, we can justify the condition $p' \sqsubseteq p$ on the positions p and p' in Definition 77, i.e. $p' \leq p$ or $p \parallel p'$, while composing unit outward growths as follows. The application of a unit outward growth at a position p followed by an application of another unit outward growth at a *lower* position p' might lead to an undesired result since the new position at which we would like to apply the second outward growth might change. This possible change of the position does not happen when the two positions p and p' are incomparable or the position p is lower than p'. As an illustration, see Example 78 bellow.

Example 78 *Let $t := \int(\partial_{\underline{x}}\underline{u}(\underline{x}))^2\, d\underline{x}$ be a term. Let τ and τ' be the added terms*

$$\begin{cases} \tau = \texttt{Indexed}(\bot, i), \\ \tau' = \sum_i(\bot). \end{cases}$$

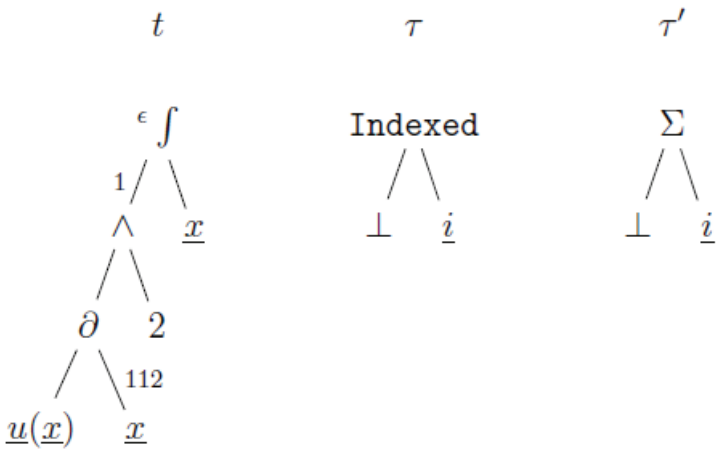


Figure 2.8: The term $t = \int (\partial_{\underline{x}} \underline{u}(\underline{x}))^2 \, d\underline{x}$ and the added terms $\tau = \texttt{Indexed}(\bot, i)$ and $\tau' = \sum_i (\bot)$.

Let $\mathcal{G}_{\tau,112}$ and $\mathcal{G}_{\tau',1}$ be the outward growths to the positions 112 and 1 respectively, and associated with the added terms τ and τ' respectively. The term t, the positions 1 and 112, and the added terms τ and τ' are depicted in Figure 2.8.

Since $1 < 112$, the composition $\mathcal{G}_{\tau,112}; \mathcal{G}_{\tau',1}$ is well defined. The result of the application of $\mathcal{G}_{\tau,112}; \mathcal{G}_{\tau',1}$ to t is depicted in Figure 2.9. This is done in two steps: firstly we apply $\mathcal{G}_{\tau,112}$ to t, yielding the term t_1, then we apply $\mathcal{G}_{\tau',1}$ to t_1.

However, the application of $\mathcal{G}_{\tau',1}$ followed by the application to t of $\mathcal{G}_{\tau,112}$ yields an undesired result as shown in Figure 2.10. Notice that after the application of $\mathcal{G}_{\tau',1}$ to t that give the term w_1, the position of w_1 at which we would like to apply $\mathcal{G}_\tau$ has changed. In other words, to obtain the desired result, the outward growth $\mathcal{G}_\tau$ has to be applied at the position 1112 of w_1 instead of 112.

In order to be able to construct complex outward growths, we slightly generalize the notion of composition of two unit outward growths given in Definition 77 so that we can compose two unit outward growths to two positions independently on their relative order. The generalized composition of unit outward growths is called *combination*. Its definition follows.

Definition 79 (Combination of two unit outward growths) *The combination of two unit outward growths $\mathcal{G}_{\tau,p}$ and $\mathcal{G}_{\tau',p'}$, denoted by $\mathcal{G}_{\tau,p} \Diamond \mathcal{G}_{\tau',p'}$, is defined as follows:*

$$\mathcal{G}_{\tau,p} \Diamond \mathcal{G}_{\tau',p'} = \begin{cases} \mathcal{G}_{\tau,p}; \mathcal{G}_{\tau',p'} & \text{if } p \sqsubseteq p', \\ \mathcal{G}_{\tau',p'}; \mathcal{G}_{\tau,p} & \text{otherwise.} \end{cases}$$

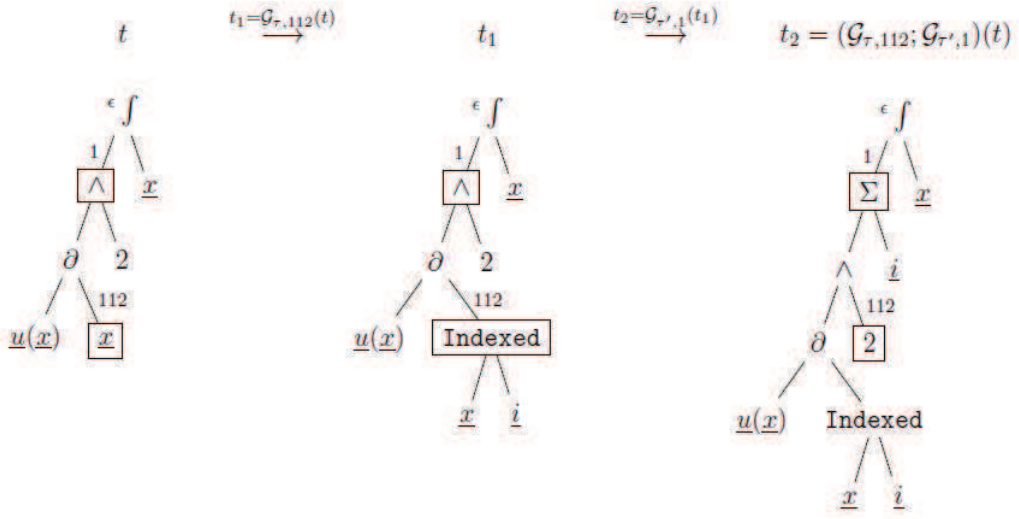


Figure 2.9: The application of the composition $\mathcal{G}_{\tau',112};\mathcal{G}_{\tau',1}$ to t.

Notice that the combination operation $\Diamond$ is associative but not commutative. However it can be commutative if the positions to witch the outward growths are applied are distinct as stated in the following Proposition.

Proposition 80 *Let τ_1, τ_2 be two added terms and let q_1, q_2 be two positions. If $q_1 \neq q_2$ then*

$$\mathcal{G}_{\tau_1,q_1} \Diamond \mathcal{G}_{\tau_2,q_2} = \mathcal{G}_{\tau_2,q_2} \Diamond \mathcal{G}_{\tau_1,q_1}.$$

2.5.3 Outward growths and their combination

Definition 81 (Outward growth) *Let $\vec{\tau} = (\tau_1, ..., \tau_n)$ be a tuple of n added terms and let $\vec{q} = (q_1, ..., q_n)$ be a tuple of n positions with $p_1 \geq p_2 \geq \ldots \geq p_n$. The outward growth $\mathcal{G}_{\vec{\tau},\vec{q}}$ on the added terms $\vec{\tau}$ to the positions $\vec{q}$ is the composition of the n unit outward growths $\mathcal{G}_{\tau_1,q_1}, \ldots, \mathcal{G}_{\tau_n,q_n}$. That is,*

$$\mathcal{G}_{\vec{\tau},\vec{q}} = \mathcal{G}_{\tau_1,q_1}; \ldots;\ \mathcal{G}_{\tau_n,q_n}.$$

In the following we shall define the operation of *combination* of two outward growths $\mathcal{G}_{\vec{\tau},\vec{q}}$ and $\mathcal{G}_{\vec{\tau}',\vec{q}'}$, where $\vec{\tau} = (\tau_1, \ldots, \tau_n)$, $\vec{q} = (q_1, \ldots, q_n)$, $\vec{\tau}' = (\tau'_1, \ldots, \tau'_m)$ and $\vec{q}' = (q'_1, ..., q'_m)$. This operation generalizes the operation of combination of unit outward growths at different positions given in Definition 77. Firstly, we need to perform some treatment on the vectors of positions $\vec{q}$ and $\vec{q}'$ as well as on their related vectors of added terms $\vec{\tau}$ and $\vec{\tau}'$.

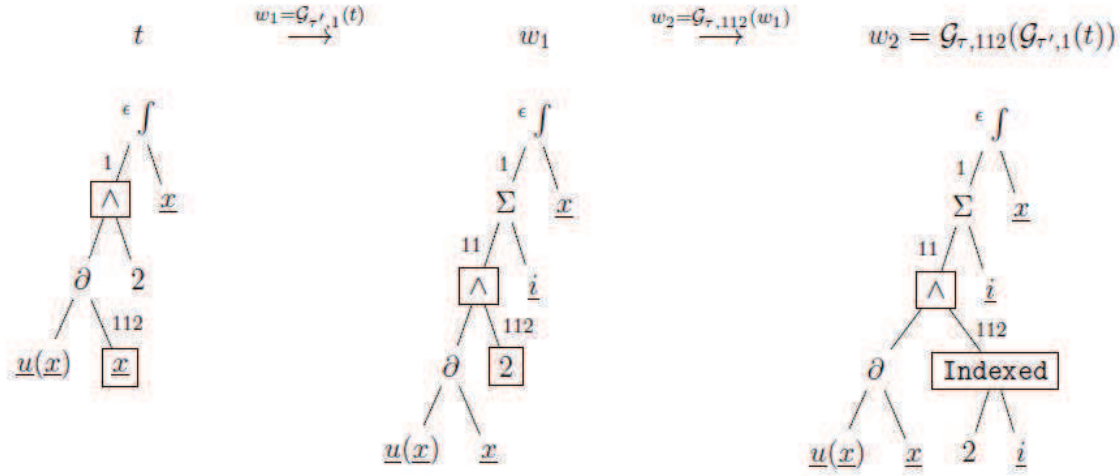


Figure 2.10: The application $\mathcal{G}_{\tau,112}(\mathcal{G}_{\tau',1}(t))$ yields an undesired result.

Definition 82 *Let $\vec{\tau} = (\tau_1, \ldots, \tau_n)$ and $\vec{\tau}' = (\tau_{n+1}, \ldots, \tau_{n+m})$ be two tuples of added terms. Let $\vec{q} = (q_1, \ldots, q_n)$ and $\vec{q}' = (q_{n+1}, \ldots, q_{n+m})$ be two tuples of positions, where the positions $q_1, \ldots, q_{n+m}$ are pairwise comparable, i.e. either $q_i \leq q_j$ or $q_j \leq q_i$ for all $i, j \in \{1, \ldots, n+m\}$. Define the mapping f as $f(q_i) = \tau_i$, for all $i \in \{1, \ldots, n+m\}$. We define the product $(\vec{\tau}, \vec{q}) \otimes (\vec{\tau}', \vec{q}')$ as follows.*

1. *Firstly, sort the tuple $(q_1, \ldots, q_{n+m})$ in the descending order. That is, let $(q'_1, \ldots, q'_{n+m})$ be such that:*

   i.) $\{q'_1, \ldots, q'_{n+m}\} = \{q_1, \ldots, q_{n+m}\}$, and

   ii.) $q'_i \leq q'_j$ iff $i < j$ for all $i, j \in \{1, \ldots, n+m\}$.

2. *Secondly, delete the redundant positions from $(q'_1, \ldots, q'_{n+m})$. That is, let*

$$\vec{q}'' = (q''_1, \ldots, q''_r) \tag{2.15}$$

   be such that $\{q''_1, \ldots, q''_r\} = \{q'_1, \ldots, q'_{n+m}\}$, and $q''_i > q''_{i+1}$ for all $i \in \{1, \ldots, r-1\}$. This yields a surjective function $g : \{1, \ldots, n+m\} \to \{1, \ldots, r\}$ s.t. $g(i) = j$ iff $q''_i = q'_j$.

3. *Thirdly, replace all the added terms in $(f(q'_1), \ldots, f(q'_{n+m}))$ which are to the same position by their composition. That is, let*

$$\vec{\tau}'' = (\tau''_1, \ldots, \tau''_r) \tag{2.16}$$

   be such that: $\tau'_i = f(q'_{k_1})//\ldots//f(q'_{k_d})$ iff $g^{-1}(i) = \{k_1, \ldots, k_d\}$ and $k_1 < k_2 < \ldots < k_d$ for all $i \in \{1, \ldots, r\}$.

4. Finally, we let

$$(\vec{\tau},\vec{q})\otimes(\vec{\tau}',\vec{q}') \stackrel{def}{=} (\vec{\tau}'',\vec{q}'')$$

where $\vec{\tau}''$ is defined in Eq. (2.16) and $\vec{q}''$ is defined in Eq. (2.15) above.

The following Proposition is not hard to prove.

Proposition 83 *The operation $\otimes$ is associative.*

However, the operation $\otimes$ is not commutative in general, but it can be under commutative under some assumptions, namely when each position of $\vec{q}$ is distinct than each position of $\amalg'$:

Proposition 84 *Let $\vec{\tau}$ and $\vec{\tau}'$ be a two tuples of n added terms. Let $\vec{q}=(q_1,...,q_n)$ and $\vec{q}'=(q'_1,...,q'_n)$ be two tuples of n positions with $q_1\geq q_2\geq\ldots\geq q_n$ and $q'_1\geq q'_2\geq\ldots\geq q'_n$. Then,*

$$\text{if } \forall i=1,\ldots,n,\ \ q_i\neq q'_i \quad \text{then} \quad (\vec{\tau},\vec{q})\otimes(\vec{\tau}',\vec{q}')=(\vec{\tau}',\vec{q}')\otimes(\vec{\tau},\vec{q})$$

Now we are ready to define the combination of two outward growths.

Definition 85 (Combination of two outward growths) *The combination of two outward growths $\mathcal{G}_{\vec{\tau},\vec{q}}$ and $\mathcal{G}_{\vec{\tau}',\vec{q}'}$ is defined by*

$$\mathcal{G}_{\vec{\tau},\vec{q}}\Diamond\mathcal{G}_{\vec{\tau}',\vec{q}'} \stackrel{def}{=} \mathcal{G}_{\vec{\tau}'',\vec{q}''}, \qquad \text{where} \quad (\vec{\tau}'',\vec{q}'')=(\vec{\tau},\vec{q})\otimes(\vec{\tau}',\vec{q}').$$

Proposition 86 *The operation $\Diamond$ of combination of outward growths is associative.*

Proof. The associativity of $\Diamond$ follows from the associativity of the product operation $\otimes$, see Proposition 83. ■

The combination operation $\Diamond$ is not commutative in general since $\otimes$ is not commutative. However, we can generalize the Proposition 80 and claim that the operation $\Diamond$ can be commutative under some conditions:

Proposition 87 *Let $\vec{\tau}$ and $\vec{\tau}'$ be a two tuples of n added terms. Let $\vec{q}=(q_1,...,q_n)$ and $\vec{q}'=(q'_1,...,q'_n)$ be two tuples of n positions with $q_1\geq q_2\geq\ldots\geq q_n$ and $q'_1\geq q_2\geq\ldots\geq q'_n$. Then,*

$$\text{if } \forall i=1,\ldots,n,\ \ q_i\neq q'_i \quad \text{then} \quad \mathcal{G}_{(\vec{\tau},\vec{q})}\Diamond\mathcal{G}_{(\vec{\tau}',\vec{q}')}=\mathcal{G}_{(\vec{\tau}',\vec{q}')}\Diamond\mathcal{G}_{(\vec{\tau},\vec{q})}$$

Proof. The proof follows from Proposition 84. ■

The following Proposition relates the outward growths to the unit outward growths by means of the operation $\Diamond$.

Proposition 88 *Let $\vec{\tau} = (\tau_1, \ldots, \tau_n)$ a tuple of added terms and let $\vec{q} = (q_1, \ldots, q_n)$ be a tuple of positions where $q_1 \geq \ldots \geq q_n$. Then,*

$$\mathcal{G}_{\vec{\tau},\vec{q}} = \mathcal{G}_{\tau_1,q_1} \Diamond \ldots \Diamond \mathcal{G}_{\tau_n,q_n}.$$

Proof. Immediate from the definition of $\otimes$, that is, $(\vec{\tau},\vec{q}) = (\tau_1,q_1) \otimes \ldots \otimes (\tau_n,q_n)$. ■

Remark 89 *Let $\vec{\tau}_1, \ldots, \vec{\tau}_n$ be a n tuples of added terms, and $\vec{q}_1, \ldots, \vec{q}_n$ be n tuples of positions where $|\vec{\tau}_i| = |\vec{q}_i|$ for all $i \in \{1, \ldots, n\}$. From Proposition 86 on the associativity of the operation $\Diamond$ of the combination of outward growths, it follows that there exist a tuple of added terms $\vec{\tau}$ and a tuple of positions $\vec{q}$ such that*

$$\mathcal{G}_{\vec{\tau},\vec{q}} = \mathcal{G}_{\vec{\tau}_1,\vec{q}_1} \Diamond \ldots \Diamond \mathcal{G}_{\vec{\tau}_n,\vec{q}_n}.$$

Example 90 (Combination of outward growths) *Let t be the term*

$$t := \int \underline{a} \partial_{\underline{x}} \underline{u}(\underline{x})\, d\underline{x}$$

depicted on the top left of Figure 2.11. Consider the following subterms of t with their related positions:

$$\begin{aligned} t|_1 &= \underline{a} \partial_{\underline{x}} \underline{u}(\underline{x}), \\ t|_{11} &= \underline{a}, \\ t|_{121} &= \underline{u}(\underline{x}), \text{ and} \\ t|_{122} &= \underline{x}. \end{aligned}$$

Consider the added terms τ_1, τ_{11}, τ_{122}, τ'_1, τ'_{11} and τ'_{121}:

$$\begin{aligned} \tau_1 &= \sum_i (\bot), \\ \tau_{11} = \tau_{122} &= \texttt{Indexed}(\bot, i), \\ \tau'_1 &= \sum_j (\bot), \text{ and} \\ \tau'_{11} = \tau'_{121} &= \texttt{Indexed}(\bot, j). \end{aligned}$$

Consider the outward growths $\mathcal{G}_{\vec{\tau},\vec{p}}$ and $\mathcal{G}_{\vec{\tau}',\vec{p}'}$:

$$\begin{aligned} \mathcal{G}_{\vec{\tau},\vec{p}} &= \mathcal{G}_{\tau_{122},122} \Diamond \mathcal{G}_{\tau_{11},11} \Diamond \mathcal{G}_{\tau_1,1}, \text{ and} \\ \mathcal{G}_{\vec{\tau}',\vec{p}'} &= \mathcal{G}_{\tau'_{121},121} \Diamond \mathcal{G}_{\tau'_{11},11} \Diamond \mathcal{G}_{\tau'_1,1}. \end{aligned}$$

A straightforward application of Definition 85 gives

$$\begin{cases} \vec{\tau} & = (\tau_{122}, \tau_{11}, \tau_1), \\ \vec{p} & = (122, 11, 1), \\ \vec{\tau}' & = (\tau'_{121}, \tau'_{11}, \tau'_1), \text{ and} \\ \vec{p'} & = (121, 11, 1). \end{cases}$$

Now we shall compute the outward growth $\mathcal{G}_{\vec{\tau}'', \vec{p}''}$*:*

$$\mathcal{G}_{\vec{\tau}'', \vec{p}''} = \mathcal{G}_{\vec{\tau}, \vec{p}} \Diamond \mathcal{G}_{\vec{\tau}, \vec{p}}$$

That is, we need to compute $\vec{\tau}''$ *and* $\vec{p}''$ *which, according to Definition 85, are defined by*

$$(\vec{\tau}'', \vec{p}'') = (\vec{\tau}, \vec{p}) \otimes (\vec{\tau}', \vec{p}').$$

Notice that $11 > 1$ *and both the positions* 122 *and* 121 *are incomparable with the positions* 11 *and* 1*. Besides, the positions* 122 *and* 121 *are incomparable. On the other hand,* $\vec{p}$ *and* $\vec{p}'$ *share the positions* 11 *and* 1*. Therefore, from Definition 82 it follows that*

$$\begin{cases} \vec{p}'' = (122, 121, 11, 1), \text{ and} \\ \vec{\tau}'' = (\tau_{122}, \tau'_{121}, \tau_{11} // \tau'_{11}, \tau_1 // \tau'_1) \end{cases}$$

Notice that, from Proposition 88, it follows that the outward growth $\mathcal{G}_{\vec{\tau}'', \vec{p}''}$ *can be written as a combination of unit outward growths as follows:*

$$\mathcal{G}_{\vec{\tau}'', \vec{p}''} = \mathcal{G}_{\tau_{122}, 122} \Diamond \mathcal{G}_{\tau'_{121}, 121} \Diamond \mathcal{G}_{(\tau_{11} // \tau'_{11}), 11} \Diamond \mathcal{G}_{(\tau_1 // \tau'_1), 1} \tag{2.17}$$

According to Definition 79, the combination of unit outward growths in Eq. (2.17) can be written as a composition of unit outward growths as follows:

$$\mathcal{G}_{\vec{\tau}'', \vec{p}''} = \mathcal{G}_{\tau_{122}, 122} \,;\, \mathcal{G}_{\tau'_{121}, 121} \,;\, \mathcal{G}_{(\tau_{11} // \tau'_{11}), 11} \,;\, \mathcal{G}_{(\tau_1 // \tau'_1), 1} \tag{2.18}$$

Using the formulation of the outward growth $\mathcal{G}_{\vec{\tau}'', \vec{p}''}$ *given in Eq. (2.18), the application of* $\mathcal{G}_{\vec{\tau}'', \vec{p}''}$ *to the term* t *is illustrated in Figure 2.11. It yields the term:*

$$\mathcal{G}_{\vec{\tau}'', \vec{p}''}(t) = \int \sum_{\underline{i}} \sum_{\underline{j}} \underline{a_{ij}} \partial_{\underline{x_i}} \underline{u_j}(\underline{x}) \; d\underline{x}.$$

2.6 Outward growths as second-order rewriting rules

We follow the extension approach established in Section 2.5. In this section we formulate the outward growths of the previous section as well as their combination as SO-strategies. For readability, we call them *second-order outward growths*.

2.6.1 Second-order outward growth

A SO-unit outward growth is a SO-order rule $l \rightrightarrows r$ where its right-hand side term r is the result of the application of a FO-outward growth to l at some position, see Definition 91 bellow. We notice that we only deal with the SO-outward growths applied to the root since it is enough to consider the application of a SO-outward growth (i.e. a SO-rule) to a FO-rule to the root. In other words, the left-hand term l above is considered as a FO-rule (that possibly contains SO-variables) and the SO-outward growth $l \rightrightarrows r$ will be applied to a FO-rule (to the root). The formal definition of SO-unit outward growth to the root follows.

Definition 91 (Second-order unit outward growth to the root) *Let $\tau \in \mathcal{T}^{add}(\mathcal{F}, \mathcal{X})$ be an added term, p be a position, and l a SO-term. The SO-unit outward growth to the root $\mathcal{G}^l_{\tau,p}$ is the SO-rewrite rule:*

$$\mathcal{G}^l_{\tau,p} \stackrel{def}{=} l \rightrightarrows \mathcal{G}_{\tau,p}(l)$$

SO-outward growths to the root can be defined similarly to SO-unit outward growths to the root.

Definition 92 (Second-order outward growth to the root) *Let $\vec{\tau}$ be a tuple of n added terms, $\vec{p}$ be a tuple of n positions in the decreasing order, and l a SO-term. The SO-outward growth to the root $\mathcal{G}^l_{\vec{\tau},\vec{p}}$ is the SO-rule:*

$$\mathcal{G}^l_{\vec{\tau},\vec{p}} \stackrel{def}{=} l \rightrightarrows \mathcal{G}_{\vec{\tau},\vec{p}}(l)$$

The application of $\mathcal{G}^l_{\vec{\tau},\vec{p}}$ to a SO-term is defined in the usual way.

We recall that the notion of the most general unifier of a unification problem E, denoted by $\mathtt{mgu}(E)$, was given in Definition 52.

2.6.2 Combination of second-order outward growths

The notion of the combination of SO-outward growths to the root can be defined in a natural way by means of the combination of their related (FO-)outward growths as follows.

Definition 93 (Combination of two SO-outward growths) *Let $\mathcal{G}^{l}_{\vec{\tau},\vec{p}}$ and $\mathcal{G}^{l'}_{\vec{\tau}',\vec{p}'}$ be two SO-outward growths where $\mathcal{V}ar^1(l) \cap \mathcal{V}ar^1(l') = \emptyset$. Assume that the* **mgu** *of the unification problem $\{l \doteq l'\}$ with respect to the second-order variables is decidable. The combination $\mathcal{G}^{l}_{\vec{\tau},\vec{p}} \Diamond \mathcal{G}^{l'}_{\vec{\tau}',\vec{p}'}$ is defined by*

$$\mathcal{G}^{l}_{\vec{\tau},\vec{p}} \Diamond \mathcal{G}^{l'}_{\vec{\tau}',\vec{p}'} \stackrel{def}{=} \mathcal{G}^{l''}_{\vec{\tau}'',\vec{p}''} \text{ where } \begin{cases} \mathcal{G}_{\vec{\tau}'',\vec{p}''} = \mathcal{G}_{\vec{\tau},\vec{p}} \Diamond \mathcal{G}_{\vec{\tau}',\vec{p}'}, \text{ and} \\ l'' = \sigma(l) = \sigma(l'), \text{ where } \sigma = \mathtt{mgu}(\{l \doteq l'\}). \end{cases}$$

Notice that if $\mathcal{V}ar^1(l) \cap \mathcal{V}ar^1(l') \neq \emptyset$, then one can rename the SO-variables in both l and l' so that $\mathcal{V}ar^1(l) \cap \mathcal{V}ar^1(l') = \emptyset$. Notice also that from Definition 93 it follows that the combination of two SO-outward growth is a SO-outward growth.

Proposition 94 *The combination operation $\Diamond$ of SO-outward growths is associative.*

Proof. The claim follows, on the one hand, from the associativity of the composition of outward growths, see Proposition 86, and on the other hand from the fact that $\mathtt{mgu}(\{\sigma_{l,l'} \doteq l''\}) = \mathtt{mgu}(\{l \doteq \sigma_{l',l''}\})$, where $\sigma_{l,l'} = \mathtt{mgu}(\{l \doteq l'\})$ and $\sigma_{l',l''} = \mathtt{mgu}(\{l' \doteq l''\})$. ■

Example 95 *Let*

$$\begin{cases} l_1 &= \underline{L^2}(\underline{u}(\underline{x})) \to \int v^2 \, dz, \\ \tau_1 &= \mathtt{Indexed}(\bot, \underline{i}), \\ p_1 &= \mathcal{P}os(v, l_1), \end{cases} \quad \text{and} \quad \begin{cases} l_2 &= \underline{L^2}(\underline{u}'(\underline{x}')) \to \int v' \, dz', \\ \tau_2 &= \sum(\bot, \underline{i}), \\ p_2 &= \mathcal{P}os(v', l_2), \end{cases}$$

where

$$\begin{aligned} \underline{\Omega} &\equiv \mathtt{Reg}(\Omega, d), \\ \underline{x} &\equiv \mathtt{Var}(x, \underline{\Omega}), \\ \underline{i} &\equiv \mathtt{Index}(i, \mathtt{Set}(I, \{1, d\})), \\ \underline{u}(\underline{x}) &\equiv \mathtt{Fun}(u, [\underline{x}], \textit{unknown}), \end{aligned}$$

and $u, x, \Omega, d, v, z, u, x, \Omega', d', v', z'$ are SO-variables in $\mathcal{X}^1$ and i is a constant in $\mathcal{F}^0$. Let $\mathcal{G}^{l_1}_{\tau_1,p_1}$ and $\mathcal{G}^{l_2}_{\tau_2,p_2}$ be two SO-unit outward growths. A simple computation yields:

$$\begin{cases} \mathcal{G}_{\tau_1,p_1}(l_1) &= \underline{L^2}(\underline{u}(\underline{x})) \to \int (v_{\underline{i}})^2 \, dz, \\ \quad \textit{and} \\ \mathcal{G}_{\tau_2,p_2}(l_2) &= \underline{L^2}(\underline{u}'(\underline{x}')) \to \int \sum_{\underline{i}} v' \, dz'. \end{cases}$$

where

$$v_{\underline{i}} \equiv \texttt{Indexed}(v, \underline{i}).$$

Therefore we have:

$$\begin{aligned}\mathcal{G}^{l_1}_{\tau_1,p_1} &\stackrel{def}{=} l_1 \rightrightarrows \mathcal{G}_{\tau_1,p_1}(l_1)\\ &= \big(\underline{L^2}(\underline{u}(\underline{x})) \to \int (v)^2\ dz\big) \rightrightarrows \big(\underline{L^2}(\underline{u}(\underline{x})) \to \int (v_{\underline{i}})^2\ dz\big),\end{aligned} \tag{2.19}$$

and

$$\begin{aligned}\mathcal{G}^{l_2}_{\tau_2,p_2} &\stackrel{def}{=} l_2 \rightrightarrows \mathcal{G}_{\tau_2,p_2}(l_2)\\ &= \big(\underline{L^2}(\underline{u}'(\underline{x}')) \to \int v'\ dz'\big) \rightrightarrows \big(\underline{L^2}(\underline{u}'(\underline{x}')) \to \int \sum_{\underline{i}} v'\ dz'\big).\end{aligned} \tag{2.20}$$

The tree structure of $\mathcal{G}^{l_1}_{\tau_1,p_1}(l_1)$ and $\mathcal{G}^{l_2}_{\tau_2,p_2}(l_2)$ is depicted in Figure 2.12 and Figure 2.13, respectively.

Now we compute the combination $\mathcal{G}^{l_1}_{\tau_1,p_1} \Diamond \mathcal{G}^{l_2}_{\tau_2,p_2}$, which is defined (see Definition 93) by:

$$\mathcal{G}^{l_1}_{\tau_1,p_1} \Diamond \mathcal{G}^{l_2}_{\tau_2,p_2} \stackrel{def}{=} \mathcal{G}^{l}_{\vec{\tau},\vec{p}} \text{ where } \begin{cases}\mathcal{G}_{\vec{\tau},\vec{p}} = \mathcal{G}_{\tau_1,p_1} \Diamond \mathcal{G}_{\tau_2,p_2}, \text{ and}\\ l = \sigma(l_1) = \sigma(l_2), \text{ where } \sigma = \texttt{mgu}(\{l_1 \doteq l_2\}).\end{cases}$$

On the one hand, since $p_1 > p_2$, it follows from Definitions 85 and 82 that:

$$\begin{cases}\vec{p} &= (p_1, p_2), \quad \text{and}\\ \vec{\tau} &= (\tau_1, \tau_2)\end{cases}$$

On the other hand, we need to compute the substitution σ which is the `mgu` *of the unification problem:*

$$\begin{cases}u &\doteq u'\\ x &\doteq x'\\ v^2 &\doteq v'\\ z &\doteq z'\end{cases}$$

We get:

$$\sigma = \{u' \mapsto u, x' \mapsto x, v' \mapsto v^2, z' \mapsto z\}.$$

Finally,

$$\begin{aligned}\mathcal{G}^{l_1}_{\tau_1,p_1} \Diamond \mathcal{G}^{l_2}_{\tau_2,p_2} &\stackrel{def}{=} \mathcal{G}^{l}_{\vec{\tau},\vec{p}} \\ &= \mathcal{G}^{\sigma(l_1)}_{(\tau_1,\tau_2),(p_1,p_2)} \\ &= \sigma(l_1) \rightrightarrows \mathcal{G}_{(\tau_1,\tau_2),(p_1,p_2)}(\sigma(l_1)) \\ &= \left(\underline{L^2}(\underline{u}(\underline{x})) \to \int v^2 \; dz\right) \rightrightarrows \left(\underline{L^2}(\underline{u}(\underline{x})) \to \int \sum_{\underline{i}} (v_{\underline{i}})^2 \; dz\right).\end{aligned}$$

2.7 Extension of first-order terms by combining outward growths and parametrizations

In order to construct richer extensions it is natural to combine the extension tools that we have at our disposal so far. That is, the combination of outward growths and parametrizations gives arise to richer mechanism called *generalization*.

2.7.1 A motivating example

Let Ω be a d dimensional domain, u a scalar function defined on Ω, and $\mathbf{u} = (u_1, ..., u_n)$ a vector function defined on Ω. The L^2 norm of u and $\mathbf{u}$ are respectively defined by:

$$\begin{cases} ||u||_{L^2(\Omega)} &= \left(\int_\Omega |u|^2\right)^{1/2}, \\ ||\mathbf{u}||_{L^2(\Omega)} &= \left(\sum_{i=1}^{n} \int_\Omega |u_i|^2\right)^{1/2}. \end{cases}$$

Their formulation by means of rewriting rules is given by the FO-rewriting rules s and s', respectively, as follows:

$$\begin{cases} s &:= L^2\left(\underline{u}\left(\underline{x}\right)\right) \to \left(\int_{\underline{\Omega}} |\underline{u}\left(\underline{x}\right)|^2 d\underline{x}\right)^{1/2}, \\ s' &:= L^2\left(\underline{u}_{\underline{i}}\left(\underline{x}\right)\right) \to \left(\sum_{\underline{i}=1}^{n} \int_{\underline{\Omega}} |\underline{u}_{\underline{i}}\left(\underline{x}\right)|^2 d\underline{x}\right)^{1/2}, \end{cases}$$

where

$$\begin{cases} \underline{\Omega} &= \texttt{Reg}\left(\Omega, d\right), \\ \underline{x} &= \texttt{Var}\left(x, \underline{\Omega}\right), \\ \underline{u} &= \texttt{Fun}\left(u, \underline{x}\right), \\ \underline{i} &= \texttt{Index}\left(i, \texttt{Set}\left(I, \{1, ..., n\}\right)\right), \end{cases}$$

and Ω, x, u, I, i are FO-variables in $\mathcal{X}^0$ and d, n are constants in $\mathcal{F}^0$. By applying the notions and techniques developed in Section 2.3, we show next how to build the FO-rules s and s' by means of SO-rules. For this purpose, we need the SO-rule s^0 and s^1 defined as follows:

$$\begin{cases} s^0 & := L^2\left(\underline{u}_{\underline{i}}\left(\underline{x}\right)\right) \rightarrow \left(\sum\limits_{\underline{i}=1}^{1} \int_{\underline{\Omega}} |\underline{u}_{\underline{i}}\left(\underline{x}\right)|^2 d\underline{x}\right)^{1/2}, \\ s^1 & := L^2\left(\underline{u}_{\underline{i}'}\left(\underline{x}\right)\right) \rightarrow \left(\sum\limits_{\underline{i}'=1}^{r} \int_{\underline{\Omega}} |\underline{u}_{\underline{i}'}\left(\underline{x}\right)|^2 d\underline{x}\right)^{1/2}, \end{cases}$$

where

$$\begin{cases} \underline{i} = \texttt{Index}\left(i, \texttt{Set}\left(I, \{1, ..., 1\}\right)\right), \\ \underline{i}' = \texttt{Index}\left(i, \texttt{Set}\left(I, \{1, ..., r\}\right)\right), \end{cases}$$

and r is a FO-variable in $\mathcal{X}^0$.

We define the SO-rules S^0 and S^1 as follows:

$$\begin{cases} S^0 & := s \rightrightarrows s^0, \\ S^1 & := s \rightrightarrows s^1. \end{cases}$$

The following claims are not hard to prove:

Fact 96 *The following hold:*

1. *The SO-rule S^0 is a semantic conservation SO-rule w.r.t the rewriting system $\mathcal{R}$ defined in Eq (2.14) of Section 2.3.*
2. *S^1 is a parametrized SO-rule in the sense of Definition 56 of Section 2.3.*
3. *The SO-rule S^1 is admissible with respect to S^0.*
4. *The FO-rule s' is a generalization of the FO-rule s in the sense of Definition 61 of Section 2.3.*

Item 2 follows from the fact that

$$\mathcal{V}ar^0(S^1) = \mathcal{V}ar^0(s^1) - \mathcal{V}ar^0(s) = \{r\} \neq \emptyset.$$

Item 3 follows from the fact that

$$\sigma\left(S^1\right) = S^0, \quad \text{where } \sigma = \{r \mapsto 1\}.$$

Item 4 follows from the fact that S^1 is an admissible SO-rule and that

$$S^1(s) = s' \quad \text{(modulo } \alpha\text{-conversion)}$$

We give next an equivalent formulation of S^0 and S^1 in terms of a combination of outward growths and parametrization, where parametrization means the replacement of a FO-term by a FO-variable. For this purpose we introduce two unit outward growths. Let τ_1 and τ_2 be the added terms:

$$\begin{aligned}\tau_1 &= \mathtt{Indexed}\left(\bot, \mathtt{Index}\left(i, \mathtt{Set}\left(I, \{1, ..., 1\}\right)\right)\right),\\ \tau_2 &= \mathtt{Oper}\left(\mathtt{Sum}, \bot, \mathtt{Index}\left(i, \mathtt{Set}\left(I, \{1, ..., 1\}\right)\right), \emptyset\right).\end{aligned}$$

They are depicted in Figure 2.14.

Let p_1, p_2 and p_3 be the positions of s defined by:

$$\begin{cases} p_1 &= 22,\\ p_2 &= 32,\\ p_3 &= 32222. \end{cases}$$

Notice that $p_1 \parallel p_2$ and $p_1 \parallel p_3$ and $p_2 < p_3$. The tree structure of s and the related positions are depicted in Figure 2.15.

We define $\mathcal{G}_{\vec{\tau},\vec{p}}$ as follows:

$$\begin{aligned}\mathcal{G}_{\vec{\tau},\vec{p}} &\stackrel{def}{=} \mathcal{G}_{\tau_1,p_1} \Diamond \mathcal{G}_{\tau_1,p_3} \Diamond \mathcal{G}_{\tau_2,p_2}\\ &= \mathcal{G}_{\tau_1,p_1}; \mathcal{G}_{\tau_1,p_3}; \mathcal{G}_{\tau_2,p_2}\\ &= \mathcal{G}_{(\tau_1,\tau_1,\tau_3),(p_1,p_3,p_2)}\end{aligned}$$

We have that

$$\mathcal{G}_{\vec{\tau},\vec{p}}(s) = s_0.$$

Let q_1, q_2 and q_3 be the positions in $\mathcal{P}os\left(s^0\right)$ defined by:

$$\begin{cases} q_1 &= 22222,\\ q_2 &= 322222222,\\ q_3 &= 32322. \end{cases}$$

Notice that $q_1 \parallel q_2$ and $q_2 \parallel q_3$ and $q_1 \parallel q_3$. Let r be a FO-variable in $\mathcal{X}^0$. We define the parametrization $\mathcal{P}_{(\vec{r},\vec{q})}$ as follows

$$\begin{aligned}\mathcal{P}_{(\vec{r},\vec{q})} &\stackrel{def}{=} \mathcal{P}_{(r,r,r),(q_1,q_2,q_3)}\\ &\stackrel{def}{=} \mathcal{P}_{r,q_1}; \mathcal{P}_{r,q_2}; \mathcal{P}_{r,q_3}\end{aligned}$$

where $\mathcal{P}_{r,q}(t)$ stands for the replacement of the subterm of t at the position q (i.e. $t|_q$) by r. Finally we have that

$$\begin{aligned}(\mathcal{G}_{\vec{r},\vec{p}};\, \mathcal{P}_{(\vec{r},\vec{q})})(s) &= \mathcal{P}_{(\vec{r},\vec{q})}(\mathcal{G}_{\vec{r},\vec{p}}(s)) \\ &= \mathcal{P}_{(\vec{r},\vec{q})}(s_0) \\ &= s_1.\end{aligned}$$

The tree structure of the rules s_0 and s_1 are depicted in Figure 2.17 and 2.18.

Discussion. The example 2.7.1 above shows the constant symbols 1 in unit outward growths upon the added terms τ_1 and τ_2, must be repalced by a FO-variable. Therefore, while combining outward growths and parametrizations, one has to apply the outward growths first then the parametrizations. In what follows we shall define the combination of two parametrizations

$$\mathcal{P}_{x_1,q_1} \Diamond \mathcal{P}_{x_2,q_2}$$

as well as the composition of outward growth with parametrization

$$\mathcal{G}_{\tau,p} \Diamond \mathcal{P}_{x,q}$$

2.7.2 Unit parametrizations, parametrizations and their combination

The parametrization consists in replacing a term by a FO-variable at a given position.

Definition 97 (Unit parametrization) *Let t be a term, q a position of t and x a FO-variable in $\mathcal{X}^0$. A unit parametrization $\mathcal{P}_{x,q} : \mathcal{X}^0 \mapsto \mathcal{T}(\mathcal{F}^0, \mathcal{X}^0)$ is a mapping:*

$$\mathcal{P}_{x,q} : t \longmapsto t\,[x]_q\,.$$

A composition of unit parametrizations applied to incomparable positions yields the notion of parametrization:

Definition 98 (Parametrization) *Let $\vec{q} = (q_1, \cdots, q_n)$ be a tuple of $n \geq 1$ positions such that $q_i \parallel q_j$ for all $i, j \in \{1, \ldots, n\}$ and $i \neq j$. Let $\vec{x} = (x_1, \cdots, x_n)$ be a tuple of FO-variables in $\mathcal{X}^0$. A parametrization $\mathcal{P}_{\vec{x},\vec{q}}$ is defined by*

$$\mathcal{P}_{\vec{x},\vec{q}} \stackrel{def}{=} \mathcal{P}_{x_1,q_1}; \ldots; \mathcal{P}_{x_n,q_n}.$$

Definition 99 (The combination of two parametrizations) *Let $\mathcal{P}_{\vec{x},\vec{p}}$ and $\mathcal{P}_{\vec{y},\vec{q}}$ be two parametrizations, where $\vec{p} = (p_1, \cdots, q_n)$ and $\vec{q} = (q_1, \cdots, q_m)$ are two tuples of positions, and $\vec{x} = (x_1, \ldots, x_n)$ and $\vec{y} = (y_1, \ldots, y_m)$ are two tuples of FO-variables in $\mathcal{X}^0$. The combination of $\mathcal{P}_{\vec{x},\vec{p}}$ and $\mathcal{P}_{\vec{y},\vec{q}}$ is defined if and only when*

$$p_i \parallel q_j \text{ for all } i \in \{1, \ldots, n\} \text{ and } j \in \{1, \ldots, m\},$$

as the parametrization $\mathcal{P}_{\vec{z},\vec{r}}$:

$$\mathcal{P}_{\vec{x},\vec{p}} \Diamond \mathcal{P}_{\vec{y},\vec{q}} \stackrel{def}{=} \mathcal{P}_{\vec{z},\vec{r}}, \qquad \text{where } \begin{cases} \vec{z} & = (x_1, \ldots, x_n, y_1, \ldots, x_m), \text{ and} \\ \vec{r} & = (p_1, \ldots, p_n, q_1, \ldots, q_m) \end{cases}$$

2.7.3 Unit generalizations, generalizations and their combination

The definition of unit generalization follows.

Definition 100 (Unit generalization) *Let q and p be two positions. Let τ be an added term and x be a FO-variable in $\mathcal{X}^0$. A unit generalization $\mathbb{G}^{x,p}_{\tau,q}$ is defined by*

$$\mathbb{G}^{x,p}_{\tau,q} = \begin{cases} \mathcal{G}_{\tau,q}; \mathcal{P}_{x,p} & \text{if } p \sqsubset q \\ \text{undefined,} & \text{otherwise} \end{cases}$$

where $\mathcal{G}_{\tau,q}$ is a unit outward growth (see definition 73) and $\mathcal{P}_{x,p}$ is a unit parametrization (see definition 97).

We notice that while composing an outward growth $\mathcal{G}_{\tau,q}$ and a parametrization $\mathcal{P}_{x,p}$ to build a generalization $\mathbb{G}^{x,p}_{\tau,q} = \mathcal{G}_{\tau,q}; \mathcal{P}_{x,p}$, it is, on the one hand more flexible to start with the application of the outward growth first since this allows, among other things, to apply the parametrization to the added term. On the hand, the condition $p \sqsubset q$ in Definition 100 on the positions q and p (in which the outward growth and the parametrization are applied respectively) is natural and ensures that a parametrization can either

i) operate on a *proper* subterm of $t_{|q}$, i.e. in this case we have $p < q$, or

ii) operate on a subterm of t that does not overlap with $t_{|q}$, i.e. in this case we have $p \parallel q$.

Definition 101 (Generalization) *Let $\overrightarrow{q} = (q_1, ..., q_n)$ and $\overrightarrow{p} = (p_1, ..., p_m)$ be two tuples of positions such that $q_i \parallel q_j$ for all $i, j \in \{1, \ldots, n\}$ and $i \neq j$, and*

$p_i \parallel p_j$ for all $i, j \in \{1, \ldots, m\}$ and $i \neq j$. Let $\overrightarrow{\tau} = (\tau_1, ..., \tau_n)$ be a tuple of added terms and $\overrightarrow{x} = (x_1, ..., x_m)$ be a tuple of FO-variables in $\mathcal{X}^0$.

A generalization $\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}}$ is defined by

$$\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}} = \begin{cases} \mathcal{G}_{\vec{\tau},\vec{q}}\,;\, \mathcal{P}_{\vec{x},\vec{p}} & \text{if } p_i \sqsubset q_j, \forall i \in \{1, \ldots, n\} \text{ and } \forall j \in \{1, \ldots, m\} \\ \text{undefined}, & \text{otherwise} \end{cases}$$

where $\mathcal{G}_{\vec{\tau},\vec{q}}$ is an outward growth (see Definition 81) and $\mathcal{P}_{\vec{x},\vec{p}}$ is a parametrization (see Definition 98).

We generalize the relation $\sqsubset$ between positions (Item (2) of Definition 45) to pairs of positions.

Definition 102 *Let q_1, q_2, p_1 and p_2 be positions. Define the binary relation $\sqsubset$ between pairs of positions as follows:*

$$(q_1, p_1) \sqsubset (q_2, p_2) \quad \text{iff} \quad q_1 \sqsubseteq q_2 \text{ and } p_1 \sqsubset q_2 \text{ and } p_1 \sqsubset p_2$$

Definition 103 (Composition of two unit generalizations) *Let $\mathbb{G}^{x_1,p_1}_{\tau_1,q_1}$ and $\mathbb{G}^{x_2,p_2}_{\tau_2,q_2}$ be two unit generalizations. Their composition, denoted by $\mathbb{G}^{x_1,p_1}_{\tau_1,q_1}\,;\,\mathbb{G}^{x_2,p_2}_{\tau_2,q_2}$, is defined as follows:*

$$\left(\mathbb{G}^{x_1,p_1}_{\tau_1,q_1}\,;\,\mathbb{G}^{x_2,p_2}_{\tau_2,q_2}\right)(t) = \begin{cases} \mathbb{G}^{x_2,p_2}_{\tau_2,q_2}(\mathbb{G}^{x_1,p_1}_{\tau_1,q_1}(t)) & \text{if } (q_1, p_1) \sqsubset (q_2, p_2) \\ \text{undefined}, & \text{otherwise.} \end{cases}$$

We notice that the condition $(q_1, p_1) \sqsubset (q_2, p_2)$ on the positions in Definition 103 are natural since:

i) $q_1 \sqsubseteq q_2$ ensures that the composition of the outward growths $\mathcal{G}_{\tau_1,q_1}\ \mathcal{G}_{\tau_2,q_2}$ can be done correctly, see Definition 77.

ii) $p_1 \sqsubset q_2$ ensures that the outward growth $\mathcal{G}_{\tau_2,q_2}$ can not be applied at a position bellow p_1 since the subterm at p_1 has been replaced by a variable by means of the parametrization $\mathcal{P}_{x_1,p_1}$.

iii) similarly, $p_1 \sqsubset p_2$ ensures that the parametrization $\mathcal{P}_{x_2,p_2}$ can not be applied at a position bellow p_1 since the subterm at p_1 has been replaced by a variable by means of the parametrization $\mathcal{P}_{x_1,p_1}$.

Lemma 104 *The composition of two unit generalizations is a generalization.*

Proof. Let $\mathbb{G}^{x_1,p_1}_{\tau_1,q_1}$ and $\mathbb{G}^{x_2,p_2}_{\tau_2,q_2}$ be two unit generalizations with $(q_1,p_1) \sqsubset (q_2,p_2)$. To prove the Lemma it is enough to compute $\vec{\tau}$, $\vec{q}$, $\vec{x}$, $\vec{p}$ such that

$$\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}} = \mathbb{G}^{x_1,p_1}_{\tau_1,q_1} ; \mathbb{G}^{x_2,p_2}_{\tau_2,q_2}$$

This can be achieved by considering many cases depending on the relative position of p_1, p_2, q_1 and q_2. ■

Definition 105 (Combination of two unit generalizations) *Let $\mathbb{G}^{x_1,p_1}_{\tau_1,q_1}$ and $\mathbb{G}^{x_2,p_2}_{\tau_2,q_2}$ be two unit generalizations. Their combination, denoted by $\mathbb{G}^{x_1,p_1}_{\tau_1,q_1} \Diamond \mathbb{G}^{x_2,p_2}_{\tau_2,q_2}$, is defined as follows:*

$$\mathbb{G}^{x_1,p_1}_{\tau_1,q_1} \Diamond \mathbb{G}^{x_2,p_2}_{\tau_2,q_2} = \begin{cases} \mathbb{G}^{x_1,p_1}_{\tau_1,q_1} ; \mathbb{G}^{x_2,p_2}_{\tau_2,q_2} & \text{if } (q_1,p_1) \sqsubset (q_2,p_2) \\ \mathbb{G}^{x_2,p_2}_{\tau_2,q_2} ; \mathbb{G}^{x_1,p_1}_{\tau_1,q_1} & \text{if } (q_2,p_2) \sqsubset (q_1,p_1) \\ \text{undefined}, & \text{otherwise.} \end{cases}$$

Lemma 106 *The combination of two unit generalizations is a generalization.*

Proof. Follows from Lemma 106 on the composition of two unit generalizations. ■

In order to inductively define the composition of two generalizations, we need first to consider the composition of a generalization and a unit generalization. Before that we need to generalize the relation $\sqsubset$ between pairs of positions (Definition 102).

Definition 107 *Let $\vec{q} = (q_1, \ldots, q_n)$ and $\vec{p} = (p_1, \ldots, p_n)$ be two tuples of positions. Let q and p be two positions. Define the binary relation $\sqsubset$ as follows:*

$$(\vec{q},\vec{p}) \sqsubset (q,p) \quad \text{iff} \quad q_i \sqsubseteq q \text{ and } p_i \sqsubset q \text{ and } p_i \sqsubset p, \quad \text{for all } i = 1, \ldots, n$$

Definition 108 (Composition of a generalization and a unit generalization) *Let $\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}}$ be a generalization and $\mathbb{G}^{x,p}_{\tau,q}$ be a unit generalizations, where*

$$\begin{cases} \vec{\tau} = (\tau_1, \ldots, \tau_n) \\ \vec{q} = (q_1, \ldots, q_n) \\ \vec{x} = (x_1, \ldots, x_m) \\ \vec{p} = (p_1, \ldots, p_n) \end{cases}$$

The composition of $\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}}$ and $\mathbb{G}^{x,p}_{\tau,q}$, denoted by $\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}}; \mathbb{G}^{x,p}_{\tau,q}$, is defined as follows:

$$\left(\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}}; \mathbb{G}^{x,p}_{\tau,q}\right)(t) = \begin{cases} \mathbb{G}^{x,p}_{\tau,q}(\mathbb{G}^{\vec{x},\vec{p}}_{\vec{\tau},\vec{q}}(t)) & \text{if } (\vec{q},\vec{p}) \sqsubseteq (q,p) \\ \text{undefined}, & \text{otherwise.} \end{cases}$$

Similarly, once can show that the composition of a generalization and a unit generalization is actually a generalization. Therefore, one can inductively define the composition/combination of two generalizations as well.

2.8 Application to the extension of the derivation of the linear operator associated to the microscopic problem to the multi-dimensional and the vector-valued setting.

In this section we apply the technique of outward growth and their combination to extend one step of the two-scale model derivation of the stationary heat equation. More precisely, we show how to extend the rewriting rule that corresponds to the derivation of the linear operator associated to the microscopic problem in the reference proof to the multi-dimensional and the vector-valued settings as well as their combination. It turns out that such combination is nothing but the derivation of the linear operator associated to the microscopic problem of elasticity.

The derivation of the linear operator associated to the microscopic problem in the reference proof as a FO-rewriting rule.

Let s^{ref} be the FO-rewrite rule used in the reference proof that corresponds to the derivation of the linear operator associated to the microscopic problem. It is defined as follows:

$$s^{ref} := \left(\int \underline{a} \frac{\partial \underline{\mathcal{V}arphi}}{\partial \underline{x}^1} \frac{\partial \underline{w}}{\partial \underline{x}^1} \, d\underline{x}^1 = -\mu \int \underline{a} \frac{\partial \underline{w}}{\partial \underline{x}^1} \, d\underline{x}^1 \right) \rightarrow \left(\frac{\partial \underline{\mathcal{V}arphi}}{\partial \underline{x}^1} = \mu \frac{\partial \underline{\theta}}{\partial \underline{x}^1} \right) \tag{2.21}$$

where

$$\begin{cases} \underline{a} & = \mathtt{Fun}(a, x, known), \\ \underline{\mathcal{V}arphi} & = \mathtt{Fun}(\mathcal{V}arphi, x, unknown), \\ \underline{w} & = \mathtt{Fun}(w, x, test), \\ \underline{x}^1 & = \mathtt{Var}(x^1, \underline{\Omega}), \\ \underline{\Omega} & = \mathtt{Reg}(\Omega, d), \\ \underline{\theta} & = \mathtt{Fun}(\theta, \underline{x}^1, known), \end{cases}$$

and

$$\begin{cases} a, x, \mathcal{V}arphi, w, x^1, \Omega, d, \mu \text{ are FO-variables in } \mathcal{X}^0, \text{ and} \\ \text{"} = \text{"}, \theta, test \ , known \ , unknown \ \text{ are function symbols in } \mathcal{F}^0. \end{cases}$$

Notice that the equality symbol "=" in s^{ref} is considered as a function symbol in $\mathcal{F}^0$ of arity two. However, we write "$t_1 = t_2$" instead of "$= (t_1, t_2)$", where t_1 and t_2 are two terms. The tree structure of the rule s^{ref} is depicted in Figure 2.19, together with the positions $p_1, \ldots, p_{17}$. These positions will be used next to define outward growths.

The derivation of the linear operator associated to the microscopic problem in the multi-dimensional setting as a FO-rewriting.

Let s^{nd} be the FO-rewriting rule that represents the derivation of the linear operator associated to the microscopic problem in the multi-dimensional setting. It is the counterpart of the FO-rewriting rule s^{ref} (defined in Eq. (2.21)) in the multi-dimensional setting. It is defined as follows:

$$s^{nd} := \left(\sum_{\underline{i},\underline{j}} \int \underline{a}_{\underline{i}\underline{j}} \frac{\partial \underline{\underline{\mathcal{V}arphi}}}{\partial \underline{x}^1_{\underline{j}}} \frac{\partial \underline{w}}{\partial \underline{x}^1_{\underline{i}}} \, d\underline{x}^1 = - \sum_{\underline{i},\underline{j}} \underline{\mu}_{\underline{j}} \int \underline{a}_{\underline{i}\underline{j}} \frac{\partial \underline{w}}{\partial \underline{x}^1_{\underline{i}}} \, d\underline{x}^1 \right) \rightarrow \left(\frac{\partial \underline{\underline{\mathcal{V}arphi}}}{\partial \underline{x}^1_{\underline{j}}} = \sum_{\underline{p}} \underline{\mu}_{\underline{p}} \frac{\partial \underline{\theta}_{\underline{p}}}{\partial \underline{x}^1_{\underline{j}}} \right) \tag{2.22}$$

where

$$\begin{cases} \underline{i} & = \texttt{Index}\left(i, \texttt{Set}\left(I, \{1, ..., d\}\right)\right), \\ \underline{j} & = \texttt{Index}\left(j, \texttt{Set}\left(J, \{1, ..., d\}\right)\right), \\ \underline{p} & = \texttt{Index}\left(p, \texttt{Set}\left(P, \{1, ..., d\}\right)\right). \end{cases}$$

The derivation of the linear operator associated to the microscopic problem in the vector-valued setting as a FO-rule.

Let s^{v} be the FO-rewriting rule that represents the the derivation of the linear operator associated to the microscopic problem in the vector-valued setting. It is the counterpart of the FO-rewriting rule s^{ref} of Eq. (2.21) in the multi-valued setting. It is defined as follows:

$$s^{v} := \left(\sum_{\underline{k},\underline{l}} \int \underline{a}_{\underline{k}\underline{l}} \frac{\partial \underline{\mathcal{V}arphi i}_{\underline{l}}}{\partial \underline{x}^1} \frac{\partial \underline{w}_{\underline{k}}}{\partial \underline{x}^1} \, d\underline{x}^1 = - \sum_{\underline{k},\underline{l}} \underline{\mu}_{\underline{l}} \int \underline{a}_{\underline{k}\underline{l}} \frac{\partial \underline{w}_{\underline{k}}}{\partial \underline{x}^1} \, d\underline{x}^1 \right) \rightarrow \left(\frac{\partial \underline{\mathcal{V}arphi i}_{\underline{l}}}{\partial \underline{x}^1} = \sum_{\underline{q}} \underline{\mu}_{\underline{q}} \frac{\partial \underline{\theta}_{\underline{q}\underline{l}}}{\partial \underline{x}^1} \right) \tag{2.23}$$

Extension of the FO-rule (i.e. the derivation of the linear operator) of the reference proof to the multi-dimensional setting by an admissible SO-rule.

We show how to construct the FO-rule r^{nd} needed in the multi-dimensional setting (given in Eq. (2.22)) out of the FO-rule s^{ref} used in the reference proof (given in Eq. (2.21)) by means of an admissible SO-rule. That is, we need to find an admissible SO-rule $\mathcal{S}^{nd}$ such that

$$\mathcal{S}^{nd}(s^{ref}) = s^{nd} \tag{2.24}$$

Let $\mathcal{S}^{nd}$ be the SO-rule:

$$\mathcal{S}^{nd} \;:=\; \ell^{nd} \rightrightarrows r^{nd} \tag{2.25}$$

where

$$\begin{cases} \ell^{nd} & := \left(\int a \frac{\partial \underline{\mathcal{V}arphi}}{\partial x} \frac{\partial \underline{w}}{\partial x}\, dx = -\mu \int a \frac{\partial \underline{w}}{\partial x}\, dx \right) \to \left(\frac{\partial \underline{\mathcal{V}arphi}}{\partial x} = \mu \frac{\partial \underline{\theta}}{\partial x} \right), \\ \text{and} & \\ r^{nd} & := \left(\sum_{\underline{i},\underline{j}} \int a_{\underline{i}\underline{j}} \frac{\partial \underline{\mathcal{V}arphi}}{\partial x_{\underline{j}}} \frac{\partial \underline{w}}{\partial x_{\underline{i}}}\, dx = -\sum_{\underline{i},\underline{j}} \mu_{\underline{j}} \int a_{\underline{i}\underline{j}} \frac{\partial \underline{w}}{\partial x_{\underline{j}}}\, dx \right) \to \left(\frac{\partial \underline{\mathcal{V}arphi}}{\partial x_{\underline{j}}} = \sum_{\underline{p}} \mu_{\underline{p}} \frac{\partial \underline{\theta}}{\partial x_{\underline{j}}} \right), \end{cases}$$

and

$$\begin{cases} \underline{\mathcal{V}arphi} & = \mathtt{Fun}(\mathcal{V}arphi, y), \\ \underline{w} & = \mathtt{Fun}(w, y), \\ \underline{\theta} & = \mathtt{Fun}(\theta, x), \end{cases} \qquad \text{and} \qquad \begin{cases} \underline{i} & = \mathtt{Var}(i, \underline{I}), \\ \underline{j} & = \mathtt{Var}(j, \underline{I}), \\ \underline{p} & = \mathtt{Var}(p, \underline{I}), \\ \underline{I} & = \mathtt{Reg}(I, d), \end{cases}$$

and

$$\begin{cases} a, \mathcal{V}arphi, y, w, \mu, \theta \text{ are SO-variables in } \mathcal{X}^1, \text{ and} \\ i, j, d \text{ are FO-variables in } \mathcal{X}^0, \text{ and} \\ p, I \text{ are constant symbols in } \mathcal{F}^0. \end{cases}$$

The following claims can be easily checked:

i.) The SO-rule $\mathcal{S}^{nd}$ (defined in Eq. (2.25)) is parametrized in the sense of Definition 56 since

$$\begin{aligned} \mathcal{V}ar^0(\mathcal{S}^{nd}) &\overset{def}{=} \mathcal{V}ar^0(r^{nd}) \setminus \mathcal{V}ar^0(\ell^{nd}) \\ &= \{i, j, d\} \neq \emptyset. \end{aligned}$$

ii.) The SO-rule $\mathcal{S}_0^{nd}$ defined by

$$\mathcal{S}_0^{nd} = \sigma_0^{nd}(\mathcal{S}^{nd}), \quad \text{where} \quad \sigma_0^{nd} = \{d \to 1\}$$

is a semantic conservation.

iii.) Therefore, $\mathcal{S}^{nd}$ is admissible w.r.t $\mathcal{S}_0^{nd}$.

iv.) The FO-rule s^{nd} is a generalization of the FO-rule s^{ref} (in the sense of Definition 64) since $\mathcal{S}^{nd}$ is admissible and $\mathcal{S}^{nd}(s^{ref}) = s^{nd}$.

Extension of the FO-rule (i.e. the derivation of the linear operator) of the reference proof to the multi-dimensional setting by outward growths.

Now we construct an outward growth $\mathcal{G}^{nd}$ which have the same effect of the SO-rule $\mathcal{S}^{nd}$ (given in E.q (2.25)). In other words, we show how to construct the rule s^{nd} of the multi-dimensional setting (given in Eq. (2.22)) out of the rule s^{ref} of the reference model (given in Eq. (2.21)) by means of an outward growth. That is, we need to construct an outward growth $\mathcal{G}^{nd}$ such that

$$\mathcal{G}^{nd}(s^{ref}) = s^{nd} \tag{2.26}$$

The outward growth $\mathcal{G}^{nd}$ can be constructed as a combination of unit outward growth by comparing the FO-rules s^{ref} and s^{nd}. That is, this comparison allows one to enumerate the set of added terms needed in the construction of the unit outward growths. Let $\tau^i, \tau^i, \tau^p, \tau^i_s, \tau^j_s$ and τ^p_s be the added terms defined as follows:

$$\begin{cases} \tau^i & = \texttt{Indexed}(\bot, \underline{i}) \\ \tau^j & = \texttt{Indexed}(\bot, \underline{j}) \\ \tau^p & = \texttt{Indexed}(\bot, \underline{p}) \\ \tau^i_s & = \sum(\bot, \underline{i}) \\ \tau^j_s & = \sum(\bot, \underline{j}) \\ \tau^p_s & = \sum(\bot, \underline{p}) \end{cases}$$

Let $\mathcal{G}^i, \mathcal{G}^j, \mathcal{G}^p$ and $\mathcal{G}^s$ be the outward growths defined as follows:

$$\begin{aligned}\mathcal{G}^i &\stackrel{def}{=} \mathcal{G}_{\tau^i,p_6} \Diamond \mathcal{G}_{\tau^i,p_{11}} \\ &= \mathcal{G}_{(\tau^i,\tau^i),(p_6,p_{11})} && \text{(Definition 85)}\end{aligned}$$

and

$$\begin{aligned}\mathcal{G}^j &\stackrel{def}{=} \mathcal{G}_{\tau^j,p_4} \Diamond \mathcal{G}_{\tau^j,p_8} \Diamond \mathcal{G}_{\tau^j,p_{13}} \Diamond \mathcal{G}_{\tau^j,p_{17}} \\ &= \mathcal{G}_{(\tau^j,\tau^j,\tau^j,\tau^j),(p_4,p_8,p_{13},p_{17})} && \text{(Definition 85)}\end{aligned}$$

and

$$\begin{aligned}\mathcal{G}^p &\stackrel{def}{=} \mathcal{G}_{\tau^p,p_{15}} \Diamond \mathcal{G}_{\tau^p,p_{17}} \\ &= \mathcal{G}_{(\tau^p,\tau^p),(p_6,p_{11})} && \text{(Definition 85)}\end{aligned}$$

and

$$\mathcal{G}^s \stackrel{def}{=} \mathcal{G}_{\tau^s,p_{14}}$$

Finally we are ready to define the outward growth $\mathcal{G}^{nd}$:

$$\mathcal{G}^{nd} \stackrel{def}{=} \mathcal{G}^i \Diamond \mathcal{G}^j \Diamond \mathcal{G}^p \Diamond \mathcal{G}^s. \tag{2.27}$$

Extension of the FO-rule (i.e. the derivation of the linear operator) of the reference model to the vector-valued setting by an admissible rule.

We show how to construct the FO-rule r^v (given in Eq. (2.23)) needed in the vector-valued setting out of the FO-rule s^{ref} (given in Eq. (2.21)) used in the reference proof by means of an admissible SO-rule. That is, we need to find an admissible SO-rule $\mathcal{S}^v$ such that

$$\mathcal{S}^v(s^{ref}) = s^v \tag{2.28}$$

Let $\mathcal{S}^v$ be the SO-rewrite rule:

$$\mathcal{S}^v := \quad \ell^v \rightrightarrows r^v \tag{2.29}$$

where

$$\ell^v := \int a \frac{\partial \underline{\mathcal{V}arphi}}{\partial x} \frac{\partial \underline{w}}{\partial x}\, dx = -\mu \int a \frac{\partial \underline{w}}{\partial x}\, dx \to \frac{\partial \underline{\mathcal{V}arphi}}{\partial x} = \mu \frac{\partial \underline{\theta}}{\partial x}$$

and

$$r^v := \sum_{\underline{k},\underline{l}} \int a_{\underline{k}\underline{l}} \frac{\partial \underline{\mathcal{V}arphi_l}}{\partial x} \frac{\partial \underline{w_k}}{\partial x}\, dx = -\sum_{\underline{k},\underline{l}} \mu_{\underline{l}} \int a_{\underline{k}\underline{l}} \frac{\partial \underline{w_k}}{\partial x}\, dx \to \frac{\partial \underline{\mathcal{V}arphi_l}}{\partial x} = \sum_{\underline{q}} \mu_{\underline{q}} \frac{\partial \underline{\theta_{ql}}}{\partial x}$$

where

$$\begin{cases} \underline{k} & = \texttt{Var}(k, \underline{I}), \\ \underline{l} & = \texttt{Var}(l, \underline{I}), \\ \underline{q} & = \texttt{Var}(q, \underline{I}), \\ \underline{I} & = \texttt{Reg}(I, d_v), \\ \underline{\mathcal{V}arphi} & = \texttt{Fun}(\mathcal{V}arphi, y, unknown), \\ \underline{w} & = \texttt{Fun}(w, y, test), \\ \underline{\theta} & = \texttt{Fun}(\theta, x, known), \end{cases}$$

and

$$\begin{cases} a, \mathcal{V}arphi, y, x, w, \mu \in \mathcal{X}^1, \\ k, l, d_v \in \mathcal{X}^0, \text{ and} \\ I, q \in \mathcal{F}^0 \end{cases}$$

By substitution $\sigma_0^v = \{d_v \to 1\}$, we get $S_0^v = \sigma_0^v(S^v)$ which a semantic conservation SO-rule for s^{ref} and S^v is admissible for S_0^v.

The following claims can be easily checked:

i.) The SO-rule $\mathcal{S}^v$ (defined in Eq. (2.29)) is parametrized in the sense of Definition 56 since

$$\begin{aligned} \mathcal{V}ar^0(\mathcal{S}^v) &\overset{def}{=} \mathcal{V}ar^0(r^v) \setminus \mathcal{V}ar^0(\ell^v) \\ &= \{k, l, d_v\} \neq \emptyset. \end{aligned}$$

ii.) The SO-rule $\mathcal{S}_0^v$ defined by

$$\mathcal{S}_0^v = \sigma_0^v(\mathcal{S}^v), \quad \text{where} \quad \sigma_0^v = \{d_v \to 1\}$$

is a semantic conservation.

iii.) Therefore, $\mathcal{S}^v$ is admissible w.r.t $\mathcal{S}_0^v$.

iv.) The FO-rule s^v is a generalization of the FO-rule s^{ref} (in the sense of Definition 64) since $\mathcal{S}^v$ is admissible and $\mathcal{S}^v(s^{ref}) = s^v$.

Extension of the FO-rule (i.e. the derivation of the linear operator) of the reference proof to the vector-valued setting by SO-outward growths.

Now we construct an outward growth $\mathcal{G}^v$ which have the same effect of the SO-rule

$\mathcal{S}^v$ (given in E.q (2.29)). In other words, we show how to construct the rule s^{nd} of multi-dimensional setting (given in Eq. (2.22)) out of the rule s^{ref} of the reference model (given in Eq. (2.21)) by means of an outward growth. That is, we need to construct an outward growth $\mathcal{G}^v$ such that

$$\mathcal{G}^v(s^{ref}) = s^v \tag{2.30}$$

Again, the outward growth $\mathcal{G}^v$ can be constructed as a combination of unit outward growths. We need to enumerate the set of added terms needed in the construction of these unit outward growths. Let $\tau^k, \tau^l, \tau^q, \tau^k_s, \tau^l_s$ and τ^q_s be the added terms defined as follows:

$$\begin{cases} \tau^k & = \texttt{Indexed}(\bot, \underline{k}) \\ \tau^l & = \texttt{Indexed}(\bot, \underline{l}) \\ \tau^q & = \texttt{Indexed}(\bot, \underline{q}) \\ \tau^k_s & = \sum(\bot, \underline{k}) \\ \tau^l_s & = \sum(\bot, \underline{l}) \\ \tau^q_s & = \sum(\bot, \underline{q}) \end{cases}$$

Let $\mathcal{G}^k, \mathcal{G}^l, \mathcal{G}^q$ and $\mathcal{G}^s$ be the outward growths defined as follows:

$$\begin{aligned} \mathcal{G}^k &\stackrel{def}{=} \mathcal{G}_{\tau^k,p_2} \Diamond \mathcal{G}_{\tau^k,p_9} \Diamond \mathcal{G}_{\tau^k,p_5} \Diamond \mathcal{G}_{\tau^k,p_{10}} \\ &= \mathcal{G}_{(\tau^k,\tau^k,\tau^k,\tau^k),(p_2,p_9,p_5,p_{10})} && \text{(Definition 85)} \end{aligned}$$

and

$$\begin{aligned} \mathcal{G}^l &\stackrel{def}{=} \mathcal{G}_{\tau^l,p_2} \Diamond \mathcal{G}_{\tau^l,p_9} \Diamond \mathcal{G}_{\tau^l,p_3} \Diamond \mathcal{G}_{\tau^l,p_8} \Diamond \mathcal{G}_{\tau^l,p_{12}} \Diamond \mathcal{G}_{\tau^l,p_{16}} \\ &= \mathcal{G}_{(\tau^l,\tau^l,\tau^l,\tau^l,\tau^l,\tau^l),(p_2,p_9,p_3,p_8,p_{12},p_{16})} && \text{(Definition 85)} \end{aligned}$$

and

$$\begin{aligned} \mathcal{G}^q &\stackrel{def}{=} \mathcal{G}_{\tau^q,p_{15}} \Diamond \mathcal{G}_{\tau^q,p_{16}} \\ &= \mathcal{G}_{(\tau^q,\tau^q),(p_{15},p_{16})} && \text{(Definition 85)} \end{aligned}$$

and

$$\mathcal{G}^s \stackrel{def}{=} \mathcal{G}_{(\tau^k_s,\tau^k_s),(p_1,p_7)} \Diamond \mathcal{G}_{(\tau^l_s,\tau^l_s),(p_1,p_7)} \Diamond \mathcal{G}_{\tau^q_s,p_{14}}$$

Finally we are ready to define the outward growth $\mathcal{G}^v$:

$$\mathcal{G}^v \stackrel{def}{=} \mathcal{G}^k \Diamond \mathcal{G}^l \Diamond \mathcal{G}^q \Diamond \mathcal{G}^s. \tag{2.31}$$

Extension of the FO-rule (i.e. the derivation of the linear operator) of the reference proof to the elasticity setting.

Thanks to the two outward growths $\mathcal{G}^{nd}$ and $\mathcal{G}^v$, defined respectively in Eq. (2.27) and Eq. (2.31), we are able to construct the FO-rewriting rule that corresponds

to the derivation of the linear operator associated to the microscopic problem of elasticity. That is, we able to construct the counterpart of the FO-rule s^{ref}, defined in Eq. (2.21), for the elasticity setting. Consider the outward growth $\mathcal{G}^{el}$:

$$\mathcal{G}^{el} \stackrel{def}{=} \mathcal{G}^{nd} \Diamond \mathcal{G}^{v} \tag{2.32}$$

The application of $\mathcal{G}^{el}$ to s^{ref} yields the FO-rule:

$$\mathcal{G}^{el}(s^{ref}) = \left(\sum_{\underline{k,l,i,j}} \int \underline{a_{ijkl}} \frac{\partial \underline{\mathcal{V}arphi_l}}{\partial \underline{x_j}^1} \frac{\partial \underline{w_k}}{\partial \underline{x_i}^1} \, d\underline{x}^1 = - \sum_{\underline{k,l,i,j}} \underline{\mu_{jl}} \int \underline{a_{ijkl}} \frac{\partial \underline{w_k}}{\partial \underline{x_i}^1} \, d\underline{x}^1 \right)$$

$$\rightarrow \left(\frac{\partial \underline{\mathcal{V}arphi_l}}{\partial \underline{x_j}^1} = \sum_{\underline{q,p}} \underline{\mu_{qp}} \frac{\partial \underline{\theta_{lqp}}}{\partial \underline{x_j}^1}. \right)$$

Example 109 *Let s, s', s'' and s''' be the FO-strategies:*

$$s := \underline{u} \rightarrow \frac{d\underline{u}}{d\underline{x}}$$

$$s' := \underline{u_i} \rightarrow \frac{d\underline{u_i}}{d\underline{x}}$$

$$s'' := \underline{u^d} \rightarrow \frac{\partial \underline{u^d}}{\partial \underline{x^d}_j}$$

$$s''' := \underline{u^d}_i \rightarrow \frac{\partial \underline{u^d}_i}{\partial \underline{x^d}_j}$$

where the underlined shortcut terms have been introduced in (2.12), we reproduce them next:

$$\begin{aligned}
\underline{i} &= \texttt{Index}\left(i, \texttt{Set}\left(I, \{1, ..., d_i\}\right)\right) \\
\underline{j} &= \texttt{Index}\left(j, \texttt{Set}\left(J, \{1, ..., d_j\}\right)\right) \\
\underline{x} &= \texttt{Var}\left(x, \texttt{Reg}\left(\Omega, 1\right)\right) \\
\underline{u} &= \texttt{Fun}\left(u, \underline{x}\right) \\
\underline{x}^d &= \texttt{Var}\left(x^d, \texttt{Reg}\left(\Omega, d_j\right)\right) \\
\underline{u}^d &= \texttt{Fun}\left(u, \underline{x}^d\right).
\end{aligned}$$

Therefore the strategy s, s', s'' and s''' can be explicitly rewritten as follows:

$$s := \underline{u} \rightarrow \texttt{Oper}\left(\texttt{Deriv}, \underline{u}, \underline{x}, \emptyset\right)$$

$$s' := \texttt{Indexed}\left(\underline{u}, \underline{i}\right) \rightarrow \texttt{Oper}\left(\texttt{Deriv}, \texttt{Indexed}\left(\underline{u}, \underline{i}\right), \underline{x}, \emptyset\right)$$

$$s'' := \underline{u}^d \rightarrow \texttt{Oper}\left(\texttt{Deriv}, \underline{u}^d, \texttt{Indexed}\left(\texttt{Var}\left(x, \texttt{Reg}\left(\Omega, d\right)\right), \underline{j}\right), \emptyset\right)$$

$$s''' := \texttt{Indexed}\left(\underline{u}^d, \underline{i}\right) \rightarrow \texttt{Oper}\left(\texttt{Deriv}, \texttt{Indexed}\left(\underline{u}^d, \underline{i}\right), \texttt{Indexed}\left(\texttt{Var}\left(x, \texttt{Reg}\left(\Omega, d\right)\right), \underline{j}\right), \emptyset\right)$$

where $k, d \in \mathcal{X}^0$. The tree structure of the strategies s, s', s'' and s''' is depicted in Figures 2.20, 2.21, 2.22 and 2.23.

In fact, the strategy s corresponds to the derivative of a scalar function defined on one dimensional domain Ω, the application of s yields a scalar. The strategy s' corresponds to the derivative of a vector function defined on one dimensional domain Ω, the result of the applicatuib of s is a vector. The strategy s'' corresponds to the derivative of a scalar function defined on muti-dimensional domain Ω, the result is a vector. Finally, the strategy s''' corresponds to the derivative of a vector function defined on muti-dimensional domain Ω, the result of the application of s''' is a matrix.

Give the -strategies S, S', S'' such that $S(s) = s'$, $S'(s) = s''$ and $S''(s) = s'''$, in grammar form

$$S : \underline{u} \to \mathtt{Oper}\left(\mathtt{Deriv}, \underline{u}, \underline{x}, \emptyset\right) \rightrightarrows \mathtt{Indexed}\left(\underline{u}, \underline{i}\right) \to \mathtt{Oper}\left(\mathtt{Deriv}, \mathtt{Indexed}\left(\underline{u}, \underline{i}\right), \underline{x}, \emptyset\right)$$

in which $y, v \in \mathcal{X}^1$, the needed unit outward growth $\tau = \mathtt{Indexed}(\bot, k)$ which will apply to position p_{12} on the left hand-side and position p_{133} on the right hand-side of strategy s.

$$\begin{aligned} S(s) &= s\left[\tau\left[s|_{p_{12}}\right]_q\right]_{p_{12}} \to s\left[\tau\left[s|_{p_{132}}\right]_q\right]_{p_{132}} \\ &= \mathcal{G}_{\tau,(p_{12},p_{132})}(s) \end{aligned}$$

$$\begin{aligned} &S' : \mathtt{Fun}\left(u, \mathtt{Var}\left(x, \mathtt{Reg}\left(\Omega, 1\right)\right)\right) \\ &\to \mathtt{Oper}\left(\mathtt{Deriv}, \mathtt{Fun}\left(u, \mathtt{Var}\left(x, \mathtt{Reg}\left(\Omega, 1\right)\right)\right), \mathtt{Var}\left(x, \mathtt{Reg}\left(\Omega, 1\right)\right), \emptyset\right) \\ &\rightrightarrows \\ &\underline{u}^d \to \mathtt{Oper}\left(\mathtt{Deriv}, \underline{u}^d, \mathtt{Indexed}\left(\mathtt{Var}\left(x, \mathtt{Reg}\left(\Omega, d\right)\right), \underline{j}\right), \emptyset\right) \end{aligned}$$

a subsitution σ' that can change 1 into d at positions p_{12222} on the left hand-side and p_{13222}, p_{13322} on the right hand-side of strategy s (need a grammar for it ???), a unit outward growth $\tau'_1 = \mathtt{Indexed}\left(\bot, \underline{j}\right)$ applies to postions p_{133} on the right hand-side of strategy s.

$$S'(s) = \mathcal{G}_{\sigma',(p_{12222},p_{13222},p_{13322})}; \mathcal{G}_{\tau'_1,p_{133}}(s)$$

S'' can be written as a combination of S and S'

$$\begin{aligned} S''(s) &= \mathcal{G}_{\sigma',(p_{12222},p_{13222},p_{13322})}; \mathcal{G}_{\tau'_1,p_{133}}; \mathcal{G}_{\tau,(p_{12},p_{132})}(s) \\ &= S'; S(s) \end{aligned}$$

2.9 Perspectives

We end up this Chapter with some perspectives and concluding remarks.

2.9.1 Extention mechanisms as strategies: outerward growth, parametrization and generalization as strategies

In section 2.5 (resp. section 2.7), the outward growths (resp. parameterizations and generalization) by means of static positions. That is, one needs to specify the exact positions on which the outward growths and the parameterizations are applied. Despite the fact that this formulation in terms of positions is useful to understand many issues related to the composition and the combination of the outward growths and parameterizations, it has clear drawbacks. Basically, it is not practical since one has to enumerate the set of all positions on which he would like to apply the extension. We illustrate another approach that consists in the formulation of the outward growths and parametrizations in terms of strategies.

More precisely, instead of providing the set of positions on with the outward growth has to be applied, we provide a *pattern* on which the outward growth has to be applied. Then, an adequate traversal strategies, namely the `InnerMost` strategy, is used to explore the term and search for the pattern. However, the formulation of the combination of outward growths and parameterizations in terms of strategies remains an open problem. It turns out that these two formulations are not equivalent in general, but it is possible to establish some conditions under which the two formulations are equivalent. In what follows, u and τ are FO-terms, and x is a FO-variable. The outward growth (resp. parametrization) formulated in terms of a strategy will be denoted by $\mathcal{G}_{\tau,u}$ (resp. $\mathcal{P}_{x,u}$) in order to distinguish them from the usual outward growth $\mathcal{G}_{\tau,p}$ (resp. parametrization $\mathcal{P}_{x,p}$). We shall call them pattern outward growth and pattern parametrization, or P-outward growth and P-parametrization for short.

$$\widehat{\mathcal{G}}_{\tau,u} \stackrel{def}{=} u \to \big(\texttt{let}(\bot := u)\ \texttt{in}\ \tau\big) \qquad \text{(P-Outward Growth at the root)}$$

$$\mathcal{G}_{\tau,u} \stackrel{def}{=} \texttt{InnerMost}(\widehat{\mathcal{G}}_{u,\tau}) \qquad \text{(P-Outward Growth at the inner most positions)}$$

$$\mathcal{G}^{\star}_{\tau,u} \stackrel{def}{=} \texttt{BottomUp}(\widehat{\mathcal{G}}_{\tau,u}) \qquad \text{("Vectorial" P-Outward Growth from the bottom)}$$

$$\widehat{\mathcal{P}}_{x,u} \stackrel{def}{=} u \to x \qquad \text{(Parametrization at the root)}$$

$$\mathcal{P}_{x,u} \stackrel{def}{=} \texttt{InnerMost}(\widehat{\mathcal{P}}_{x,u}) \qquad \text{(P-Parametrization)}$$

2.9.2 Second-order pattern matching modulo alpha-conversion and second-order unification

In Definition 54, Section 2.3, our SO-pattern matching is not done modulo α-conversion of the FO-order variables. That is, the SO-pattern matching algorithm considers the FO-variables as constants, while it would be convenient to rename them. Let us illustrate this idea through an example. Let S be the SO-rule:

$$S := (f(x) \to f(x)) \rightrightarrows (f(x) \to f(x)),$$

where x is a FO-variable. Let s be the FO-rule:

$$s := f(y) \to f(y),$$

where y is a FO-variable. According to our definition 54, the application $S(s)$ fails because $f(y) \to f(y)$ does not match $f(x) \to f(x)$ since x and y are considered as constants. However, this is a severe limitation since, morally, the SO-rule S tends to transform a FO-rule $f(x) \to f(x)$ to $g(x) \to g(x)$ *for any FO-variable* x. Therefore, the SO-pattern matching algorithm has to α-convert the FO-variables if necessary, e.g. by renaming y by x in s. Another problem is that we need to give syntactic conditions so that the SO-unification modulo α-conversion is decidable, see e.g. [19]. This is necessary for the computability of the operation of combination of SO-outward growths given in Definition 93.

2.10 Appendix

2.10.1 Proofs of Section 2.2

Proposition 110 *Let s, t, r be terms and p, q be strings. The following hold.*

1. *If $pq \in \mathcal{P}os(s)$, then $s|_{pq} = (s|_p)|_q$.*
2. *If $p \in \mathcal{P}os(s)$ and $q \in \mathcal{P}os(t)$, then*

$$\begin{aligned} \left(s[t]_p\right)|_{pq} &= t|_q, \\ \left(s[t]_p\right)[r]_{pq} &= s\left[t[r]_q\right]_p. \end{aligned}$$

3. *If $pq \in \mathcal{P}os(s)$, then*

$$\begin{aligned} \left(s[t]_{pq}\right)|_p &= (s|_p)[t]_q, \\ \left(s[t]_{pq}\right)[r]_p &= s[r]_p. \end{aligned}$$

4. If p and q are parallel positions in s (i.e. $p \parallel q$), then

$$\begin{aligned}\left(s\left[t\right]_p\right)|_q &= s|_q,\\ \left(s\left[t\right]_p\right)\left[r\right]_q &= \left(s\left[r\right]_q\right)\left[t\right]_p.\end{aligned}$$

Proof. A detailed proof can be found in [4], page 37 and 38. We reproduce here the main arguments. In order to prove (1), we assume that $p = i_1...i_n$,then $s|_{pq} = s|_{i_1...i_nq} = f\left(s_1,...,s_{n_1}\right)|_{i_1...i_nq} = s_{i_1}|_{i_2...i_nq} = f\left(s_{i_11},...,s_{i_1n_2}\right)|_{i_2...i_nq} = ... = s_{i_1...i_n}|_q = s_p|_q = \left(s|_p\right)|_q$. In order to prove $(2a)$,we know that $pq \in \mathcal{P}os\left(s\left[t\right]_p\right)$, apply (1), we have $\left(s\left[t\right]_p\right)|_{pq} = \left(\left(s\left[t\right]_p\right)|_p\right)|_q = t|_q$. In order to prove $(2b)$, we denote $s^l = \left(s\left[t\right]_p\right)\left[r\right]_{pq}$ and $s^r = s\left[t\left[r\right]_q\right]_p$. From $(1)\,(2a)$, $s^l|_{pq} = s^r|_{pq} = r$. Therefore, we need to compare the structures of s^r and s^l except positon pq, the position of r. Since the remain structures of both s^r, s^l are built from s and t by changing $s|_p$ by t, we have $s^l = s^r$. In order to prove $(3a)$, we denote $s^l = \left(s\left[t\right]_{pq}\right)|_p, s^r = \left(s|_p\right)\left[t\right]_q, s^0 = s\left[t\right]_{pq}$, we have $s^l = s^0|_p = s^0_p$. Since $s^0 = f\left(s_1,...,s_{i_1}\left[t\right]_{p'q},...,s_{n_1}\right)$, we have $s^0_{i_1} = s^0|_{i_1} = s_{i_1}\left[t\right]_{p'q}$. Since $s_{i_1}\left[t\right]_{p'q} = f\left(s_{i_11},...,s_{i_1i_2}\left[t\right]_{p''q},...,s_{i_1n}\right)$, we have $s^0_{i_1i_2} = s^0_{i_1}|_{i_2} = s_{i_1i_2}\left[t\right]_{p''q}$. Continue the same step, we have $s^0_p = s_p\left[t\right]_q = \left(s|_p\right)_q = s^r$. This result leads to if we change the subterm $s^0|_p$ actually we will chang the term $\left(s|_p\right)\left[t\right]_q$ which includes t, so that the remain structure of s^0 keeps the same structure of s except position p. Now we will prove $(4a)$, since p and q are parallel positions in term s, i.e. $p \parallel q$ or there is no k such that $pk = q$ or $qk = p$, we denote $s^l = \left(s\left[t\right]_p\right)|_q, s^r = s|_q$ and $s^0 = s\left[t\right]_p$. We have $\forall \alpha \in \mathcal{P}os\left(s\right) \setminus \left\{pj \mid j \in \mathcal{P}os\left(s|_p\right)\right\} : s^0|_\alpha = s|_\alpha$ and from assumption $q \notin \left\{pj \mid j \in \mathcal{P}os\left(s|_p\right)\right\}$, so that $s_0|_q = s|_q$ or $s_l = s_r$. This result leads to the fact that p and q are not in the same branch, so that we can replace $s|_p$ or $s|_q$ first without changing the another position, which leads to the property $(4b)$. ■

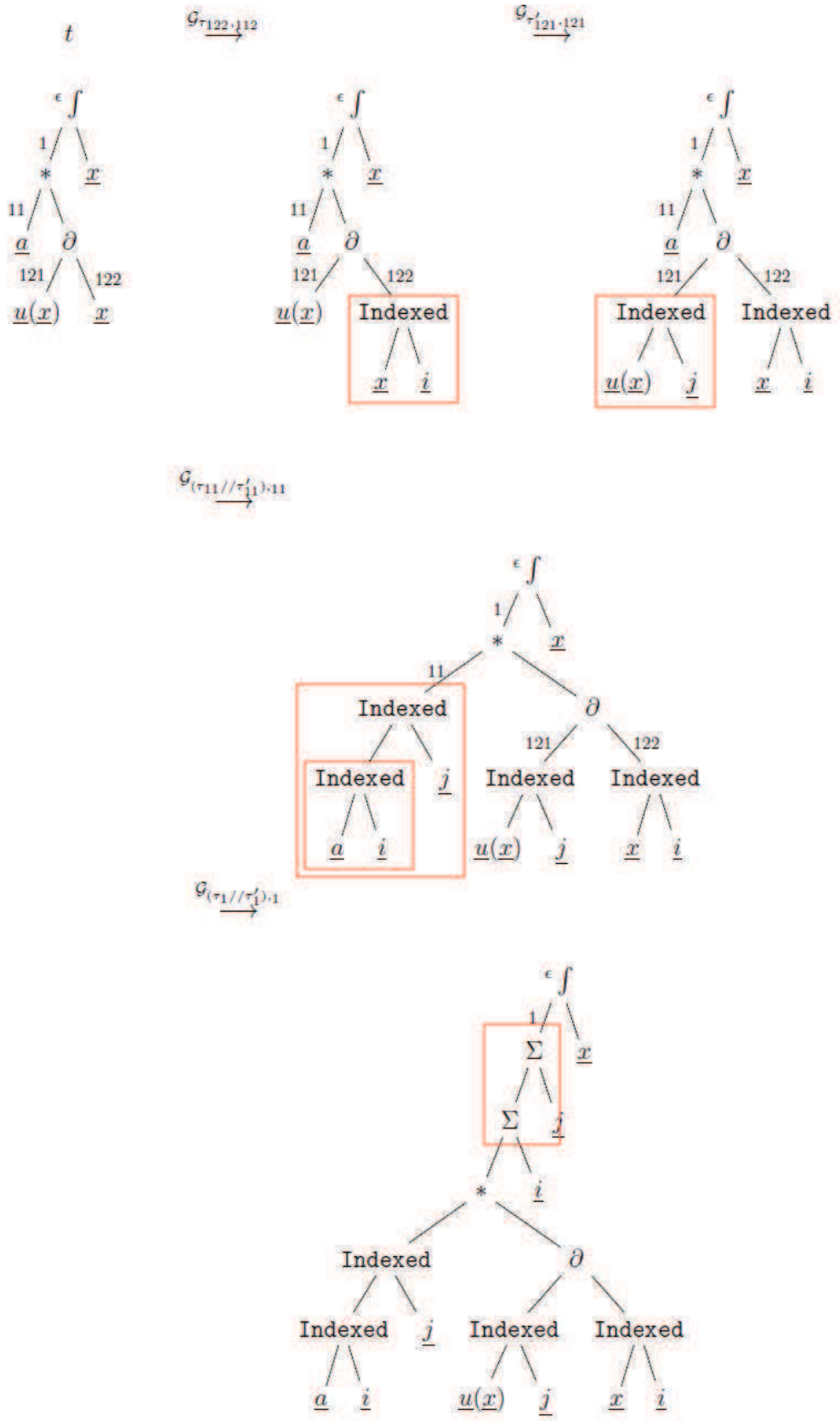


Figure 2.11: Application of a combination of outward growths to the term t.

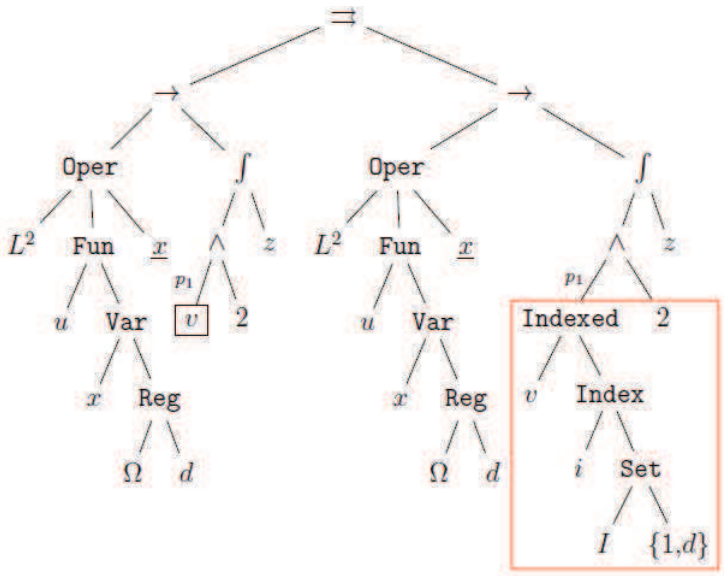


Figure 2.12: The SO-unit outward growth $\mathcal{G}^{l_1}_{\tau_1,p_1}$ defined in Eq. (2.19).

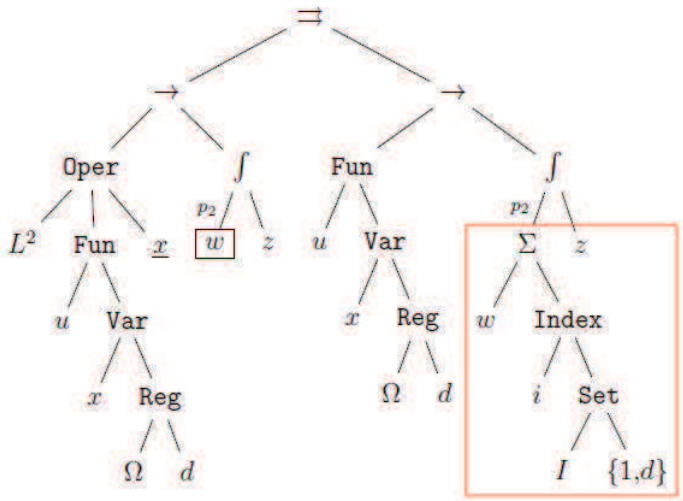


Figure 2.13: The SO-unit outward growth $\mathcal{G}^{l_2}_{\tau_2,p_2}$ defined in Eq. (2.20).

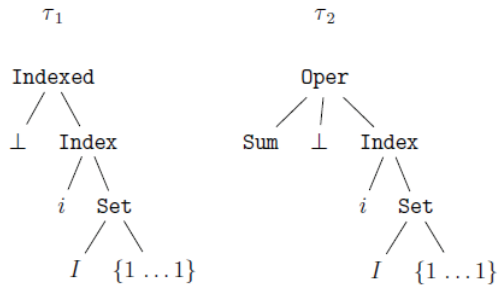


Figure 2.14: The tree structure of the added terms τ_1 and τ_2.

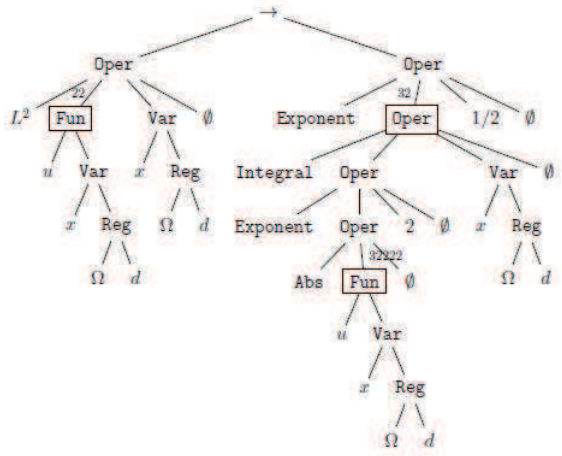


Figure 2.15: The tree structure of the FO-rule $s = L^2\left(\underline{u}\left(\underline{x}\right)\right) \rightarrow \left(\int_{\underline{\Omega}} |\underline{u}\left(\underline{x}\right)|^2 d\underline{x}\right)^{1/2}$.

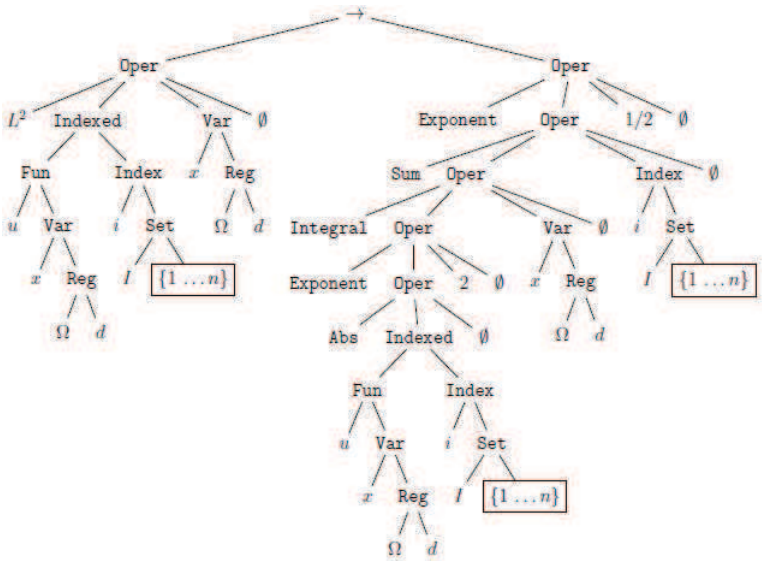


Figure 2.16: The tree structure of the FO-rule s'.

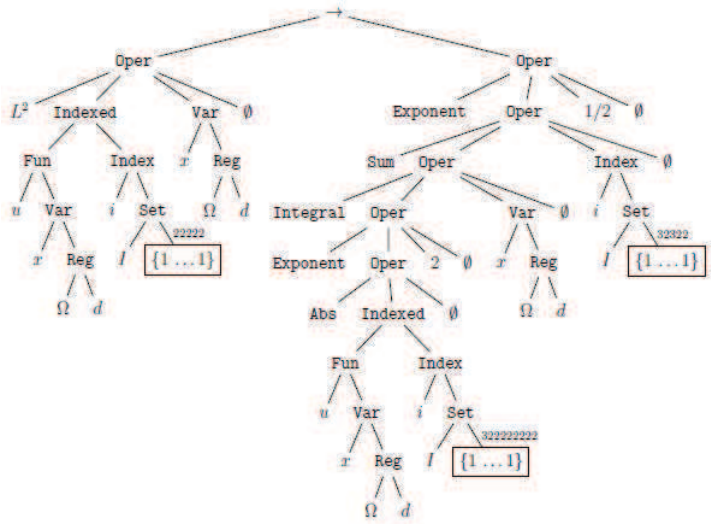


Figure 2.17: The tree structure of FO-rule $s_0 = \mathcal{G}_{\vec{\tau},\vec{p}}(s)$.

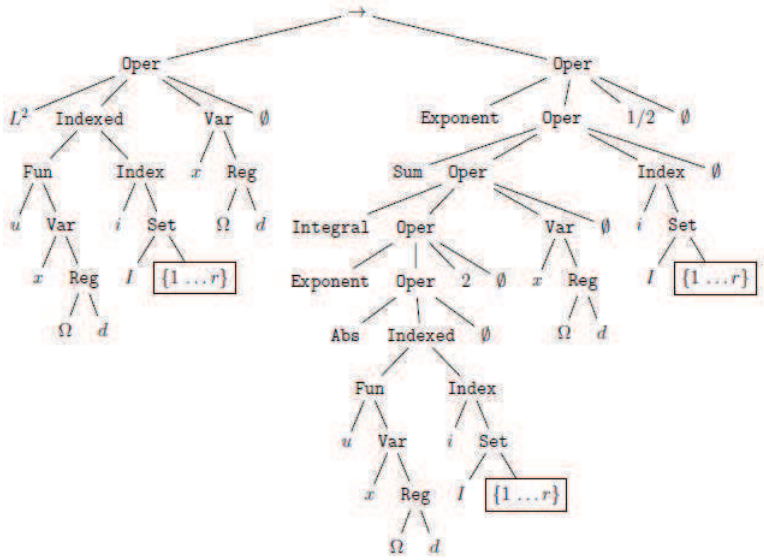


Figure 2.18: The tree structure of the FO-rule $s_1 = (\mathcal{G}_{\vec{r},\vec{p}}; \mathcal{P})(s) = \mathcal{P}(s_0)$.

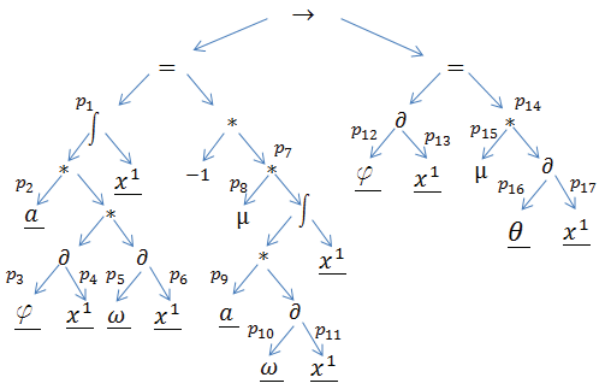


Figure 2.19: The tree structure of the FO-rewrite rule s^{ref} defined in Eq. (2.21).

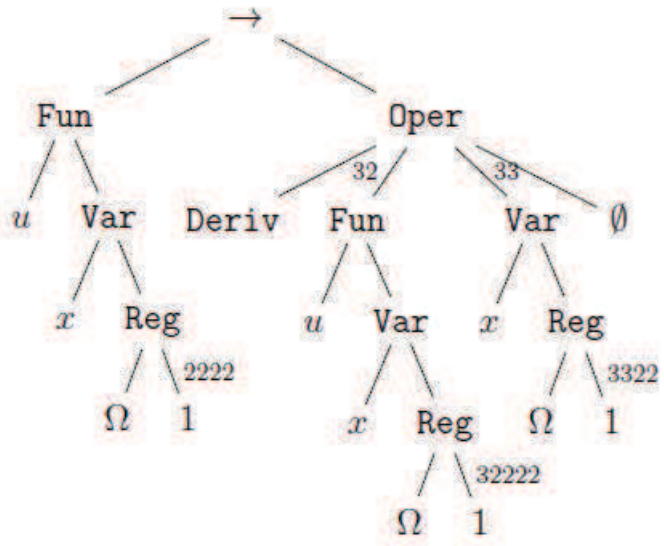


Figure 2.20: The FO-strategy $s := \underline{u} \to \frac{d\underline{u}}{d\underline{x}}$.

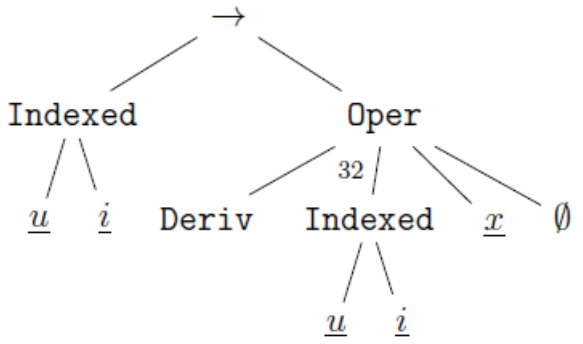


Figure 2.21: The FO-strategy $s' := \underline{u_i} \to \frac{d\underline{u_i}}{d\underline{x}}$.

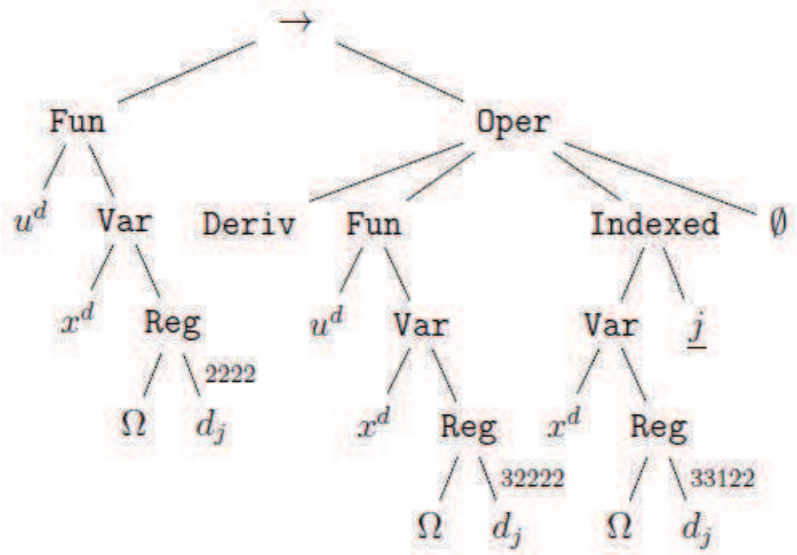


Figure 2.22: The FO-strategy $s'' := \underline{u^d} \to \frac{\partial \underline{u^d}}{\partial \underline{x^d_j}}$.

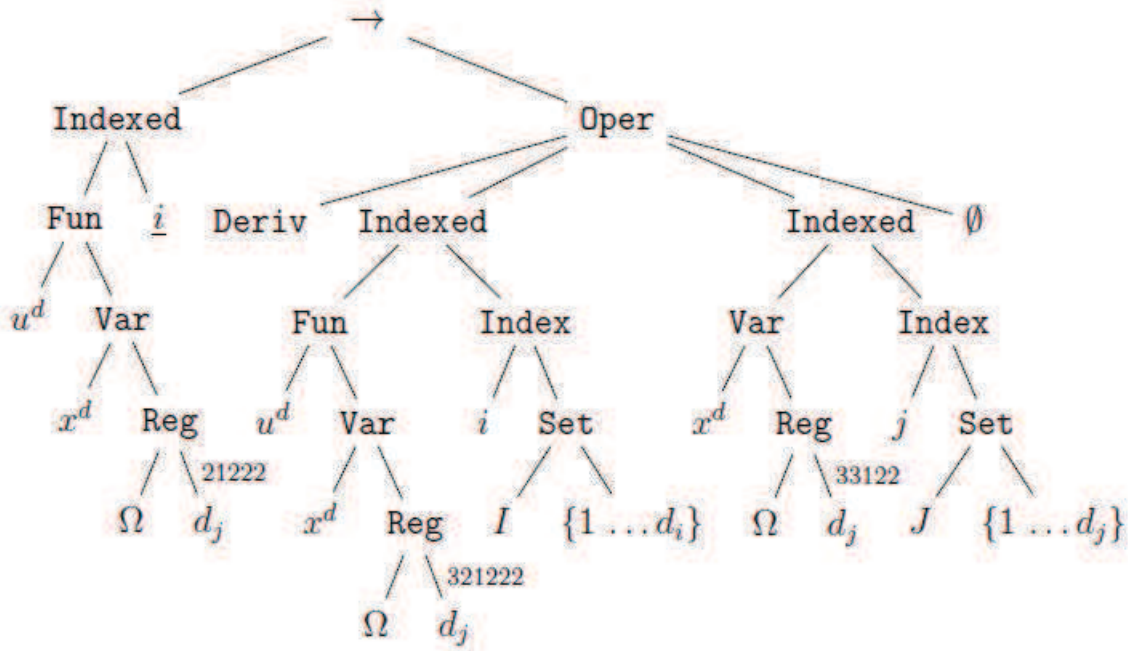


Figure 2.23: The FO-strategy $s''' := \underline{u^d_i} \to \frac{\partial \underline{u^d_i}}{\partial \underline{x^d_j}}$.

Chapter 3

A two-scale model derivation for a SThM probe

Abstract. *In this chapter we state the two-scale model derivation for an SThM probe developed in the NANOHEAT project. In the derivation, the mathematic approach proposed in 1 is followed. In the new proof, the features (i) the multi-dimensional domain, (ii) thin domain, (iii) sub-domains with different physics, (iv) vector solution and (v) multi-physics are taken into account. By taking into account these new features, mathematical rules used in the reference proof in 1 are extended and new steps are added. Then follow the same framework, the homogenized model for the Joule-heating thermoelasticity is derived.*

3.1 Introduction

This chapter is devoted to derive a two-scale model for an SThM probe developed in the NANOHEAT project. The derivation is presented in the perspective of its use to enrich extensions of the reference proof introduced in Chapter 1. The features to be taken into account are: (i) the multi-dimensional domain of $\mathbb{R}^3$, (ii) thin domain, (iii) sub-domains with different physics, (iv) vector solution, (v) multi-physics ie the coupling between thermal effects, elasticity deformations and the electric current flowing in the conductive parts. Other features are also taken into account but they are due to technical reason and will appear later. To put this model in our framework, we consider, in addition to the thinness of the domain, that the coefficients are periodic and get an homogenized model in a thin structure as in [18] [21] and [22]. We notice that one of the differences with the latter references is that the asymptotic behavior regarding the periodicity and the thinness are taken into account through a single technique, that is the technique used in the reference proof. Moreover, we bring a simplification of the proofs

by replacing in some places the two-scale convergence, based on the two-scale transform (ie this used in the unfolding method) by the two-scale convergence of G. Nguetseng and G. Allaire.

3.1.1 Organization of the Chapter

The chapter is organized as follows: in Section 3.2, the physical problem is stated. The rest of the chapter has the structure of the reference proof. In the first part of Section 3.3, the definitions and properties of two-scale transform operators are discussed. In the second part, the weak limits of two-scale transform of first order derivatives of solutions are derived. The last section is focused on the derivation of the two-scale model and then of the homogenized model.

3.2 Physical model description

The probe is designed as a thin three-layered structure and is located in a domain denoted by Ω. See Figure 4(a) and Figure 4(b). For illustration, we notice that in the last fabrication Ω_{Si} the silicon (Si) supporting layer is 5 μm thin and it is covered by a 50 nm silicon dioxide (SiO2) insulator layer Ω_{SiO2}. Finally, a 100 nm thick platinum (Pt) track Ω_{Pt} used for both a heating circuit and a sensing circuit is deposited. A current source is applied to one end $\Gamma^{\varepsilon}_{01}$ of the platinum track, and the other end $\Gamma^{\varepsilon}_{02}$ is electrically grounded. The conductive tip is heated through the Joule heating effect and the heat flux through the tip-sample interface is measured by the sensing circuit through the variation of the tip voltage.

The behavior of the SThM probe is governed by the thermoelasticity equation with Joule heating. The electric resistivity of the platinum layer affects the Joule heating effect in the probe. It varies with the temperature. We use $\mathbf{C}^{\varepsilon}$, $\mathbf{M}^{\varepsilon}$, $\mathbf{k}^{\varepsilon}$ and $\mathbf{a}^{\varepsilon}$ to denote the elasticity coefficient tensor, the matrix of thermal expansion coefficients, the matrix of thermal conductivity and the matrix of electric conductivity. Obviously, $\mathbf{C}^{\varepsilon}$, $\mathbf{M}^{\varepsilon}$ and $\mathbf{k}^{\varepsilon}$ are piecewise constant functions and we assume that $\mathbf{C}^{\varepsilon}$, $\mathbf{k}^{\varepsilon}$ and $\mathbf{a}^{\varepsilon}$ satisfy the usual ellipticity conditions. We use $\mathbf{u}^{\varepsilon} = (u^{\varepsilon}_1, u^{\varepsilon}_2, u^{\varepsilon}_3)$, θ^{ε} and φ^{ε} to denote the mechanical displacement vector, the difference of the temperature to the ambient temperature and the electric potential respectively. Since the SiO2 layer is a good insulator, the electric potential φ^{ε} is only defined in Ω_{Pt}. The Joule heating is the only heat source of the probe.

The thermoelasticity equations with Joule heating are:

$$\left\{\begin{array}{r} -\operatorname{div}(\boldsymbol{\sigma}^\varepsilon) = \mathbf{f}^{M,\varepsilon} \text{ in } \Omega \\ -\operatorname{div}\mathbf{q}^\varepsilon = (\nabla\varphi^\varepsilon)^T\mathbf{a}^\varepsilon\nabla\varphi^\varepsilon \text{ in } \Omega_{\mathrm{Pt}} \\ -\operatorname{div}\mathbf{q}^\varepsilon = 0 \text{ in } \Omega_{\mathrm{Si}}\cup\Omega_{\mathrm{SiO2}} \\ -\operatorname{div}(\mathbf{a}^\varepsilon\nabla\varphi^\varepsilon) = 0 \text{ in } \Omega_{\mathrm{Pt}}, \end{array}\right. \tag{3.1}$$

where $\boldsymbol{\sigma}^\varepsilon = \mathbf{C}^\varepsilon\mathbf{s}(\mathbf{u}^\varepsilon)+\mathbf{M}^\varepsilon\theta^\varepsilon$ is the tensor of stresses, $\mathbf{s}(\mathbf{u}^\varepsilon) = \frac{1}{2}(\nabla\mathbf{u}^\varepsilon+(\nabla\mathbf{u}^\varepsilon)^T)$ is the tensor of strains, $\mathbf{f}^{M,\varepsilon}$ is the body force load, $\mathbf{q}^\varepsilon = \mathbf{k}^\varepsilon\nabla\theta^\varepsilon$ is the heat flux, $\mathbf{a}^\varepsilon = (1+\lambda\theta^\varepsilon)^{-1}\mathbf{a}^{ref,\varepsilon}$ is the electric conductivity, λ is the temperature coefficient and $\mathbf{a}^{ref}$ is the tensor of electric conductivity at ambient temperature. Regarding the boundary conditions, the cantilever is clamped and with an imposed temperature on a part Γ_0^ε of the boundary, i.e. $\mathbf{u}^\varepsilon = 0$ and $\theta^\varepsilon = \theta_0$, and is mechanically free loaded and thermally insulated on the other part Γ_1, i.e. $\boldsymbol{\sigma}^\varepsilon\mathbf{n} = \mathbf{g}^{M,\varepsilon}$ and $\mathbf{q}^\varepsilon\mathbf{n} = \mathbf{0}$ where $\mathbf{n}$ denotes the outward normal vector to the boundary. Finally, a current source j^ε is applied to Γ_{01} ie $\int_{\Gamma_{01}^\varepsilon}\mathbf{a}^\varepsilon\nabla\varphi^\varepsilon\mathbf{n}\,dx^\varepsilon = j^\varepsilon$, Γ_{02} is grounded ie $\varphi^\varepsilon = 0$ and the other boundaries are electrically insulated ie $\mathbf{a}^\varepsilon\nabla\varphi^\varepsilon\mathbf{n} = 0$ on $\partial\Omega/(\Gamma_{01}\cup\Gamma_{02})$.

The weak formulation is obtained by choosing test functions $\mathbf{v}^{M,\varepsilon}$, $v^{H,\varepsilon}$, and $v^{E,\varepsilon}$ satisfying the boundary conditions $\mathbf{v}^{M,\varepsilon} = 0$, $v^{H,\varepsilon} = 0$ on Γ_0 and $v^{E,\varepsilon} = 0$ on Γ_{02}. After some usual calculation, we get the weak form of Equation (3.1) with a scaling $\kappa^0 = 1/|\Omega|$,

$$\begin{aligned} &\kappa^0\int_\Omega(\mathbf{C}^\varepsilon\mathbf{s}(\mathbf{u}^\varepsilon)+\mathbf{M}^\varepsilon\theta^\varepsilon)\mathbf{s}(\mathbf{v}^{M,\varepsilon})\,dx + \kappa^0\int_\Omega\mathbf{k}^\varepsilon\nabla\theta^\varepsilon\,\nabla v^{H,\varepsilon}\,dx + \kappa^0\int_{\Omega_{\mathrm{Pt}}}\mathbf{a}^\varepsilon\nabla\varphi^\varepsilon\,\nabla v^{E,\varepsilon}\,dx \\ = \;&\kappa^0\int_\Omega\mathbf{f}^{M,\varepsilon}\mathbf{v}^{M,\varepsilon}\,dx + \kappa^0\int_{\Omega_{\mathrm{Pt}}}\mathbf{a}^\varepsilon\nabla\varphi^\varepsilon\,\nabla\varphi^\varepsilon\,v^{H,\varepsilon}\,dx + \kappa^0 j^\varepsilon\int_{\Gamma_{01}}v^{E,\varepsilon}\,dx^\varepsilon + \kappa^0\int_{\Gamma_1}\mathbf{g}^{M,\varepsilon}\mathbf{v}^{M,\varepsilon}\,dx \end{aligned}$$

with the Dirichlet-like conditions $\mathbf{u}^\varepsilon = \mathbf{v}^{M,\varepsilon} = 0$ and $\theta^\varepsilon = v^{H,\varepsilon} = 0$ on Γ_0, $\varphi^\varepsilon = v^{E,\varepsilon} = 0$ on Γ_{02}. We notice that the boundary condition θ_0 has been taken equal to zero for simplicity, and this is also sufficient for the current application.

In the following asymptotic analysis, the whole probe is assumed to be thin, ie its thickness (which is in the range of a small parameter ε) is small compared to its lengths in the two other directions and the coefficients are assumed to be periodic with period ε, which includes the case with constant coefficients. Moreover, the thermal conductivity in the insulating layer made of silicon dioxide is assumed to be in the range of ε^2 when it is the range of 1 in the other components. From the mathematical point of view, we say that this coefficient is strongly heterogeneous.

For the asymptotic model derivation with respect to the small parameter ε, we will assume (without proof) some usual uniform estimates of the data and of the

solution. To simplify, we introduce the scaled L^2-norm for functions defined over a domain A

$$|||v|||_A^2 = \frac{1}{|A|}\int_A v^2\ dx.$$

We assume that the data are uniformly bounded,

$$|||f_\alpha^{M,\varepsilon}|||_\Omega^2 \text{ and } |||\varepsilon^{-1}f_3^{M,\varepsilon}|||_\Omega^2 \ \leq\ C \tag{3.2}$$

$$|j^\varepsilon| \ \leq\ C \tag{3.3}$$

and that the solution $\mathbf{u}^\varepsilon$, θ^ε and φ^ε satisfy the a priori estimates, inspired from [26], [15] and [22],

$$|||(u_i^\varepsilon)_{i\in\{1,2\}}|||_\Omega^2 \leq C,\ |||\varepsilon u_3^\varepsilon|||_\Omega^2 \leq C,\ |||\mathbf{s}(\mathbf{u}^\varepsilon)|||_\Omega^2 \ \leq\ C \tag{3.4}$$

$$|||\theta^\varepsilon|||_\Omega^2,\ |||\nabla\theta^\varepsilon|||_{\Omega_{\rm Pt}}^2 \leq C,\ |||\nabla\theta^\varepsilon|||_{\Omega_{\rm Si}}^2 \leq C \text{ and } |||\varepsilon\nabla\theta^\varepsilon|||_{\Omega_{\rm SiO2}}^2 \ \leq\ C \tag{3.5}$$

$$|||\varphi^\varepsilon|||_{\Omega_{\rm Pt}}^2,\ |||\nabla\varphi^\varepsilon|||_{\Omega_{\rm Pt}}^2 \ \leq\ C, \tag{3.6}$$

C denoting various constants independent of ε. These assumptions take the place of assumption $f \in L^2(\Omega)$ and assumption (1.15) for unknowns in the reference proof.

To conclude this section, we list the additional features taken into account in comparison with those already present in the reference proof:

- it is posed in a multi-dimensional (three-dimensional) domain;
- the domain is thin;
- several subdomains (the three layers where the coefficients are constant) are distinguished;
- the solution is comprised with several fields $\mathbf{u}^\varepsilon = (u_1^\varepsilon, u_2^\varepsilon, u_3^\varepsilon)$, θ^ε and φ^ε;
- the matrix $\mathbf{k}^\varepsilon$ has strongly heterogeneous coefficients ie $\mathbf{k}^\varepsilon \sim \varepsilon^2$ in $\Omega_{\rm SiO2}$ which implies the uniform estimate of $|||\varepsilon\nabla\theta^\varepsilon|||_{\Omega_{\rm SiO2}}^2$;
- the scaled field $\varepsilon u_3^\varepsilon$ satisfies a uniform L^2-estimate.

3.3 The SThM Probe model derivation

3.3.1 Notations, Definitions and Propositions

Notations, definitions and proposition of the reference proof are extended to cover the present case and new ones are added. All domains and variables are multi-dimensional without to be explicitely said in each case. Notice that, in the current status, the propositions are not defined in an optimized manner for further extensions. They are chosen to work for the current application.

Convention 111 *(i) Latin indices and exponents: $i, j, h, k, ...$, take their values in the set $\{1, 2, 3\}$, unless otherwise indicated.*

(ii) Greek indices and exponents: $\alpha, \beta, \theta, ...$, take their values in the set $\{1, 2\}$, unless otherwise indicated.

(iii) The repeated index summation conventions is systematically used in conjunction with rules (i) and (ii).

Notation 112 ***[Kronecker delta function]***

$$\delta_{ij} = \begin{cases} 1 \text{ if } i = j, \\ 0 \text{ if } i \neq j \end{cases}$$

Notation 113 ***[Characteristic function]*** *The characteristic function is denoted by*

$$\chi_{(A)}^{(x)} = \begin{cases} 1 \text{ if } x \in A, \\ 0 \text{ otherwise} \end{cases}$$

where x is variable and A is a set or a domain.

Notation 114 ***[Mean value of integral]*** $\oint_\Omega dz = \frac{1}{|\Omega|} \int_\Omega dz$.

Notation 115 ***[Strain operator]*** $\mathbf{u}$ *is a vector valued function defined in a domain A, x is the coordinate variable, then the strain operator with respect to x is*

$$s_{ij}^x(\mathbf{u}) = \frac{1}{2} \left(\partial_{x_i} u_j + \partial_{x_j} u_i \right).$$

Property 116 ***[Integral rule for subdomain]****Suppose $A = A_1 \cup A_2$ and $A_1 \cap A_2 = \varnothing$, then*

$$\int_A dz = \int_{A_1} dz + \int_{A_2} dz.$$

Property 117 ***[Integral rule for subdomain]*** *Suppose $A_1 \subset A$ and $a(x)$ is a function defined in A_1, then the integral of $a(x)$ is extended to A by*

$$\int_A a \; dz = \int_{A_1} \chi_{(A_1)}^{(x)} a(x) \; dz.$$

Property 118 ***[Interpretation of a weak equality]*** *For $u \in L^2(A)$ and for any $v \in C_0^\infty(A)$,*

$$\text{if } \int_A u(x) \; v(x) \; dx = 0 \text{ then } u = 0$$

in the sense of $L^2(A)$ functions.

Property 119 ***[Interpretation of a periodic boundary condition]*** *For $u \in H^1(A)$ and for any $v \in \mathcal{C}^\infty_\sharp(A)$,*

$$\text{if } \int_{\partial A} u(x)\ v(x)\ n_{x_\alpha}(x)\ dx = 0 \text{ then } u \text{ is } x_\alpha\text{-periodic in } A,$$

where n_{x_α} is the α component of the outward normal vector n.

Property 120 *Suppose A is a rectangle, $\mathbf{u} = (u_1, u_2)$ is a vector valued function in A, if for $\alpha, \beta \in \{1,2\}$ and $v \in C^\infty_\sharp(A)$, $\int_{\partial A}(n_{x_\alpha}u_\beta + n_{x_\beta}u_\alpha)v\ dx = 0$ then $\mathbf{u}$ is x_α-periodic in A.*

Property 121 *For u a periodic function in A and for any $v \in \mathcal{C}^\infty_\sharp(A)$, we have*

$$\int_{\partial A} uv(x) n_{\partial A}(x)\ dx = 0.$$

Property 122 (Linear dependency) *For u a function defined in A and x the coordinate variable, a is any function independent of x, if $\partial_x u = a$, then*

$$u(x) = xa + \widetilde{u}$$

where $\widetilde{u}$ is a function independent of x.

Property 123 *If $u(x) = x_\alpha a(x) + b$ is x_α-periodic, then $a(x) = 0$.*

Property 124 *Suppose A is a rectangle, $\mathbf{u} = (u_1, u_2)$ is an A-periodic vector valued function in A, if for $\alpha, \beta \in \{1,2\}$, $\partial_{x_\alpha}u_\beta + \partial_{x_\beta}u_\alpha = 0$, then $\mathbf{u}$ is a constant in A.*

Property 125 *A is a domain and Γ_0 is a part of its boundary with out normal vector $\mathbf{n}$, u is a scalar function defined in A, if for $\alpha \in \{1,2\}$ and $\forall v \in \mathcal{C}^\infty(A)$ so that*

$$\int_{\Gamma_0} u n_\alpha v\ dx = 0,$$

then $u = 0$ on Γ_0.

Property 126 *$\mathbf{u} = (u_1, u_2)$ is a vector valued function defined in A, Γ_0 is a part of its boundary with out normal vector $\mathbf{n} = (0, b)$ for $b \neq 0$, if for $\forall v \in \mathcal{C}^\infty(A)$ and $\alpha, \beta \in \{1,2\}$, so that*

$$\int_{\Gamma_0} (u_\alpha n_\beta + u_\beta n_\alpha)\, v\ dx = 0,$$

then $u_1 = 0$ and $u_2 = 0$ on Γ_0.

Property 127 ***[Green Rule]*** *If u, $v \in H^1(\Omega)$ then the traces of u and v on Γ are well defined and*

$$\int_\Omega u\partial_{x_i} v \; dx = \int_\Gamma tr(u)\; tr(v)\; n_{x_i}\; ds(x) - \int_\Omega v\partial_{x_i} u \; dx.$$

Property 128 (Introduction of a Kronecker symbol) *For $i, j \in \{1,2,3\}$, $\alpha, \beta \in \{1,2\}$, then*

$$a_\alpha + \sum\nolimits_i a_i = \sum\nolimits_i a_i(1+\delta_{i\alpha}),\; b_{\alpha\beta} + \sum\nolimits_{i,j} b_{ij} = \sum\nolimits_{i,j} b_{ij}(1+\delta_{i\alpha}\delta_{j\beta}).$$

In the following, the two-scale transform related notations and properties are introduced.

Notation 129 ***[Physical and microscopic Domains]*** *We consider an domain $\Omega = \bigcup_{c=1}^{N(\varepsilon)} \Omega_c^{1,\varepsilon} \subset \mathbb{R}$ divided into $N(\varepsilon)$ periodic cells $\Omega_c^{1,\varepsilon}$, of size $\varepsilon > 0$, indexed by c, and with center x_c. The translation and magnification $(\Omega_c^{1,\varepsilon} - x_c)/\varepsilon$ is called the unit cell and is denoted by Ω^1. The variables in Ω and in Ω^1 are denoted by x^ε and x^1.*

The two-scale transform T is an operator mapping functions defined in the physical domain Ω to functions defined in a two-scale domain $\Omega^\sharp \times \Omega^1$. The configuration of Ω, $\Omega^\sharp$ and Ω^1 in 1-dimensional and 2-dimensional case have been explaned in Chapter 1. The same principle is applied in 3-dimensional case also. We notice that the dimension of $\Omega^\sharp$ is less or equal to the dimension of Ω and the relation just depends on the configuration of Ω.

Notation 130 (Macroscopic domain indices) *We denote by $I^\sharp$ the set of coordinate indices of variables of the macroscopic domain $\Omega^\sharp$ and denote by I the set of coordinate indices of variables of the physical domain Ω.*

In the SThM probe model, $I^\sharp = \{1,2\}$ and $I = \{1,2,3\}$.

Definition 131 ***[Two-Scale Transform]*** *The two-scale transform T is the linear operator defined by*

$$(Tu)(x_c, x^1) = u(x_c + \varepsilon x^1) \tag{3.7}$$

and then by extension $T(u)(x^0, x^1) = u(x_c + \varepsilon x^1)$ for all $x^0 \in \Omega_c^{1,\varepsilon}$ and each c in $1, .., N(\varepsilon)$.

The operator T enjoys the following properties.

Property 132 ***[Product Rule]*** *For two functions u, v defined in Ω,*

$$T(uv) = T(u)T(v).$$

Property 133 ***[Derivative Rule]*** *If u and its partial derivative are defined in Ω then*

$$\text{for } \forall i \in I,\ T\left(\partial_{x_i} u\right) = \frac{1}{\varepsilon}\partial_{x_i^1} T(u). \tag{3.8}$$

Property 134 ***[Integral Rule]*** *If a function $u \in L^1(\Omega)$ then $T(u) \in L^1(\Omega^\sharp \times \Omega^1)$ and*

$$\oint_\Omega u\ dx = \oint_{\Omega^\sharp \times \Omega^1} T(u)\ dx^0 dx^1.$$

The next two properties are corollaries of the previous ones.

Property 135 ***[Inner Product Rule]*** *For two functions u, $v \in L^2(\Omega)$,*

$$\oint_\Omega u\ v\ dx = \oint_{\Omega^\sharp \times \Omega^1} T(u)\ T(v)\ dx^0 dx^1.$$

Property 136 ***[Norm Rule]*** *For a function $u \in L^2(\Omega)$,*

$$|||u|||_\Omega^2 = |||T(u)|||_{\Omega^\sharp \times \Omega^1}^2. \tag{3.9}$$

Definition 137 ***[Two-Scale Convergence]*** *A sequence $u^\varepsilon \in L^2(\Omega)$ is said to be two-scale strongly (respect. weakly) convergent in $L^2(\Omega^\sharp \times \Omega^1)$ to a limit $u^0(x^0, x^1)$ if $T(u^\varepsilon)$ is strongly (respect. weakly) convergent towards u^0 in $L^2(\Omega^\sharp \times \Omega^1)$.*

Definition 138 ***[Adjoint or Dual of T]*** *As T is a bounded linear operator from $L^2(\Omega)$ to $L^2(\Omega^\sharp \times \Omega^1)$, its adjoint T^* is a bounded linear operator from $L^2(\Omega^\sharp \times \Omega^1)$ to $L^2(\Omega)$ defined by*

$$\oint_\Omega T^*(v)\ u\ dx = \oint_{\Omega^\sharp \times \Omega^1} v\ T(u)\ dx^0 dx^1. \tag{3.10}$$

The expression of T^* can be detailed, it maps regular functions in $\Omega^\sharp \times \Omega^1$ to piecewise-constant functions in Ω. The next definition introduce an operator used as a smooth approximation of T^*.

Definition 139 ***[Regularization of T^*]*** *The operator B is the linear continuous operator defined from $L^2(\Omega^\sharp \times \Omega^1)$ to $L^2(\Omega)$ by*

$$Bv = v(x, \frac{x}{\varepsilon}). \tag{3.11}$$

The nullity condition of a function $v(x^0, x^1)$ on the boundary $\partial\Omega^\sharp \times \Omega^1$ is transferred to the range Bv as follows.

Property 140 ***[Boundary Conditions of Bv]*** *If $v \in \mathcal{C}^\infty_{\Gamma^\sharp}(\Omega^\sharp; \mathcal{C}^\infty(\Omega^1))$ then $Bv \in \mathcal{C}^\infty_\Gamma(\Omega)$.*

Property 141 ***[Derivation Rule for B]*** *If v and its partial derivatives are defined on $\Omega^\sharp \times \Omega^1$ then*

$$\text{for } i \in I,\ \partial_{x_i}(Bv) = \chi_{(I^\sharp)}(i) B(\partial_{x_i^0} v) + \varepsilon^{-1} B(\partial_{x_i^1} v). \tag{3.12}$$

The next proposition states that the operator B is actually an approximation of the operator T^* for Ω^1-periodic functions.

Property 142 ***[Approximation between T^* and B]*** *If $v(x^0, x^1)$ is continuous, continuously differentiable in x^0 and Ω^1-periodic in x^1 then*

$$T^*(v) = B(v - \varepsilon \sum\nolimits_{i \in I^\sharp} x_i^1 \partial_{x_i^0} v) + \varepsilon O_s(\varepsilon). \tag{3.13}$$

Conversely,

$$B(v) = T^*(v + \varepsilon \sum\nolimits_{i \in I^\sharp} x_i^1 \partial_{x_i^0} v) + \varepsilon O_s(\varepsilon). \tag{3.14}$$

The next two proposition are used for the homogenized model derivation, they are extension of Proposition 20.

Proposition 143 ***[The linear operator associated to the Microscopic problem H]*** *Here we assume a convention of summation over α from 1 to n. For any $\boldsymbol{\mu} \in \mathbb{R}^n$, under ellipticity condition on c^0, i.e. there exists $\alpha > 0$ such that*

$$\forall \xi \in \mathbb{R}^2, \qquad \sum_{i,j=1}^{2} c^0_{ij}\xi_i\xi_j \geq \alpha|\xi|^2,$$

there exist $\boldsymbol{\zeta}^\mu \in H^1_\sharp(\Omega^1)$ solutions to the linear weak formulation

$$\int_{\Omega^1} c^0_{ij}\frac{\partial \zeta^\mu}{\partial x^1_j}\frac{\partial w}{\partial x^1_i}\ dx^1 = -\mu_\alpha \int_{\Omega^1} c^0_{i\alpha}\frac{\partial w}{\partial x^1_i}\ dx^1 \text{ for all } w \in \mathcal{C}^\infty_\sharp(\Omega^1), \tag{3.15}$$

with unique derivatives $\frac{\partial \zeta^\mu}{\partial x^1_j}$. Since the mapping $\boldsymbol{\mu} \mapsto \nabla_{x^1}\zeta^\mu$ from $\mathbb{R}^n$ to $L^2(\Omega^1)^n$ is linear,

$$\frac{\partial \zeta^\mu}{\partial x^1_j} = \mu_\alpha \frac{\partial \zeta^1_\alpha}{\partial x^1_j}, \tag{3.16}$$

where ζ^1_α is solution to (3.15) for $\mu_\alpha = 1$ and $\mu_\beta = 0$ for $\beta \neq \alpha$,

$$\int_{\Omega^1} c^0_{ij}\frac{\partial \zeta^1_\alpha}{\partial x^1_j}\frac{\partial w}{\partial x^1_i}\ dx^1 = -\int_{\Omega^1} c^0_{i\alpha}\frac{\partial w}{\partial x^1_i}\ dx^1 \text{ for all } w \in \mathcal{C}^\infty_\sharp(\Omega^1). \tag{3.17}$$

Moreover, the relation (3.15) can be extended to any $\boldsymbol{\mu} \in L^2(\Omega^\sharp)^n$.

Proposition 144 ***[The linear operator associated to the Microscopic problem M]*** *Here we assume a convention of summation over h, k from 1 to n. Under usual ellipticity condition of c^0, i.e. there exists $\alpha > 0$ such that*

$$\forall \xi = (\xi_{ij}) \in \mathbb{R}^6, \quad \text{such that } \xi_{ij} = \xi_{ji} \quad (i,j) \in \{1,2,3\}^2,$$
$$\sum_{i,j=1}^{3} c^0_{ijkl}\xi_{ij}\xi_{kl} \geq \alpha|\xi|^2,$$

for $\boldsymbol{\mu} \in \mathbb{R}^{n\times n}$, there exist $\boldsymbol{\zeta}^\mu \in H^1_\sharp(\Omega^1)^n$ solutions to the linear weak formulation

$$\int_{\Omega^1} c^0_{ijhk}S^{x^1}_{hk}(\boldsymbol{\zeta}^\mu)S^{x^1}_{ij}(\mathbf{w})\ dx^1 = -\mu_{hk}\int_{\Omega^1} c^0_{ijhk}S^{x^1}_{ij}(\mathbf{w})\ dx^1 \text{ for all } \mathbf{w} \in \mathcal{C}^\infty_\sharp(\Omega^1)^n, \tag{3.18}$$

and $S^{x^1}_{hk}(\boldsymbol{\zeta}^\mu)$ is unique. Since the mapping $\boldsymbol{\mu} \mapsto S^{x^1}_{hk}(\boldsymbol{\zeta}^\mu)$ from $\mathbb{R}^{n\times n}$ to $L^2(\Omega^1)^{n\times n}$ is linear,

$$S^{x^1}_{hk}(\boldsymbol{\zeta}^\mu) = \mathrm{L}_{pqhk}\mu_{pq} \tag{3.19}$$

where $\mathrm{L}_{pqhk} = S^{x^1}_{hk}(\boldsymbol{\zeta}^1_{pq})$ *and* $\zeta^1_{pq} \in H^1(\Omega^1)^n$ *is the solution to (3.18) for* $\mu_{pq} = 1$,

$$\int_{\Omega^1} c^0_{ijhk} S^{x^1}_{hk}(\boldsymbol{\zeta}^1_{pq}) S^{x^1}_{ij}(\mathbf{w})\ dx^1 = -\int_{\Omega^1} c^0_{ijpq} S^{x^1}_{ij}(\mathbf{w})\ dx^1 \text{ for all } \mathbf{w} \in \mathcal{C}^\infty_\sharp(\Omega^1)^n.$$

Moreover, the relation (3.19) can be extended to any $\boldsymbol{\mu} \in L^2(\Omega^\sharp)^{n\times n}$.

Proposition 145 *Suppose* A *is a rectangle,* Γ^+ *and* Γ^- *are the top and bottom surface,* Γ^{Lat} *is the lateral boundary,* k_{ij} *for* $i,j \in \{1,2\}$ *is a constant matrix,* a *and* b *are two constants, if a function* $\theta \in H^1(A)$ *enjoys*

$$\begin{cases} -\sum_i \partial_{x_i}(\sum_j (k_{ij}\partial_{x_j}\theta)) = 0 \text{ in } A \\ (\sum_j k_{ij}\partial_{x_j}\theta) n_{x_i} = 0 \text{ on } \Gamma^{Lat} \\ \theta = a \text{ on } \Gamma^+ \\ \theta = b \text{ on } \Gamma^-, \end{cases}$$

then $\theta = a\theta^+ + b\theta^-$, *where* θ^+ *and* θ^- *are solutions to*

$$\begin{cases} -\sum_i \partial_{x_i}(\sum_j (k_{ij}\partial_{x_j}\theta^+)) = 0 \text{ in } A \\ (\sum_j k_{ij}\partial_{x_j}\theta^+) n_{x_i} = 0 \text{ on } \Gamma^{Lat} \\ \theta^+ = 1 \text{ on } \Gamma^+ \\ \theta^+ = 0 \text{ on } \Gamma^-, \end{cases} \tag{3.20}$$

$$\begin{cases} -\sum_i \partial_{x_i}(\sum_j (k_{ij}\partial_{x_j}\theta^-)) = 0 \text{ in } A \\ (\sum_j k_{ij}\partial_{x_j}\theta^-) n_{x_i} = 0 \text{ on } \Gamma^{Lat} \\ \theta^- = 0 \text{ on } \Gamma^+ \\ \theta^- = 1 \text{ on } \Gamma^-. \end{cases} \tag{3.21}$$

Proposition 146 *Suppose* A *is a rectangle with a boundary* Γ, Γ^- *is the bottom surface of* A, k_{ij} *for* $i,j \in \{1,2\}$ *is a constant matrix,* a *is a constant, if a function* $\theta \in H^1(A)$ *enjoys*

$$\begin{cases} -\sum_i \partial_{x_i}(\sum_j (k_{ij}\partial_{x_j}\theta)) = 0 \text{ in } A \\ (\sum_j k_{ij}\partial_{x_j}\theta) n_{x_i} = 0 \text{ on } \Gamma - \Gamma^- \\ \theta = a \text{ on } \Gamma^- \end{cases}$$

then $\theta = a$.

Proposition 147 ***[Solution to microscopic problem]*** *If* $(\lambda_k)_{k=1,2,3}$ *is* x_α*-periodic in* A *and* $\partial_{x_h}\lambda_k = \delta_{h\alpha}\delta_{k3}$, *then* $\lambda_k = x_3\delta_{k3}\delta_{h\alpha}$.

Proposition 148 ***[Zero solution for free load elasticity]*** *Suppose* A *is a cubic with elastic coefficient tensor* c_{ijhk}, $(u_i)_{i=1,2,3}$ *is the displacement filed and is periodic on the lateral directions, if for* $\forall (v_i)_{i=1,2,3} \in \mathcal{C}^\infty_\sharp(A)$,

$$\begin{cases} \int_A c_{ijhk}\partial_{x_h}u_k\partial_{x_i}v_j\ dx = 0 \\ (u_i)_{i=1,2,3} \text{ is } x_\alpha\text{-periodic on } \partial A, \end{cases}$$

then $(u_i)_{i=1,2,3} = 0$.

In the previous part, the general notations, properties and propositions have been introduced. In the following, we introduce specific notations that are used to simplify the presentation of the SThM probe model.

Notation 149 ***[Domain decomposition]*** *The domain Ω is decomposed in parts with regard to their number of layers: Ω_2 is the two-layered subdomain and Ω_3 is the three-layered subdomain. We denote by Ω_2^{Si} and Ω_2^{SiO2} the silicon layer and the silicon dioxide layer in Ω_2: $\Omega_2^{\mathrm{Si}} = \Omega_{\mathrm{Si}} \cap \Omega_2$ and $\Omega_2^{\mathrm{SiO2}} = \Omega_{\mathrm{SiO2}} \cap \Omega_2$. Similarly, notations Ω_3^{Si} and Ω_3^{SiO2} are defined by $\Omega_3^{\mathrm{Si}} = \Omega_{\mathrm{Si}} \cap \Omega_3$ and $\Omega_3^{\mathrm{SiO2}} = \Omega_{\mathrm{SiO2}} \cap \Omega_3$.*

The configuration of the probe is shown in Figure 3.1.

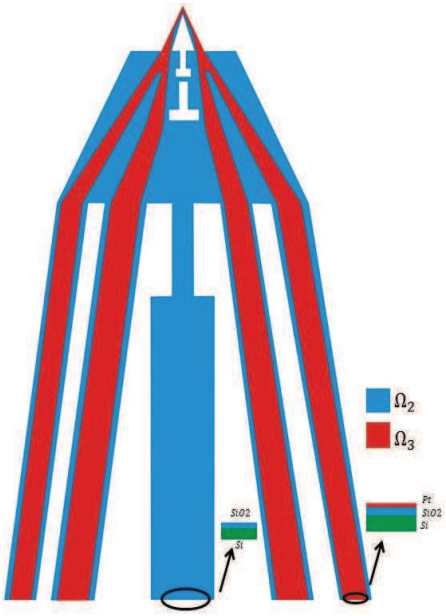


Figure 3.1: Configuration of the probe

Notation 150 ***[Two-scale domains]*** *The subdomains Ω_2 and Ω_3 are partitioned in cylindrical cells that intersect the x-y plane by $\varepsilon\times\varepsilon$-squares. The cells are denoted as Ω_2^c and Ω_3^c, which after shift by x_c and scaling by ε^{-1} yield the scaled cells Ω_2^1 and Ω_3^1. Considering the multi-layered structures of Ω_2^1 and Ω_3^1, they are decomposed into $\Omega_2^1 = \Omega_{\mathrm{Si}}^1 \cup \Omega_{\mathrm{SiO2}}^1$ and $\Omega_3^1 = \Omega_{\mathrm{Si}}^1 \cup \Omega_{\mathrm{SiO2}}^1 \cup \Omega_{\mathrm{Pt}}^1$. The domains $\Omega_2^\sharp$ and $\Omega_3^\sharp$ are the projections of Ω_2 and Ω_3 on the x-y plane. Then the two-scale domains corresponding to Ω_2^{Si} and Ω_2^{SiO2} are $\Omega_2^\sharp \times \Omega_{\mathrm{Si}}^1$ and $\Omega_2^\sharp \times \Omega_{\mathrm{SiO2}}^1$, when those of Ω_3^{Si}, Ω_3^{SiO2} and Ω_{Pt} are $\Omega_3^\sharp \times \Omega_{\mathrm{Si}}^1$, $\Omega_3^\sharp \times \Omega_{\mathrm{SiO2}}^1$ and $\Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1$, and those of Ω_2 and Ω_3 are $\Omega_2^\sharp \times \Omega_2^1$ and $\Omega_3^\sharp \times \Omega_3^1$. The projection of Γ_0 and Γ_{02} on the x-y plane is denoted by $\Gamma_0^\sharp$ and $\Gamma_{02}^\sharp$.*

Notation 151 ***[Volume Ratios]*** *The volume ratios of each component of the whole probe is denoted by:* $r_2^{\mathrm{Si}} = \left|\Omega_2^{\mathrm{Si}}\right| |\Omega|^{-1}$, $r_2^{\mathrm{SiO2}} = \left|\Omega_2^{\mathrm{SiO2}}\right| |\Omega|^{-1}$, $r_3^{\mathrm{Si}} = \left|\Omega_3^{\mathrm{Si}}\right| |\Omega|^{-1}$, $r_3^{\mathrm{SiO2}} = \left|\Omega_3^{\mathrm{SiO2}}\right| |\Omega|^{-1}$, $r^{\mathrm{Pt}} = \left|\Omega^{\mathrm{Pt}}\right| |\Omega|^{-1}$, $r_2 = |\Omega_2| |\Omega|^{-1}$ *and* $r_3 = |\Omega_3| |\Omega|^{-1}$.

3.3.2 Two-Scale Approximation of Derivatives

This section is aimed to compute the two-scale limits of strains and gradients of temperature and electric potential. This is an extension of Section 1.3.2. Considering the configuration of the microscopic domains, the physical domain Ω is separated to the two-layered subdomain Ω_2 and the three-layered subdomain Ω_3. The computation of the weak limits of the two-scale transform of $s^x_{\alpha\beta}(\mathbf{u}^\varepsilon)$, $\nabla\theta^\varepsilon$, $\varepsilon\nabla\theta^\varepsilon$ and $\nabla\varphi^\varepsilon$ are discussed in Ω_2 and Ω_3 separately because of the different configuration of the microscopic domains. On the other hand, the derivation for each term on Ω_2 and Ω_3 are very similar, so the discussion is only detailed in Ω_3. In the following, we introduce assumptions of the two-scale approximations of the fields $\mathbf{u}^\varepsilon$, θ^ε and φ^ε designed accordingly to the a priori estimates.

Assumption 152 ***[Two-scale approximation of*** u***]*** *There exist* $(u_i^0, u_i^1, u_i^2)_{i=1,3}$, θ^0, $\theta^1 \in L^2(\Omega_3^\sharp \times \Omega_3^1)$ *and* φ^0, $\varphi^1 \in L^2(\Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1)$ *such that*

$$\text{for } i \in \{1,2,3\},\ \fint_{\Omega_3} \varepsilon^{\delta_{i3}} u_i^\varepsilon\ Bv\ dx - \fint_{\Omega_3^\sharp \times \Omega_3^1} u_i^0\ v\ dx^0 dx^1 = O(\varepsilon), \tag{3.22}$$

$$\text{for } m \in \{\mathrm{Si}, \mathrm{SiO2}, \mathrm{Pt}\},\ \fint_{\Omega_3^m} \theta^\varepsilon\ Bv\ dx - \fint_{\Omega_3^\sharp \times \Omega_m^1} \theta^0\ v\ dx^0 dx^1 = O(\varepsilon), \tag{3.23}$$

and

$$\fint_{\Omega_{\mathrm{Pt}}} \varphi^\varepsilon\ Bv\ dx - \fint_{\Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1} \varphi^0\ v\ dx^0 dx^1 = O(\varepsilon), \tag{3.24}$$

for all $v \in \mathcal{C}^\infty(\Omega_3^\sharp \times \Omega_3^1)$,

$$\text{for } i \in \{1,2,3\} : \fint_{\Omega_3} \varepsilon^{\delta_{i3}} u_i^\varepsilon\ Bv\ dx - \fint_{\Omega_3^\sharp \times \Omega_3^1} (u_i^0 + \varepsilon u_i^1 + \varepsilon^2 u_i^2)\ v\ dx^0 dx^1 = \varepsilon O(\varepsilon), \tag{3.25}$$

$$\text{for } m \in \{\mathrm{Si}, \mathrm{SiO2}, \mathrm{Pt}\},\ \fint_{\Omega_3^m} \theta^\varepsilon\ Bv\ dx - \fint_{\Omega_3^\sharp \times \Omega_m^1} (\theta^0 + \varepsilon\theta^1)\ v\ dx^0 dx^1 = O(\varepsilon), \tag{3.26}$$

and

$$\fint_{\Omega_{\mathrm{Pt}}} \varphi^\varepsilon\ Bv\ dx - \fint_{\Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1} (\varphi^0 + \varepsilon\varphi^1)\ v\ dx^0 dx^1 = \varepsilon O(\varepsilon) \tag{3.27}$$

for all $v \in \mathcal{D}(\Omega_3^\sharp; \mathcal{C}_\sharp^\infty(\Omega_3^1))$.

In fact, θ^0 and θ^1 are functions depending on the microscopic layers. For example, $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}$, $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}$ and $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}$ are three functions, but we do not distinguish them for simplicity. The following Proposition extends Proposition 21.

Proposition 153 ***[Two-scale Limit of a Derivative]*** *If $(u^\varepsilon_\alpha)_{\alpha\in\{1,2\}}$, $\varepsilon u^\varepsilon_3$, θ^ε and φ^ε are sequences bounded as in (3.4,3.5,3.6) and satisfying (3.22-3.27), then $(\widetilde{u}^0_\alpha)_{\alpha\in\{1,2\}}$, u^0_3, u^1_3, $\theta^1_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}\cup\Omega_3^\sharp\times\Omega^1_{\rm Si}}$ and φ^0 are independent of x^1, $(u^1_\alpha)_{\alpha\in\{1,2\}}$, u^2_3, $\theta^1_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}\cup\Omega_3^\sharp\times\Omega^1_{\rm Si}}$ and φ^1 are x^1_α-periodic, and*

$$
\begin{aligned}
\text{for } \alpha,\beta\in\{1,2\}: \fint_{\Omega_3}(\partial_{x_\alpha}u^\varepsilon_\beta+\partial_{x_\beta}u^\varepsilon_\alpha)Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega_3^1}\eta^M_{\alpha\beta}v\ dx^0dx^1=O(\varepsilon),\\
\text{for } \alpha\in\{1,2\}: \fint_{\Omega_3}(\partial_{x_3}u^\varepsilon_\alpha+\partial_{x_\alpha}u^\varepsilon_3)Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega_3^1}\eta^M_{\alpha3}v\ dx^0dx^1=O(\varepsilon),\\
\fint_{\Omega_3}\partial_{x_3}u^\varepsilon_3Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega_3^1}\eta^M_{33}v\ dx^0dx^1=O(\varepsilon),\\
\fint_{\Omega_{\rm Pt}}\partial_{x_i}\theta^\varepsilon Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}}\eta^H_iv\ dx^0dx^1=O(\varepsilon),\\
\fint_{\Omega^{\rm Si}_3}\partial_{x_i}\theta^\varepsilon Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega^1_{\rm Si}}\eta^H_iv\ dx^0dx^1=O(\varepsilon),\\
\fint_{\Omega_{\rm SiO2}}\varepsilon\partial_{x_i}\theta^\varepsilon Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}\eta^h_iv\ dx^0dx^1=O(\varepsilon),\\
\fint_{\Omega_{\rm Pt}}\partial_{x_i}\varphi^\varepsilon Bv\ dx-\fint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}}\eta^E_iv\ dx^0dx^1=O(\varepsilon),
\end{aligned}
$$

where

$$
\begin{aligned}
\eta^M_{\alpha\beta} &= -x^1_3\partial^2_{x^0_\alpha x^0_\beta}u^0_3+\partial_{x^0_\beta}\widetilde{u}^0_\alpha+\partial_{x^0_\alpha}\widetilde{u}^0_\beta+\partial_{x^1_\beta}u^1_\alpha+\partial_{x^1_\alpha}u^1_\beta\ \text{ in } \Omega_3^\sharp\times\Omega_3^1,\\
\eta^M_{\alpha3} &= \partial_{x^0_\alpha}u^1_3+\partial_{x^1_\alpha}u^2_3+\partial_{x^1_3}u^1_\alpha\ \text{ in } \Omega_3^\sharp\times\Omega_3^1,\\
\eta^M_{33} &= \partial_{x^1_3}u^2_3\ \text{ in } \Omega_3^\sharp\times\Omega_3^1,\\
\eta^H_i &= \chi_{\{1,2\}}(i)\partial_{x^0_i}\theta^0+\partial_{x^1_i}\theta^1\ \text{ in } \Omega_3^\sharp\times\Omega^1_{\rm Pt},\\
\eta^H_i &= \chi_{\{1,2\}}(i)\partial_{x^0_i}\theta^0+\partial_{x^1_i}\theta^1\ \text{ in } \Omega_3^\sharp\times\Omega^1_{\rm Si},\\
\eta^h_i &= \partial_{x^1_i}\theta^0\ \text{ in } \Omega_3^\sharp\times\Omega^1_{\rm SiO2},\\
\eta^E_i &= \chi_{\{1,2\}}(i)\partial_{x^0_i}\varphi^0+\partial_{x^1_i}\varphi^1\ \text{ in } \Omega_3^\sharp\times\Omega^1_{\rm Pt}.
\end{aligned}
$$

Moreover, if $\mathbf{u}^\varepsilon=0$, $\theta^\varepsilon=0$ on Γ_0, $\varphi^\varepsilon=0$ on Γ_{02}, then $\mathbf{u}^0=0$ and $\theta^0=0$ on $\Gamma_0^\sharp\cap\partial\Omega_3^0$ and $\varphi^0=0$ on $\Gamma_{02}^\sharp$.

The proof of Proposition 153 is decomposed into seven lemmas extending those of the reference proof, which are proved for each set of assumptions. The new steps in the extensions are remarked by *Substep* of the main steps in the reference proof.

Lemma 154 ***[First Block-1: Constraint of u^0]*** *(a) $\partial_{x^1_\beta}u^0_\alpha+\partial_{x^1_\alpha}u^0_\beta=0$, (b) u^0_3 is independent of x^1_α, (c) $\partial_{x^1_3}u^0_\alpha+\partial_{x^0_\alpha}u^0_3+\partial_{x^1_\alpha}u^1_3=0$, (d) u^0_3 is independent of x^1_3, (e) u^1_3 is independent of x^1_3 in $\Omega_3^\sharp\times\Omega_3^1$ (f) θ^0 is independent of x^1 in $\Omega_3^\sharp\times\Omega^1_{\rm Pt}$, (g) θ^0 is independent of x^1 in $\Omega_3^\sharp\times\Omega^1_{\rm Si}$, (h) φ^0 is independent x^1 in $\Omega_3^\sharp\times\Omega^1_{\rm Pt}$.*

Proof. **a-Source term.** For each $\alpha, \beta \in \{1,2\}$, we set the initial term

$$\Psi = \varepsilon \fint_{\Omega_3} (\partial_{x_\beta} u_\alpha^\varepsilon + \partial_{x_\alpha} u_\beta^\varepsilon) Bv \; dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$. From the Cauchy-Schwartz inequality and (3.4), $\lim_{\varepsilon\to 0} \Psi = 0$.

We follow *Step 1 - Step 5* in the proof of Lemma 22 in Chapter 1. Instead of using the propositions in Section 1.3.1, we use their extended form posed in Section 3.3.1, and for the assumptions for the two-scale convergence, we use (3.22).

b-Source term. For each $\alpha \in \{1,2\}$, the initial term is

$$\Psi = \varepsilon^2 \fint_{\Omega_3} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) Bv \; dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$. The proof is the same as for Lemma 154(a).

c-Source term. For each $\alpha \in \{1,2\}$, the initial term is

$$\Psi = \varepsilon \fint_{\Omega_3} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) Bv \; dx \tag{3.28}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$. From the Cauchy-Schwartz inequality and (3.4), $\lim_{\varepsilon\to 0} \Psi = 0$.

- **Step c-1.** Propositions 127 and 140 $\Longrightarrow$

$$\Psi = -\varepsilon \fint_{\Omega_3} u_\alpha^\varepsilon \partial_{x_3} Bv + u_3^\varepsilon \partial_{x_\alpha} Bv \; dx.$$

- **Step c-2.** Proposition 141 and the boundness (3.4) $\Longrightarrow$

$$\Psi = \fint_{\Omega_3} u_\alpha^\varepsilon B \partial_{x_3^1} v + \frac{1}{\varepsilon} \varepsilon u_3^\varepsilon B(\varepsilon \partial_{x_\alpha^0} v + \partial_{x_\alpha^1} v) \; dx + O(\varepsilon).$$

- **Step c-3.** Assumption (3.22) and (3.25) $\Longrightarrow$

$$\fint_{\Omega_3^\sharp \times \Omega_3^1} u_\alpha^0 \partial_{x_3^1} v + (u_3^0 + \varepsilon u_3^1)(\partial_{x_\alpha^0} v + \varepsilon^{-1} \partial_{x_\alpha^1} v) \; dx^0 dx^1 = O(\varepsilon).$$

- **Substep c-3-1.** Expand the second term

$$\oint_{\Omega_3^\sharp\times\Omega_3^1}\Big(u_\alpha^0\partial_{x_3^1}v+u_3^0\partial_{x_\alpha^0}v+u_3^0\varepsilon^{-1}\partial_{x_\alpha^1}v+\varepsilon u_3^1\partial_{x_\alpha^0}v+u_3^1\partial_{x_\alpha^1}v\Big)\ dx^0dx^1=O(\varepsilon).$$

- **Step c-4.** Proposition 127 and $v=0$ on $\Omega_3^\sharp\times\partial\Omega_3^1\Longrightarrow$

$$\oint_{\Omega_3^\sharp\times\Omega_3^1}(\partial_{x_3^1}u_\alpha^0+\partial_{x_\alpha^0}u_3^0+\varepsilon^{-1}\partial_{x_\alpha^1}u_3^0+\varepsilon\partial_{x_\alpha^0}u_3^1+\partial_{x_\alpha^1}u_3^1)v\ dx^0dx^1=O(\varepsilon)$$

- **Substep c-4-1.** Lemma 154(b) $\Longrightarrow$

$$\oint_{\Omega_3^\sharp\times\Omega_3^1}(\partial_{x_3^1}u_\alpha^0+\partial_{x_\alpha^0}u_3^0+\varepsilon\partial_{x_\alpha^0}u_3^1+\partial_{x_\alpha^1}u_3^1)v\ dx^0dx^1=O(\varepsilon)$$

  Passing to the limit when $\varepsilon\to 0\Longrightarrow$

$$\oint_{\Omega_3^\sharp\times\Omega_3^1}(\partial_{x_3^1}u_\alpha^0+\partial_{x_\alpha^0}u_3^0+\partial_{x_\alpha^1}u_3^1)v\ dx^0dx^1=0$$

- **Step c-5.** Proposition 118 $\Longrightarrow$

$$\partial_{x_3^1}u_\alpha^0+\partial_{x_\alpha^0}u_3^0+\partial_{x_\alpha^1}u_3^1=0.$$

d-Source term. The initial term is

$$\Psi=\varepsilon^2\oint_{\Omega_3}\partial_{x_3}u_3^\varepsilon Bv\ dx$$

with $v\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp;\mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$. The proof is the same as for Lemma 154(a).

e-Source term. The initial term is

$$\Psi=\varepsilon\oint_{\Omega_3}\partial_{x_3}u_3^\varepsilon Bv\ dx$$

with $v\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp;\mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$. The proof is the same as for Lemma 154(c).

f-Source term. The initial term is

$$\Psi=\varepsilon\oint_{\Omega_{\rm Pt}}\partial_{x_i}\theta^\varepsilon Bv\ dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_{\rm Pt}}(\Omega^1_{\rm Pt}))$. The proof is the same as for Lemma 154(a).

g-Source term. The initial term is

$$\Psi = \varepsilon \oint_{\Omega_3^{\rm Si}} \partial_{x_i}\theta^\varepsilon B v \; dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_{\rm Si}}(\Omega^1_{\rm Si}))$. The proof is the same as for Lemma 154(a).

h-Source term. The initial term is

$$\Psi = \varepsilon \oint_{\Omega_{\rm Pt}} \partial_{x_i}\varphi^\varepsilon B v \; dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_{\rm Pt}}(\Omega^1_{\rm Pt}))$. The proof is the same as for Lemma 154(a). ■

Lemma 155 ***[Second Block-1: Two-Scale Limit of the Derivative]*** *(a)* $\eta^M_{\alpha\beta} = \partial_{x^0_\beta} u^0_\alpha + \partial_{x^0_\alpha} u^0_\beta + \partial_{x^1_\beta} u^1_\alpha + \partial_{x^1_\alpha} u^1_\beta$, *(b)* $\eta^M_{\alpha 3} = \partial_{x^0_\alpha} u^1_3 + \partial_{x^1_3} u^1_\alpha + \partial_{x^1_\alpha} u^2_3$, *(c)* $\eta^M_{33} = \partial_{x^1_3} u^2_3$ *in* $\Omega_3^\sharp \times \Omega^1_3$, *(d)* $\eta^H_i = \chi_{\{1,2\}}(i)\partial_{x^0_i}\theta^0 + \partial_{x^1_i}\theta^1$ *in* $\Omega_3^\sharp \times \Omega^1_{\rm Pt}$, *(e)* $\eta^H_i = \chi_{\{1,2\}}(i)\partial_{x^0_i}\theta^0 + \partial_{x^1_i}\theta^1$ *in* $\Omega_3^\sharp \times \Omega^1_{\rm Si}$, *(f)* $\eta^h_i = \partial_{x^1_i}\theta^0_3$ *in* $\Omega_3^\sharp \times \Omega^1_{\rm SiO2}$ *(g)* $\eta^E_i = \chi_{\{1,2\}}(i)\partial_{x^0_i}\varphi^0 + \partial_{x^1_i}\varphi^1$ *in* $\Omega_3^\sharp \times \Omega^1_{\rm Pt}$.

Proof. **a-Source term.** The initial term is

$$\Psi = \oint_{\Omega_3} (\partial_{x_\beta} u^\varepsilon_\alpha + \partial_{x_\alpha} u^\varepsilon_\beta) B v \; dx \tag{3.29}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_3}(\Omega^1_3))$.

The steps are the same as the proof of Lemma 23 in Chapter 1 and we get the conclusion (a).

b-Source term.

$$\Psi = \oint_{\Omega_3} (\partial_{x_3} u^\varepsilon_\alpha + \partial_{x_\alpha} u^\varepsilon_3) B v \; dx \tag{3.30}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_3}(\Omega^1_3))$.

- **Step b-1.** The Green formula (127), Proposition 141 and the linearity of integrals $\Longrightarrow$

$$\Psi = -\oint_{\Omega_3} u^\varepsilon_\alpha \varepsilon^{-1} B(\partial_{x^1_3} v) + \varepsilon u^\varepsilon_3 \varepsilon^{-1} B(\partial_{x^0_\alpha} v + \varepsilon^{-1}\partial_{x^1_\alpha} v) \; dx.$$

- **Step b-2.** Assumption 3.25 and 3.25 $\Longrightarrow$

$$\Psi = \oint_{\Omega_3^\sharp \times \Omega_3^1} (\varepsilon^{-1} u_\alpha^0 + u_\alpha^1)\partial_{x_3^1} v + (u_3^0 + \varepsilon u_3^1 + \varepsilon^2 u_3^2)\varepsilon^{-1}(\partial_{x_\alpha^0} v + \varepsilon^{-1}\partial_{x_\alpha^1} v)\, dx^0 dx^1 + O(\varepsilon).$$

- **Substep b-2-1.** Expand and factorizing by exponent of ε $\Longrightarrow$

$$\Psi = \oint_{\Omega_3^\sharp \times \Omega_3^1} \varepsilon^{-2} u_3^0 \partial_{x_\alpha^1} v\, dx^0 dx^1 + \oint_{\Omega_3^\sharp \times \Omega_3^1} \varepsilon^{-1} \left(u_\alpha^0 \partial_{x_3^1} v + u_3^0 \partial_{x_\alpha^0} v + u_3^1 \partial_{x_\alpha^1} v \right) dx^0 dx^1 + \oint_{\Omega_3^\sharp \times \Omega_3^1} \left(u_\alpha^1 \partial_{x_3^1} v + u_3^1 \partial_{x_\alpha^0} v + u_3^2 \partial_{x_\alpha^1} v \right) dx^0 dx^1 + O(\varepsilon).$$

- **Step b-3.** The Green formula (127) and factorizing $\Longrightarrow$

$$\Psi = \oint_{\Omega_3^\sharp \times \Omega_3^1} \varepsilon^{-2} \partial_{x_\alpha^1} u_3^0 v\, dx^0 dx^1 + \oint_{\Omega_3^\sharp \times \Omega_3^1} \varepsilon^{-1} \left(\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \partial_{x_\alpha^1} u_3^1 \right) v\, dx^0 dx^1 + \oint_{\Omega_3^\sharp \times \Omega_3^1} \left(\partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \right) v\, dx^0 dx^1 + O(\varepsilon).$$

- **Step b-4.** Lemma 154(b) and (c), passing to the limit when $\varepsilon \to 0$ $\Longrightarrow$

$$\Psi = \oint_{\Omega_3^\sharp \times \Omega_3^1} \left(\partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \right) v\, dx^0 dx^1.$$

- **Step b-5.** Proposition 118 $\Longrightarrow$

$$\eta_{\alpha 3}^M = \partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1.$$

c-Source term.

$$\Psi = \oint_{\Omega_3} \partial_{x_3} u_3^\varepsilon B v\, dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$. We follow the steps of the proof of Lemma 23 to find the conclusion.

d-Source term. The initial term is

$$\Psi = \oint_{\Omega_{\mathrm{Pt}}} \partial_{x_i} \theta^\varepsilon B v\, dx \text{ for each } i \in \{1,2,3\} \tag{3.31}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_{\mathrm{Pt}}^1}(\Omega_{\mathrm{Pt}}^1))$. We follow the steps of the proof of Lemma 23 to find the conclusion.

e-Source term. The initial term is

$$\Psi = \oint_{\Omega_3^{\rm Si}} \partial_{x_i}\theta^\varepsilon Bv\ dx \text{ for each } i \in \{1,2,3\}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_{\rm Si}}(\Omega^1_{\rm Si}))$. We follow the steps of the proof of Lemma 23 to find the conclusion.

f-Source term. The initial term is

$$\Psi = \oint_{\Omega_3^{\rm SiO2}} \varepsilon\partial_{x_i}\theta^\varepsilon Bv\ dx \text{ for each } i \in \{1,2,3\}, \tag{3.32}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_{\rm SiO2}}(\Omega^1_{\rm SiO2}))$. We follow the steps of the proof of Lemma 23 to find the conclusion.

g-Source term. The initial term is

$$\Psi = \oint_{\Omega_{\rm Pt}} \partial_{x_i}\varphi^\varepsilon Bv\ dx \text{ for each } i \in \{1,2,3\}, \tag{3.33}$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_{\rm Pt}}(\Omega^1_{\rm Pt}))$. We follow the steps of the proof of Lemma 23 to find the conclusion. ■

Lemma 156 ***[Third Block-1: Microscopic Boundary Condition]*** *(a)* u^0_α, *(b)* u^1_α, *(c)* u^1_3 *and (d)* u^2_3 *are* x^1_α*-periodic in* Ω^1_3, *(e)* $\theta^1_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}$ *is* x^1_α*-periodic in* $\Omega^1_{\rm Si}$, *(f)* $\theta^1_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}$ *and (g)* φ^1 *are* x^1_α*-periodic in* $\Omega^1_{\rm Pt}$ *and (h)* θ^0 *is continuous in* Ω^1_3.

Proof. **a-Source term.** The initial term is

$$\Psi = \varepsilon \oint_{\Omega_3} (\partial_{x_\beta} u^\varepsilon_\alpha + \partial_{x_\alpha} u^\varepsilon_\beta) Bv\ dx$$

with $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega^1_3}(\Omega^1_3))$. From the Cauchy-Schwartz inequality and (3.4), $\lim_{\varepsilon\to 0}\Psi = 0$.

- **Step a-1.** The Step 1 to Step 3 of the proof of Lemma 154(a)$\Longrightarrow$

$$-\oint_{\Omega_3^\sharp\times\Omega^1_3} (\partial_{x^1_\beta} u^0_\alpha + \partial_{x^1_\alpha} u^0_\beta)v\ dx^0dx^1 + \frac{|\partial\Omega^1_3|}{|\Omega^1_3|}\oint_{\Omega_3^\sharp\times\Gamma^1_3} (\partial_{x^1_\beta} u^0_\alpha + \partial_{x^1_\alpha} u^0_\beta)v\ dx^0dx^1 = O(\varepsilon).$$

- **Step a-2.** Lemma 154 and passing to the limit when $\varepsilon \to 0 \Longrightarrow$

$$\oint_{\Omega_3^\sharp \times \Gamma_3^1} (u_\alpha^0 n_{x_\beta^1} + u_\beta^0 n_{x_\alpha^1}) v \; dx^0 dx^1 = O(\varepsilon).$$

- **Step a-3.** Proposition 120 $\Longrightarrow$

$$\text{for } \alpha \in \{1,2\} \; u_\alpha^0 \text{ is } x_\alpha^1\text{-periodic in } \Omega_3^1.$$

b-Source term. In (3.30), we choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_\sharp(\Omega_3^1))$. The proof is the same as for Lemma 24. In Step 3, we replace Proposition 2 by Proposition 120.

c-Source term. In (3.28), we choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_\sharp(\Omega_3^1))$ and vanish on the top and bottom surface. We use $\Gamma_3^{1,Lat}$ to denote the lateral boundary of Ω_3^1.

- **Step c-1.** The steps 1-4 for the proof of Lemma 154(c) $\Longrightarrow$

$$\oint_{\Omega_3^\sharp \times \Omega_3^1} (\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \varepsilon^{-1} \partial_{x_\alpha^1} u_3^0 + \varepsilon \partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^1) v \; dx^0 dx^1$$
$$- \frac{|\Gamma_3^1|}{|\Omega_3^1|} \oint_{\Omega_3^\sharp \times \Gamma_3^{1,Lat}} (\varepsilon^{-1} u_3^0 n_{x_\alpha^1} + u_3^1 n_{x_\alpha^1}) v \; dx^0 dx^1 = O(\varepsilon)$$

- **Step c-2.** Lemma 154, Property 121 and passing to the limit when $\varepsilon \to 0 \Longrightarrow$

$$\oint_{\Omega_3^\sharp \times \Gamma_3^{1,Lat}} u_3^1 n_{x_\alpha^1} v \; dx^0 dx^1 = 0.$$

- **Step c-3.** Proposition 119 $\Longrightarrow$

$$\text{for } \alpha \in \{1,2\} \; u_3^1 \text{ is } \Omega_3^1\text{-periodic.}$$

d-Source term. Choose test function $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_\sharp(\Omega_3^1))$ and let v vanish on the top and bottom in (3.30).

- **Step d-1.** Steps b-1 to b-4 in Lemma 155, $\Longrightarrow$

$$\Psi = \oint_{\Omega_3^\sharp \times \Omega_3^1} \left(\partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \right) v \; dx^0 dx^1$$
$$- \oint_{\Omega_3^\sharp \times \Gamma_3^{1,Lat}} \left(n_{x_\alpha^1} u_3^1 + n_{x_\alpha^1} u_3^2 \right) v \; dx^0 dx^1 + O(\varepsilon).$$

- **Step d-2.** Lemma 155, Lemma 156(c), Property 121, passing to the limit when $\varepsilon \to 0$, $\Longrightarrow$

$$-\oint_{\Omega_3^\sharp \times \Gamma_3^{1,Lat}} n_{x_\alpha^1} u_3^2 v \; dx^0 dx^1 = 0.$$

- **Step d-3.** Property 119 $\Longrightarrow$

$$u_3^2 \text{ is } x_\alpha^1\text{-periodic in } \Omega_3^1.$$

The proofs of (e) (f) and (g) are the same as for the Lemma 24 in Chapter 1.

h-Source term. We choose $v \in C^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; C^\infty_{\partial\Omega_3^1}(\Omega_3^1))$, the initial term is

$$\begin{aligned}
&\frac{\varepsilon}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Pt}}^1}\eta_i^H v\; dx^0dx^1 + \frac{\varepsilon}{|\Omega_{\mathrm{Pt}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Si}}^1}\eta_i^H v\; dx^0dx^1 \\
&\qquad + \frac{1}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{Pt}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{SiO2}}^1}\eta_i^H v\; dx^0dx^1 \\
&= \frac{\varepsilon}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_{\mathrm{Pt}}}\partial_{x_i}\theta\; Bv\; dx^0dx^1 + \frac{\varepsilon}{|\Omega_{\mathrm{Pt}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_{\mathrm{Si}}}\partial_{x_i}\theta\; Bv\; dx^0dx^1 \\
&\qquad + \frac{1}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{Pt}}^1|}\oint_{\Omega_{\mathrm{SiO2}}}\varepsilon\partial_{x_i}\theta\; Bv\; dx^0dx^1 + O(\varepsilon)
\end{aligned}$$

- **Step h-1.** Follow steps 1-3 of the proof for Lemma 155.

$$\begin{aligned}
&\frac{\varepsilon}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Pt}}^1}\eta_i^H v\; dx^0dx^1 + \frac{\varepsilon}{|\Omega_{\mathrm{Pt}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Si}}^1}\eta_i^H v\; dx^0dx^1 \\
&+ \frac{1}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{Pt}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{SiO2}}^1}\eta_i^h v\; dx^0dx^1 \\
&= \frac{1}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Pt}}^1}\partial_{x_i^1}\theta^0 v\; dx^0dx^1 - \frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma_{\mathrm{Pt}}^1\cap\Gamma_{\mathrm{SiO2}}^1)}\theta^0_{|\Omega_3^\sharp\times\Omega_{\mathrm{Pt}}^1} n_{x_3^1} v\; dx^0dx^1 \\
&+ \frac{1}{|\Omega_{\mathrm{Pt}}^1|\,|\Omega_{\mathrm{SiO2}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Si}}^1}\partial_{x_i^1}\theta^0 v\; dx^0dx^1 - \frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma_{\mathrm{Si}}^1\cap\Gamma_{\mathrm{SiO2}}^1)}\theta^0_{|\Omega_3^\sharp\times\Omega_{\mathrm{Si}}^1} n_{x_3^1} v\; dx^0dx^1 \\
&+ \frac{1}{|\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{Pt}}^1|}\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{SiO2}}^1}\partial_{x_i^1}\theta^0\; v\; dx^0dx^1 - \frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma_{\mathrm{Pt}}^1\cap\Gamma_{\mathrm{SiO2}}^1)}\theta^0_{|\Omega_3^\sharp\times\Omega_{\mathrm{SiO2}}^1} n_{x_3^1} v\; dx^0dx^1 \\
&- \frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma_{\mathrm{Si}}^1\cap\Gamma_{\mathrm{SiO2}}^1)}\theta^0_{|\Omega_3^\sharp\times\Omega_{\mathrm{SiO2}}^1} n_{x_3^1} v\; dx^0dx^1 + O(\varepsilon).
\end{aligned}$$

with $A = |\Omega_{\mathrm{Si}}^1|\,|\Omega_{\mathrm{SiO2}}^1|\,|\Omega_{\mathrm{Pt}}^1|\,|\Omega_3^\sharp|$.

- **Step h-2**. Lemma 154, Lemma 155, passing to the limit when $\varepsilon \to 0 \Rightarrow$

$$\frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma^1_{\rm Pt}\cap\Gamma^1_{\rm SiO2})}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}n_{x_3^1}v\;dx^0dx^1+\frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma^1_{\rm Si}\cap\Gamma^1_{\rm SiO2})}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}n_{x_3^1}v\;dx^0dx^1$$
$$+\frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma^1_{\rm Pt}\cap\Gamma^1_{\rm SiO2})}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}n_{x_3^1}v\;dx^0dx^1+\frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma^1_{\rm Si}\cap\Gamma^1_{\rm SiO2})}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}n_{x_3^1}v\;dx^0dx^1=0.$$

- **Step h-3.** Factorizing by integration domains $\Longrightarrow$

$$\frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma^1_{\rm Pt}\cap\Gamma^1_{\rm SiO2})}\left(\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}-\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}\right)n_{x_3^1}v\;dx^0dx^1$$
$$+\frac{1}{A}\int_{\Omega_3^\sharp\times(\Gamma^1_{\rm Si}\cap\Gamma^1_{\rm SiO2})}\left(\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}-\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}\right)n_{x_3^1}v\;dx^0dx^1=0$$

- **Step h-4**. Proposition 125$\Rightarrow$

$$\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}-\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}=0 \text{ on } \Gamma^1_{\rm Pt}\cap\Gamma^1_{\rm SiO2} \text{ and } \theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}-\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm SiO2}}=0 \text{ on } \Gamma^1_{\rm Si}\cap\Gamma^1_{\rm SiO2}.$$

■

Lemma 157 ***[Fourth Block-1: Macroscopic Boundary Condition]*** *(a) u^0_α, (b) u^0_3, (c) u^1_3 (d) $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}$, (e) $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}$ vanishes on $\Gamma_0^\sharp\cap\partial\Omega_3^\sharp$ and (f) φ^0 vanishes on $\Gamma_{02}^\sharp$.*

Proof. **a-Source term.** In (3.29), we choose $v\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp-\Gamma_0^\sharp}(\Omega_3^\sharp;\mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$.

- **Step a-1.** The steps 1-3 of the proof for Lemma 155 and use $\mathbf{u}^\varepsilon=0$ on Γ_0 $\Longrightarrow$

$$\begin{aligned}\oint_{\Omega_3^\sharp\times\Omega_3^1}\eta^M_{\alpha\beta}v\;dx^0dx^1 &= \oint_{\Omega_3^\sharp\times\Omega_3^1}(\partial_{x_\beta^\sharp}u^0_\alpha+\partial_{x_\alpha^\sharp}u^0_\beta+\partial_{x_\beta^1}u^1_\alpha+\partial_{x_\alpha^1}u^1_\beta)v\;dx^0dx^1\\ &\quad-\frac{|\partial\Omega_3^\sharp|}{|\Omega_3^\sharp|}\oint_{(\Gamma_0^\sharp\cap\partial\Omega_3^\sharp)\times\Omega_3^1}(u^0_\alpha n_{x_\beta^\sharp}+u^0_\beta n_{x_\alpha^\sharp})v\;dx^0dx^1\\ &\quad+\frac{1}{\varepsilon}\oint_{\Omega_3^\sharp\times\Omega_3^1}(\partial_{x_\beta^1}u^0_\alpha+\partial_{x_\alpha^1}u^0_\beta)v\;dx^0dx^1+O(\varepsilon).\end{aligned}$$

- **Step a-2.** Lemma 154 and lemma 155, passing to the limit when $\varepsilon\to0\Longrightarrow$

$$\oint_{(\Gamma_0^\sharp\cap\partial\Omega_3^\sharp)\times\Omega_3^1}(u^0_\alpha n_{x_\beta^\sharp}+u^0_\beta n_{x_\alpha^\sharp})v\;dx^0dx^1.$$

- **Step a-3.** Proposition 126$\Longrightarrow$

$$u_\alpha^0 = 0 \text{ on } \Gamma_0^\sharp \cap \partial\Omega_3^\sharp.$$

b-Source term. We choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_0^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$, the initial term is

$$\varepsilon \oint_{\Omega_3^\sharp \times \Omega_3^1} \eta^M_{\alpha 3} v \; dx^0 dx^1 = \varepsilon \oint_{\Omega_3} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) B v \; dx + O(\varepsilon).$$

- **Step b-1.** The steps 1-4 of the proof for Lemma 154 and $\mathbf{u}^\varepsilon = 0$ on $\Gamma_0 \Longrightarrow$

$$\varepsilon \oint_{\Omega_3^\sharp \times \Omega_3^1} \eta^M_{\alpha 3} v \; dx^0 dx^1 = \oint_{\Omega_3^\sharp \times \Omega_3^1} (\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \varepsilon^{-1} \partial_{x_\alpha^1} u_3^0 + \varepsilon \partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^1) v \; dx^0 dx^1$$
$$- \frac{|\partial\Omega_3^\sharp|}{|\Omega_3^\sharp|} \oint_{(\Gamma_0^\sharp \cap \partial\Omega_3^\sharp) \times \Omega_3^1} (u_3^0 n_{x_\alpha^0} + \varepsilon u_3^1 n_{x_\alpha^0}) v \; dx^0 dx^1 + O(\varepsilon)$$

- **Step b-2.** Lemma 154, passing to the limit when $\varepsilon \to 0 \Longrightarrow$

$$\oint_{(\Gamma_0^\sharp \cap \partial\Omega_3^\sharp) \times \Omega_3^1} u_3^0 n_{x_\alpha^0} v \; dx^0 dx^1 = 0.$$

- **Step b-3.** Proposition 125 $\Longrightarrow$

$$u_3^0 = 0 \text{ on } \Gamma_0^\sharp \cap \partial\Omega_3^\sharp.$$

c-Source term. We choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_0^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_3^1}(\Omega_3^1))$, the initial term is

$$\oint_{\Omega_3^\sharp \times \Omega_3^1} \eta^M_{\alpha 3} v \; dx^0 dx^1 = \oint_{\Omega_3} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) B v \; dx + O(\varepsilon).$$

- **Step c-1.** The steps 1-3 of the proof for Lemma 155, $\Longrightarrow$

$$\begin{aligned}
\oint_{\Omega_3^\sharp \times \Omega_3^1} \eta^M_{\alpha 3} v \; dx^0 dx^1 \;=\; & \oint_{\Omega_3^\sharp \times \Omega_3^1} \varepsilon^{-2} \partial_{x_\alpha^1} u_3^0 v \; dx^0 dx^1 \\
& + \oint_{\Omega_3^\sharp \times \Omega_3^1} \varepsilon^{-1} \left(\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \partial_{x_\alpha^1} u_3^1 \right) v \; dx^0 dx^1 \\
& + \oint_{\Omega_3^\sharp \times \Omega_3^1} \left(\partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \right) v \; dx^0 dx^1 \\
& - \frac{|\partial\Omega_3^\sharp|}{|\Omega_3^\sharp|} \oint_{(\Gamma_0^\sharp \cap \partial\Omega_3^\sharp) \times \Omega_3^1} (\varepsilon^{-1} u_3^0 n_{x_\alpha^0} + u_3^1 n_{x_\alpha^0}) v \; dx^0 dx^1 + O(\varepsilon)
\end{aligned}$$

- **Step c-2.** Lemma 154, Lemma 155, Lemma 157(b), passing to the limit when $\varepsilon \to 0 \Longrightarrow$

$$\oint_{(\Gamma_0^\sharp \cap \partial\Omega_3^\sharp)\times\Omega_3^1} u_3^1 n_{x_\alpha^0} v \; dx^0 dx^1 = 0.$$

- **Step c-3.** Proposition 125 $\Longrightarrow$

$$u_3^1 = 0 \text{ on } \Gamma_0^\sharp \cap \partial\Omega_3^\sharp.$$

d-Source term. We choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_0^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_{\mathrm{Si}}^1}(\Omega_{\mathrm{Si}}^1))$, the initial term is

$$\oint_{\Omega_3^\sharp \times \Omega_{\mathrm{Si}}^1} \eta_i^H v \; dx^0 dx^1 = \oint_{\Omega_3^{\mathrm{Si}}} \partial_{x_i}\theta^\varepsilon B v \; dx + O(\varepsilon).$$

Follow steps 1-4 in the proof for Lemma 25 in Chapter 1, we get the conclusion.

e-Source term. We choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_0^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_{\mathrm{Pt}}^1}(\Omega_{\mathrm{Pt}}^1))$ the initial term is

$$\oint_{\Omega_3^\sharp \times \Omega_{\mathrm{Si}}^1} \eta_i^H v \; dx^0 dx^1 = \oint_{\Omega_3^{\mathrm{Pt}}} \partial_{x_i}\theta^\varepsilon B v \; dx + O(\varepsilon).$$

Follow steps 1-4 in the proof for Lemma 25 in Chapter [**?**], we get the conclusion.

f-Source term. We choose $v \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{02}^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_{\mathrm{Pt}}^1}(\Omega_{\mathrm{Pt}}^1))$ the initial term is

$$\oint_{\Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1} \eta_i^E v \; dx^0 dx^1 = \oint_{\Omega^{\mathrm{Pt}}} \partial_{x_i}\varphi^\varepsilon B v \; dx + O(\varepsilon).$$

Follow steps 1-4 in the proof for Lemma 25 in Chapter 1, we get the conclusion. ■

Lemma 158 *[**Constraint Reduction**] (a) u_α^0 is independent of x_α^1, (b) u_3^1 is independent of x_α^1, (c) $u_\alpha^0 = -x_3^1 \partial_{x_\alpha^0} u_3^0 + \widetilde{u}_\alpha^0(x^0)$.*

Proof. **a-Source term.** Lemma 154(a) $\partial_{x_\alpha^1} u_\beta^0 + \partial_{x_\beta^1} u_\alpha^0 = 0$ and Lemma 156(b) u_α^0 is x_α^1-periodic in Ω_3^1.

- **Step a-1.** Proposition 124 $\Longrightarrow$

$$\partial_{x_\beta^1} u_\alpha^0 = 0 \text{ for } \forall \alpha, \beta \in \{1, 2\}.$$

b-Source term. Lemma 154(c) $\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \partial_{x_\alpha^1} u_3^1 = 0$.

- **Step b-1.** Equivalent transformation $\Longrightarrow$

$$\partial_{x_\alpha^1} u_3^1 = -\left(\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0\right).$$

- **Step b-2.** Lemma 154, Lemma 158(a), Proposition 122 $\Longrightarrow$

$$u_3^1 = -x_\alpha^1 \left(\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0\right) + \widetilde{u}_3^1(x^0)$$

- **Step b-3.** Property 123 $\Longrightarrow$

$$\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 = 0$$

and u_3^1 independent of x_α^1.

c-Source term. $\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 = 0$

- **Step c-1.** Equivalent transformation $\Longrightarrow$

$$\partial_{x_3^1} u_\alpha^0 = -\partial_{x_\alpha^0} u_3^0.$$

- **Step c-2.** Lemma 154, Proposition 122, Lemma 158(a) $\Longrightarrow$

$$u_\alpha^0 = -x_3^1 \partial_{x_\alpha^0} u_3^0 + \widetilde{u}_\alpha^0(x^0).$$

■

The proofs of Proposition 153 is complete. In the following, according to another assumptions of two-scale convergence of the solutions on the two-layered subdomain, a similar proposition is stated for the two-scale limits of strains and gradient of temperature.

Assumption 159 ***[Two-scale approximation of*** u***]*** *There exist* $(u_i^0, u_i^1, u_i^2)_{i=1,3}$, θ^0, $\theta^1 \in L^2(\Omega_2^\sharp \times \Omega_2^1)$ *such that*

$$\textit{for } i \in \{1,2,3\} : \oint_{\Omega_2} \varepsilon^{\delta_{i3}} u_i^\varepsilon \; Bv \; dx - \oint_{\Omega_2^\sharp \times \Omega_2^1} u_i^0 \; v \; dx^0 dx^1 = O(\varepsilon)$$

$$\textit{for } m \in \{\mathrm{Si}, \mathrm{SiO2}\} : \oint_{\Omega_2^m} \theta^\varepsilon \; Bv \; dx - \oint_{\Omega_2^\sharp \times \Omega_m^1} \theta^0 \; v \; dx^0 dx^1 = O(\varepsilon)$$

for all $v \in \mathcal{C}^\infty(\Omega_2^\sharp \times \Omega_2^1)$,

$$\text{for } i \in \{1,2,3\} : \fint_{\Omega_2} \varepsilon^{\delta_{i3}} u_i^\varepsilon \; Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega_2^1} (u_i^0 + \varepsilon u_i^1 + \varepsilon^2 u_i^2) \; v \; dx^0 dx^1 = O(\varepsilon)$$

$$\text{for } m \in \{\mathrm{Si}, \mathrm{SiO2}\} : \fint_{\Omega_2^m} \theta^\varepsilon \; Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega_m^1} (\theta^0 + \varepsilon \theta^1) \; v \; dx^0 dx^1 = O(\varepsilon)$$

for all $v \in \mathcal{D}(\Omega_2^\sharp; \mathcal{C}_\sharp^\infty(\Omega_2^1))$.

Proposition 160 ***[Two-scale Limit of a Derivative]*** *If* $(u_\alpha^\varepsilon)_{\alpha\in\{1,2\}}$, $\varepsilon u_3^\varepsilon$, θ^ε *and* φ^ε *are sequences bounded as in (3.4,3.5,3.6) and satisfying (3.22-3.27), then* $(\widetilde{u}_\alpha^0)_{\alpha\in\{1,2\}}$, u_3^0, u_3^1 *and* $\theta^1_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}}$ *are independent of* x^1, $(u_\alpha^1)_{\alpha\in\{1,2\}}$, u_3^2 *and* $\theta^1_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}}$ *are* x_α^1*-periodic, and*

$$\begin{aligned}
\text{for } \alpha,\beta \in \{1,2\} : \fint_{\Omega_2} (\partial_{x_\alpha} u_\beta^\varepsilon + \partial_{x_\beta} u_\alpha^\varepsilon) Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega_2^1} \eta_{\alpha\beta}^M v \; dx^0 dx^1 = O(\varepsilon),\\
\text{for } \alpha \in \{1,2\} : \fint_{\Omega_2} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega_2^1} \eta_{\alpha 3}^M v \; dx^0 dx^1 = O(\varepsilon),\\
\fint_{\Omega_2} \partial_{x_3} u_3^\varepsilon Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega_2^1} \eta_{33}^M v \; dx^0 dx^1 = O(\varepsilon),\\
\fint_{\Omega_2^{\mathrm{Si}}} \partial_{x_i} \theta^\varepsilon Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} \eta_i^H v \; dx^0 dx^1 = O(\varepsilon),\\
\fint_{\Omega_2^{\mathrm{SiO2}}} \varepsilon \partial_{x_i} \theta^\varepsilon Bv \; dx - \fint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} \eta_i^h v \; dx^0 dx^1 = O(\varepsilon),
\end{aligned}$$

where

$$\begin{aligned}
\eta_{\alpha\beta}^M &= -x_3^1 \partial^2_{x_\alpha^0 x_\beta^0} u_3^0 + \partial_{x_\beta^0} \widetilde{u}_\alpha^0 + \partial_{x_\alpha^0} \widetilde{u}_\beta^0 + \partial_{x_\beta^1} u_\alpha^1 + \partial_{x_\alpha^1} u_\beta^1 \; \text{ in } \Omega_2^\sharp \times \Omega_2^1,\\
\eta_{\alpha 3}^M &= \partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \; \text{ in } \Omega_2^\sharp \times \Omega_2^1,\\
\eta_{33}^M &= \partial_{x_3^1} u_3^2 \; \text{ in } \Omega_2^\sharp \times \Omega_2^1,\\
\eta_i^H &= \chi_{\{1,2\}}(i) \partial_{x_i^0} \theta^0 + \partial_{x_i^1} \theta^1 \; \text{ in } \Omega_2^\sharp \times \Omega^1_{\mathrm{Si}},\\
\eta_i^h &= \partial_{x_i^1} \theta^0 \; \text{ in } \Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}.
\end{aligned}$$

Moreover, if $\mathbf{u}^\varepsilon = 0$, $\theta^\varepsilon = 0$ *on* Γ_0, *then* $\mathbf{u}^0 = 0$ *and* $\theta^0 = 0$ *on* $\Gamma_0^\sharp \cap \partial\Omega_2^0$.

The proof of this proposition is the same as the proof for Proposition 153. The next proposition shows that $\mathbf{u}^0$ and θ^0 are continuous on the interface $\partial\Omega_2^\sharp \cap \partial\Omega_3^\sharp$.

Proposition 161 *The weak limit* $\mathbf{u}^0$ *and* θ^0 *are continuous on* $\partial\Omega_2^\sharp \cap \partial\Omega_3^\sharp$.

Lemma 162 ***[Continuity of*** u^0 ***and*** θ^0***]*** *(a)* $(u_\alpha^0)_{\alpha\in\{1,2\}}$, *(b)* u_3^0, *(c)* u_3^1 *and (d)* $\theta^0_{|\Omega^1_{\mathrm{Si}}}$ *are continuous on* $\partial\Omega_2^\sharp \cap \partial\Omega_3^\sharp$.

Proof. For convenience of the presentation, we denote by $\Gamma_{23}^\sharp$ the intersection of $\partial\Omega_2^\sharp$ and $\partial\Omega_3^\sharp$.

a-Source term. Choose $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp; \mathcal{C}^\infty_{\Gamma_2^1}(\Omega_2^1))$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\Gamma_3^1}(\Omega_3^1))$, the initial term is

$$\begin{aligned}
&\frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2^\sharp\times\Omega_2^1}\eta^M_{\alpha\beta}v^2\ dx^0dx^1 + \frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3^\sharp\times\Omega_3^1}\eta^M_{\alpha\beta}v\ dx^0dx^1\\
=\ &\frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2}(\partial_{x_\alpha}u^\varepsilon_\beta + \partial_{x_\beta}u^\varepsilon_\alpha)v^2\ dx^0dx^1 + \frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3}(\partial_{x_\alpha}u^\varepsilon_\beta + \partial_{x_\beta}u^\varepsilon_\alpha)v^3\ dx^0dx^1.
\end{aligned}$$

- **Step a-1.** Follow the Step 1 - Step 4 of the proof of Lemma 155 $\Longrightarrow$

$$\begin{aligned}
&\frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2^\sharp\times\Omega_2^1}\eta^M_{\alpha\beta}v^2\ dx^0dx^1 + \frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3^\sharp\times\Omega_3^1}\eta^M_{\alpha\beta}v^3\ dx^0dx^1\\
=\ &\frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2^\sharp\times\Omega_2^1}(\partial_{x^0_\alpha}u^0_\beta + \partial_{x^0_\beta}u^0_\alpha + \partial_{x^1_\alpha}u^1_\beta + \partial_{x^1_\beta}u^1_\alpha)v^2\ dx^0dx^1\\
&-\frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_2^1|}\int_{\Gamma_{23}^\sharp\times\Omega_2^1}\left(n_{x^0_\alpha}u^0_\beta + n_{x^0_\beta}u^0_\alpha\right)v^2\ dx^0dx^1\\
&+\frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3^\sharp\times\Omega_3^1}(\partial_{x^0_\alpha}u^0_\beta + \partial_{x^0_\beta}u^0_\alpha + \partial_{x^1_\alpha}u^1_\beta + \partial_{x^1_\beta}u^1_\alpha)v^3\ dx^0dx^1\\
&-\frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_3^1|}\int_{\Gamma_{23}^\sharp\times\Omega_3^1}\left(n_{x^0_\alpha}u^0_\beta + n_{x^0_\beta}u^0_\alpha\right)v^3\ dx^0dx^1
\end{aligned}$$

- **Step a-2.** Lemma 155 $\Longrightarrow$

$$\begin{aligned}
&\frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_2^1|}\int_{\Gamma_{23}^\sharp\times\Omega_2^1}\left(n_{x^0_\alpha}u^0_\beta + n_{x^0_\beta}u^0_\alpha\right)v^2\ dx^0dx^1\\
&+\frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_3^1|}\int_{\Gamma_{23}^\sharp\times\Omega_3^1}\left(n_{x^0_\alpha}u^0_\beta + n_{x^0_\beta}u^0_\alpha\right)v^3\ dx^0dx^1 = 0.
\end{aligned}$$

- **Step a-3.** Let $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp)$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp)$ and $v^2 = v^3 = v$ on $\Gamma_{23}^\sharp$, factoring $\Longrightarrow$

$$\int_{\Gamma_{23}^\sharp}\left(n_{x^0_\alpha}(u^0_{\beta|\Omega_2^\sharp} - u^0_{\beta|\Omega_3^\sharp}) + n_{x^0_\beta}(u^0_{\alpha|\Omega_2^\sharp} - u^0_{\alpha|\Omega_3^\sharp})\right)v\ dx^0 = 0.$$

- **Step a-4.** Proposition 126 $\Longrightarrow$

$$\text{for } \forall\alpha,\beta\in\{1,2\},\ u^0_{\beta|\Omega_2^\sharp} - u^0_{\beta|\Omega_3^\sharp} = 0 \text{ and } u^0_{\alpha|\Omega_2^\sharp} - u^0_{\alpha|\Omega_3^\sharp} = 0 \text{ on } \Gamma_{23}^\sharp.$$

b-Source term. Choose $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp; \mathcal{C}^\infty_{\Gamma_2^1}(\Omega_2^1))$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\Gamma_3^1}(\Omega_3^1))$, for each $\alpha \in \{1,2\}$, the initial term is

$$\Psi = \varepsilon \frac{1}{|\Omega_3^\sharp|} \oint_{\Omega_2} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) B v^2 \, dx + \varepsilon \frac{1}{|\Omega_2^\sharp|} \oint_{\Omega_3} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) B v^3 \, dx,$$

From the Cauchy-Schwartz inequality and (3.4), $\lim_{\varepsilon \to 0} \Psi = 0$.

- **Step b-1.** Follow the Step c-1 to Step c-4 in Lemma 154(c) $\Longrightarrow$

$$\frac{1}{|\Omega_3^\sharp|} \oint_{\Omega_2^\sharp \times \Omega_2^1} (\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \partial_{x_\alpha^1} u_3^1) v^2 \, dx^0 dx^1 - \frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_2^1|} \int_{\Gamma_{23}^\sharp \times \Omega_2^1} n_{x_\alpha^0} u_3^0 v^2 \, dx^0 dx^1$$
$$+ \frac{1}{|\Omega_2^\sharp|} \oint_{\Omega_3^\sharp \times \Omega_3^1} (\partial_{x_3^1} u_\alpha^0 + \partial_{x_\alpha^0} u_3^0 + \partial_{x_\alpha^1} u_3^1) v^3 \, dx^0 dx^1 - \frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_3^1|} \int_{\Gamma_{23}^\sharp \times \Omega_2^1} n_{x_\alpha^0} u_3^0 v^3 \, dx^0 dx^1 = 0$$

- **Step b-2.** Lemma 154(c) $\Longrightarrow$

$$- \frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_2^1|} \int_{\Gamma_{23}^\sharp \times \Omega_2^1} n_{x_\alpha^0} u_3^0 v^2 \, dx^0 dx^1 - \frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_3^1|} \int_{\Gamma_{23}^\sharp \times \Omega_3^1} n_{x_\alpha^0} u_3^0 v^3 \, dx^0 dx^1 = 0.$$

- **Step b-3.** Let $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp)$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp)$ and $v^2 = v^3 = v$ on $\Gamma_{23}^\sharp$, factoring $\Longrightarrow$

$$\int_{\Gamma_{23}^\sharp} n_{x_\alpha^0} (u^0_{3|\Omega_2^\sharp} - u^0_{3|\Omega_3^\sharp}) v \, dx^0 = 0.$$

- **Step b-4.** Proposition 125 $\Longrightarrow$

$$u^0_{3|\Omega_2^\sharp} - u^0_{3|\Omega_3^\sharp} = 0 \text{ on } \Gamma_{23}^\sharp.$$

c-Source term. Choose $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp; \mathcal{C}^\infty_{\Gamma_2^1}(\Omega_2^1))$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\Gamma_3^1}(\Omega_3^1))$, for each $\alpha \in \{1,2\}$, the initial term is

$$\Psi = \frac{1}{|\Omega_3^\sharp|} \oint_{\Omega_2} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) B v^2 \, dx + \frac{1}{|\Omega_2^\sharp|} \oint_{\Omega_3} (\partial_{x_3} u_\alpha^\varepsilon + \partial_{x_\alpha} u_3^\varepsilon) B v^3 \, dx.$$

- **Step c-1.** Follow the Step b-1 to Step b-4 155 $\Longrightarrow$

$$\frac{1}{|\Omega_3^\sharp|} \oint_{\Omega_2^\sharp \times \Omega_2^1} \eta^M_{\alpha 3} \, v^2 \, dx^0 dx^1 + \frac{1}{|\Omega_2^\sharp|} \oint_{\Omega_3^\sharp \times \Omega_3^1} \eta^M_{\alpha 3} \, v^3 \, dx^0 dx^1$$
$$= \frac{1}{|\Omega_3^\sharp|} \oint_{\Omega_2^\sharp \times \Omega_2^1} \left(\partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \right) v^2 \, dx^0 dx^1 - \frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_2^1|} \int_{\Gamma_{23}^\sharp \times \Omega_2^1} n_{x_\alpha^0} u_3^1 v^2 \, dx^0 dx^1$$
$$+ \frac{1}{|\Omega_2^\sharp|} \oint_{\Omega_3^\sharp \times \Omega_3^1} \left(\partial_{x_\alpha^0} u_3^1 + \partial_{x_\alpha^1} u_3^2 + \partial_{x_3^1} u_\alpha^1 \right) v^3 \, dx^0 dx^1 - \frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_3^1|} \int_{\Gamma_{23}^\sharp \times \Omega_3^1} n_{x_\alpha^0} u_3^1 v^3 \, dx^0 dx^1$$

- **Step c-2.** Lemma 155(b) $\Longrightarrow$

$$-\frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_2^1|}\int_{\Gamma_{23}^\sharp\times\Omega_2^1} n_{x_\alpha^0} u_3^1 v^2 \; dx^0dx^1 - \frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_3^1|}\int_{\Gamma_{23}^\sharp\times\Omega_3^1} n_{x_\alpha^0} u_3^1 v^3 \; dx^0dx^1 = 0.$$

- **Step c-3.** Let $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp)$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp)$ and $v^2 = v^3 = v$ on $\Gamma_{23}^\sharp$, factoring $\Longrightarrow$

$$\int_{\Gamma_{23}^\sharp} n_{x_\alpha^0}(u^1_{3|\Omega_2^\sharp} - u^1_{3|\Omega_3^\sharp}) v \; dx^0 = 0.$$

- **Step c-4.** Proposition 125 $\Longrightarrow$

$$u^1_{3|\Omega_2^\sharp} - u^1_{3|\Omega_3^\sharp} = 0 \text{ on } \Gamma_{23}^\sharp.$$

d-Source term. Choose $v^2 \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp; \mathcal{C}^\infty_{\partial\Omega_{\rm Si}^1}(\Omega_{\rm Si}^1))$, $v^3 \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\partial\Omega_{\rm Si}^1}(\Omega_{\rm Si}^1))$, the initial term is

$$\Psi = \frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2^{\rm Si}} \partial_{x_i}\theta^\varepsilon B v \; dx + \frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3^{\rm Si}} \partial_{x_i}\theta^\varepsilon B v \; dx \text{ for each } i \in \{1,2,3\}.$$

- **Step d-1.** Follow the Step 1 to Step 4 in the proof of Lemma 155 $\Longrightarrow$

$$\begin{aligned}
&\frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2^\sharp\times\Omega_{\rm Si}^1} \eta_i^H \; v \; dx^0dx^1 + \frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3^\sharp\times\Omega_{\rm Si}^1} \eta_i^H \; v \; dx^0dx^1 \\
= \;& \frac{1}{|\Omega_3^\sharp|}\oint_{\Omega_2^\sharp\times\Omega_{\rm Si}^1} \left(\chi_{\{1,2\}}(i)\partial_{x_i^0}\theta^0 + \partial_{x_i^1}\theta^1\right) \; v \; dx^0dx^1 \\
&+ \frac{1}{|\Omega_2^\sharp|}\oint_{\Omega_3^\sharp\times\Omega_{\rm Si}^1} \left(\chi_{\{1,2\}}(i)\partial_{x_i^0}\theta^0 + \partial_{x_i^1}\theta^1\right) \; v \; dx^0dx^1 \\
&- \frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_{\rm Si}^1|}\int_{\Gamma_{23}^\sharp\times\Omega_{\rm Si}^1} \chi_{\{1,2\}}(i) n_{x_i^0}\theta^0_{|\Omega_2^\sharp\times\Omega_{\rm Si}^1} v \; dx^0dx^1 \\
&- \frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_{\rm Si}^1|}\int_{\Gamma_{23}^\sharp\times\Omega_{\rm Si}^1} \chi_{\{1,2\}}(i) n_{x_i^0}\theta^0_{|\Omega_3^\sharp\times\Omega_{\rm Si}^1} v \; dx^0dx^1
\end{aligned}$$

- **Step d-2.** Lemma 155(e) $\Longrightarrow$

$$\begin{aligned}
&- \frac{1}{|\Omega_3^\sharp||\Omega_2^\sharp||\Omega_{\rm Si}^1|}\int_{\Gamma_{23}^\sharp\times\Omega_{\rm Si}^1} \chi_{\{1,2\}}(i) n_{x_i^0}\theta^0_{|\Omega_2^\sharp\times\Omega_{\rm Si}^1} v \; dx^0dx^1 \\
&- \frac{1}{|\Omega_2^\sharp||\Omega_3^\sharp||\Omega_{\rm Si}^1|}\int_{\Gamma_{23}^\sharp\times\Omega_{\rm Si}^1} \chi_{\{1,2\}}(i) n_{x_i^0}\theta^0_{|\Omega_3^\sharp\times\Omega_{\rm Si}^1} v \; dx^0dx^1 = 0.
\end{aligned}$$

- **Step d-3.** Let $v^2 \in \mathcal{C}^{\infty}_{\partial\Omega_2^\sharp - \Gamma_{23}^\sharp}(\Omega_2^\sharp)$, $v^3 \in \mathcal{C}^{\infty}_{\partial\Omega_3^\sharp - \Gamma_{23}^\sharp}(\Omega_3^\sharp)$ and $v^2 = v^3 = v$ on $\Gamma_{23}^\sharp$, factoring $\Longrightarrow$

$$\int_{\Gamma_{23}^\sharp} \chi_{\{1,2\}}(i) n_{x_i^0} (\theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} - \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}}) v \, dx^0 = 0.$$

- **Step d-4.** Proposition 125 $\Longrightarrow$

$$\theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} - \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}} = 0 \text{ on } \Gamma_{23}^\sharp.$$

■

3.3.3 Homogenized Model Derivation

In the begining of this section, we introduce some assumptions used during the model derivation. They are assumptions for the boundness and regularity of the solutions, the scaling of the coefficients and the force loads.

Assumption 163 ***[Boundness of the Solution]*** *The solutions u^ε, θ^ε and φ^ε, force load $\mathbf{f}^\varepsilon$ and current source j^ε of (3.1) satisfies the boundness (3.4)-(3.6) and (3.2)-(3.3).*

Assumption 164 ***[Strong convergence of two-scale transform of solutions]*** *We assume that φ^ε and θ^ε are regular enough so that their two-scale transformations $T(\varphi^\varepsilon)$ and $T(\theta^\varepsilon)$ strongly converge to the regular function $\varphi^0(x^0, x^1)$ and $\theta^0(x^0, x^1)$ in (3.24) and (3.23).*

Assumption 165 ***[Scaling for the coefficients and source]*** *We assume that for the scaled functions C_{ijhk}, k_{ij}, a_{ij}^{ref}, f_i and j, the coefficients and the forced satisfy the following scaling*

$$\begin{aligned} C^\varepsilon_{ijhk} = C_{ijhk},\ f^\varepsilon_\alpha = f_\alpha,\ f^\varepsilon_3 = \varepsilon f_3 \ \text{in}\ \Omega \\ k^\varepsilon_{ij} = k_{ij} \ \text{in}\ \Omega_{\mathrm{Pt}} \cup \Omega_{\mathrm{Si}} \\ k^\varepsilon_{ij} = \varepsilon^2 k_{ij} \ \text{in}\ \Omega_{\mathrm{SiO2}} \\ a_{ij}^{ref,\varepsilon} = a_{ij}^{ref},\ j^\varepsilon = j \ \text{in}\ \Omega_{\mathrm{Pt}}. \end{aligned}$$

For some functions $C^0_{ijhk}(x^1)$, $k^0_{ij}(x^1)$, $a^0_{ij}(x^1)$ and $f^0_i(x^\sharp, x^1)$, the two-scale transform of the scaled functions are

$$T(C_{ijhk}) = C^0_{ijhk}(x^1),\ T(k_{ij}) = k^0_{ij}(x^1),\ T(a^{ref}_{ij}) = a^0_{ij}(x^1),\ T(f_i) = f_i^{M,0} \text{ and } T(j) = j^0.$$

For convenience of the presentation of the following proposition, we introduce some notations for the homogenized coefficients.

Notation 166 ***[Homogenized coefficients and force loads]***

- ***Electric conductivity:***

$$a_{ij}^H = \oint_{\Omega_{\rm Pt}^1} a_{ij}^0(\delta_{j\beta} + \partial_{x_j^1}\xi_\beta^{1,\rm Pt})(\delta_{i\alpha} + \partial_{x_i^1}\xi_\alpha^{1,\rm Pt})\ dx^1$$

  where $\xi_\alpha^{1,\rm Pt}$ *is the solution to (3.15) for* $c_{i\alpha}^0 = a_{i\alpha}^0$.

- ***Coefficient for elastic tensor:*** *For* $a, b \in \{D, S\}$, p',q',p,$q \in \{1, 2\}$ *and* $d \in \{2, 3\}$

$$C_{p'q'pq}^{H,ab} = \chi_{(\Omega_d^\sharp)}(x^0) \oint_{\Omega_d^1} C_{ijhk}^0 \widetilde{\rm L}_{p'q'hk}^{d,a} \widetilde{\rm L}_{pqij}^{d,b} dx^1,$$

  where $\widetilde{\rm L}_{p'q'hk}^{d,a}$ *and* $\widetilde{\rm L}_{pqij}^{d,b}$ *are defined in Proposition 144.*

- ***Thermal expansion coefficient:*** *For* $a, b \in \{D, S\}$, p,$q \in \{1, 2\}$, $m \in \{\rm Si, Pt\}$ *and* $d \in \{2, 3\}$

$$M_{pq}^{2,b} = \oint_{\Omega_2^1} \left(C_{ijhk}^0 {\rm L}_{hk}^{2,\theta_{\rm Si}} + M_{ij}\right) \widetilde{\rm L}_{pqij}^{2,b} dx^1,\ M_{pq}^{3,b,m} = \oint_{\Omega_3^1} \left(C_{ijhk}^0 {\rm L}_{hk}^{3,\theta_m} + Q_{ij}^m\right) \widetilde{\rm L}_{pqij}^{3,b} dx^1,$$

  where

$$Q_{ij}^{\rm Si} = \begin{cases} M_{ij} \text{ in } \Omega_{\rm Si}^1 \\ M_{ij}\theta^- \text{ in } \Omega_{\rm SiO2}^1 \\ 0 \text{ in } \Omega_{\rm Pt}^1, \end{cases} \quad \text{and } Q_{ij}^{\rm Pt} = \begin{cases} 0 \text{ in } \Omega_{\rm Si}^1 \\ M_{ij}\theta^+ \text{ in } \Omega_{\rm SiO2}^1 \\ M_{ij} \text{ in } \Omega_{\rm Pt}^1, \end{cases}$$

  θ^- *and* θ^+ *are solutions of Equation (3.20) and Equation (3.21).*

- ***Thermal conductivity****:*

$$\begin{aligned} k_{\alpha\beta}^{2,\rm Si} &= k_{\alpha\beta}^{3,\rm Si} = \oint_{\Omega_{\rm Si}^1} k_{ij}^0(\delta_{j\beta} + \partial_{x_j^1}\zeta_\beta^{1,\rm Si})(\delta_{i\alpha} + \partial_{x_i^1}\zeta_\alpha^{1,\rm Si})\ dx^1,\ k_3^{\rm SiO2,\pm} = \oint_{\Gamma_{\rm SiO2}^{1,\pm}} k_{3j}^0 \partial_{x_j^1}\theta^\pm\ dx^1 \\ k_{\alpha\beta}^{3,\rm Pt} &= \oint_{\Omega_{\rm Pt}^1} k_{ij}^0(\delta_{j\beta} + \partial_{x_j^1}\zeta_\beta^{1,\rm Pt})(\delta_{i\alpha} + \partial_{x_i^1}\zeta_\alpha^{1,\rm Pt})\ dx^1 \end{aligned}$$

  where $\zeta_\beta^{1,\rm Si}$, $\zeta_\beta^{1,\rm Pt}$ *are solutions to (3.15) with* $c_{i\alpha}^0 = k_{i\alpha}^0$, $\Gamma_{\rm SiO2}^{1,\pm}$ *are the top/bottom surface of* $\Omega_{\rm SiO2}^1$.

- ***Force load:***

$$q_\alpha^0 = \chi_{(\Omega_d^\sharp)}(x^0) \oint_{\Omega_d^1} x_3^1 f_\alpha^{M,0} dx^1,\ f_3^0 = \chi_{(\Omega_d^\sharp)}(x^0) \oint_{\Omega_d^1} f_3^{M,0} dx^1 \text{ for } d \in \{2, 3\}.$$

Property 167 ***[Equation Separation]*** *Weak formula (3.2) is equivalent to*

$$\begin{cases} \kappa^0 \int_\Omega (\mathbf{C}^\varepsilon \mathbf{s}(\mathbf{u}^\varepsilon) + \mathbf{M}^\varepsilon \theta^\varepsilon)\mathbf{s}(\mathbf{v}^{M,\varepsilon})\ dx = \kappa^0 \int_\Omega \mathbf{f}^{M,\varepsilon}\mathbf{v}^{M,\varepsilon}\ dx^\varepsilon + \kappa^0 \int_{\Gamma_1} \mathbf{g}^{M,\varepsilon}\mathbf{v}^{M,\varepsilon}\ dx\ (a) \\ \kappa^0 \int_\Omega \mathbf{k}^\varepsilon \nabla\theta^\varepsilon\ \nabla v^{H,\varepsilon}\ dx^\varepsilon = \kappa^0 \int_{\Omega_{\mathrm{Pt}}} \mathbf{a}^\varepsilon \nabla\varphi^\varepsilon \nabla\varphi^\varepsilon\ v^{H,\varepsilon}\ dx\ (b) \\ \kappa^0 \int_{\Omega_{\mathrm{Pt}}} \mathbf{a}^\varepsilon \nabla\varphi^\varepsilon\ \nabla v^{E,\varepsilon}\ dx = \kappa^0 j^\varepsilon \int_{\Gamma_{01}} v^{E,\varepsilon}\ dx\ (c) \end{cases} \tag{3.34}$$

The following proposition states the homogenized model for the SThM probe. Its proof is separated into three lemmas.

Proposition 168 ***[Homogenized Model]***

(a) The limit φ^0 and θ^0 are solutions of the coupled problems (a.1) and (a.2) as following:

(a.1)

$$\oint_{\Omega_3^\sharp} \frac{a^H_{\alpha\beta}}{1+\lambda\theta^0} \partial_{x^0_\beta}\varphi^0 \partial_{x^0_\alpha} v^{E,0}\ dx^0\ dx^0 = \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}^\sharp} j^0 v^{E,0}\ dx^0,$$

for all $v^{E,0} \in \mathcal{C}^\infty_{\Gamma^\sharp_{02}}(\Omega_3^\sharp)$.

(a.2)

$$r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp} k^{3,\mathrm{Pt}}_{\alpha\beta} \partial_{x^0_\beta}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} \partial_{x^0_\alpha} v_3^{H,0}\ dx^0 + r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp} \theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} \Big(\oint_{\Omega^1_{\mathrm{Pt}}} k_3^{\mathrm{SiO2},+}\ dx^1 \Big)\ v_3^{H,0}\ dx^0$$
$$= r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp} \Big(\oint_{\Omega^1_{\mathrm{Pt}}} \frac{a^0_{ij}}{1+\lambda\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}}} (\delta_{j\beta} + \partial_{x^1_j}\xi^{1,\mathrm{Pt}}_\beta)(\delta_{i\alpha} + \partial_{x^1_i}\xi^{1,\mathrm{Pt}}_\alpha)\ dx^1 \Big)\ \partial_{x^0_\beta}\varphi^0\varphi^0 \partial_{x^0_\alpha} v^{H,0}_{3\alpha}\ dx^0$$

for all $v_3^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp)$.

(b) The limit θ^0 is solution to the weak formulation

$$r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp} k^{2,\mathrm{Si}}_{\alpha\beta} \partial_{x^0_\beta}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}} \partial_{x^0_\alpha} v_2^{H,0}\ dx^0 = 0$$

for all $v_2^{H,0} \in \mathcal{C}^\infty_{\Gamma_0^\sharp\cap\partial\Omega_2^\sharp}(\Omega_2^\sharp)$.

(c) $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}$ is the solution to

$$r_3^{\mathrm{Si}} \int_{\Omega_3^\sharp} k^{3,\mathrm{Si}}_{\alpha\beta} \partial_{x^0_\beta}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} \partial_{x^0_\alpha} v_3^{H,0}\ dx^0 - r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp} \theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} \Big(\oint_{\Omega^1_{\mathrm{Pt}}} k_3^{\mathrm{SiO2},-}\ dx^1 \Big)\ v_3^{H,0}\ dx^0 = 0$$

for all $v_3^{H,0} \in \mathcal{C}^\infty_{\Gamma_0^\sharp\cap\partial\Omega_3^\sharp}(\Omega_3^\sharp)$.

(d) The limit $(u_i^0)_{i=1,2,3}$ *and* u_3^1 *satisfy* $u_\alpha^0 = -x_3^1 \partial_{x_\alpha^0} u_3^0 + \widetilde{u}_\alpha^0$, $\nabla_{x^1} u_3^0 = 0$ *and* $\nabla_{x^1} u_3^1 = 0$, *they are solutions to the weak formulation*

$$\begin{aligned}
&\int_{\Omega_2^\sharp} \left(C^{H,DD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SD}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{2,D}_{pq} \theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} \right) \cdot D^{x^0}_{pq}(v_3^0)\ dx^0 \\
&+ \int_{\Omega_2^\sharp} \left(C^{H,SD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SS}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{2,S}_{pq} \theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} \right) \cdot S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\ dx^0 \\
&+ \int_{\Omega_3^\sharp} \left(C^{H,DD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SD}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{3,D,\mathrm{Pt}}_{pq} \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} + M^{3,D,\mathrm{Si}}_{pq} \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}} \right) \cdot D^{x^0}_{pq}(v_3^0)\ dx^0 \\
&+ \int_{\Omega_3^\sharp} \left(C^{H,SD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SS}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{3,S,\mathrm{Pt}}_{pq} \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} + M^{3,S,\mathrm{Si}}_{pq} \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}} \right) \cdot S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\ dx^0 \\
&= \int_{\Omega^\sharp} -q^0_\alpha \partial_{x^0_\alpha} v_3^0 + f_3^0 v_3^0 + f_\alpha^0 \widetilde{v}_\alpha^0\ dx^0.
\end{aligned}$$

for all $\widetilde{\mathbf{v}}^0 \in H^1_{\Gamma_0^\sharp}(\Omega^\sharp)^2$, $v_3^0 \in H^1(\Omega^\sharp)$.

Lemma 169 ***[Fifth Block: Two-Scale Model]*** *(a) The couples* (φ^0, φ^1) *and* (θ^0, θ^1) *are solutions to the coupled two-scale weak formulations (a.1) and (a.2) as following*

(a.1) The (φ^0, φ^1) *solves*

$$\begin{aligned}
&\oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} (1+\alpha\theta^0)^{-1} a^0_{ij} \left(\chi_{\{1,2\}}(j) \partial_{x_j^0} \varphi^0 + \partial_{x_j^1} \varphi^1 \right) \left(\chi_{\{1,2\}}(i) \partial_{x_i^0} v^{E,0} + \partial_{x_i^1} v^{E,1} \right)\ dx^0 dx^1 \\
&= \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}^\sharp \times \Gamma^1_{01}} j^0 v^{E,0}\ dx^0 dx^1 \qquad (3.35)
\end{aligned}$$

for any $(v^{E,i})_{i=0,1} \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp, C^\infty_\sharp(\Omega^1_{\mathrm{Pt}}))$ *with condition* $\partial_{x_i^1} v^{E,0} = 0$.

(a.2) The couple (θ^0,θ^1) solves

$$
\begin{aligned}
&r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}} k^0_{ij}\left(\chi_{\{1,2\}}(j)\partial_{x_j^0}\theta^0+\partial_{x_j^1}\theta^1\right)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0}v_2^{H,0}+\partial_{x_i^1}v_2^{H,1}\right)\,dx^0dx^1\\
&+r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp\times\Omega^1_{\mathrm{SiO2}}} k^0_{ij}\partial_{x_j^1}\theta^0\partial_{x_i^1}v_2^{H,0}\,dx^0dx^1\\
&+r_3^{\mathrm{Si}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} k^0_{ij}\left(\chi_{\{1,2\}}(j)\partial_{x_j^0}\theta^0+\partial_{x_j^1}\theta^1\right)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx^0dx^1\\
&+r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} k^0_{ij}\left(\chi_{\{1,2\}}(j)\partial_{x_j^0}\theta^0+\partial_{x_j^1}\theta^1\right)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx^0dx^1\\
&+r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{SiO2}}} k^0_{ij}\partial_{x_j^1}\theta^0\partial_{x_i^1}v_3^{H,0}\,dx^0dx^1\\
&=-r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} \frac{a^0_{ij}}{1+\lambda\theta^0}\varphi^0\left(\chi_{\{1,2\}}(j)\partial_{x_j^0}\varphi^0+\partial_{x_j^1}\varphi^1\right)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx^0dx^1
\end{aligned}
\tag{3.36}
$$

for any $(v_2^{H,i})_{i=0,1}\in\mathcal{C}^\infty_{\partial\Omega_2^\sharp}(\Omega_2^\sharp,C^\infty_\sharp(\Omega_2^1))$ and $(v_3^{H,i})_{i=0,1}\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp,C^\infty_\sharp(\Omega_3^1))$ with condition $\partial_{x_i^1}v_2^{H,0}=0$ in $\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}$ and $\partial_{x_i^1}v_3^{H,0}=0$ in $\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}\cup\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}$.

(b) $(\widetilde{u}^0_\alpha)_{\alpha\in\{1,2\}}$, u_3^0, u_3^1 and $\boldsymbol{\varsigma}^1=(u_1^1,u_2^1,u_3^2)$ are solutions to the two-scale weak formulation

$$
\begin{aligned}
\textstyle\sum_d r_d \oint_{\Omega_d^\sharp\times\Omega_d^1}&\left(C^0_{ijhk}\left(-x_3^1D^{x^0}_{hk}(u_3^0)+S^{x^0}_{hk}(\widetilde{\mathbf{u}}^0)+K^{x^0}_{hk}(\mathbf{u}^1)+s^{x^1}_{hk}(\boldsymbol{\varsigma}^1)\right)+M_{ij}\theta^0\right)\cdot\\
&\left(-x_3^1D^{x^0}_{ij}(v_3^{d,0})+S^{x^0}_{ij}(\widetilde{\mathbf{v}}^{d,0})+K^{x^0}_{ij}(\mathbf{v}^{d,1})+s^{x^1}_{ij}(\mathbf{w}^{d,1})\right)\,dx^0dx^1\\
&=\textstyle\sum_d r_d \oint_{\Omega_d^\sharp\times\Omega_d^1} f^{M,0}_\alpha\left(-x_3^1\partial_{x_\alpha^0}v_3^{d,0}+\widetilde{v}_\alpha^{d,0}\right)+f_3^{M,0}v_3^{d,0}\,dx^0dx^1
\end{aligned}
\tag{3.37}
$$

for any $\widetilde{v}_\alpha^{d,0},v_3^{d,0},v_3^{d,1}\in\mathcal{C}^\infty(\Omega_d^\sharp)$, $\mathbf{w}^{d,1}=(v_1^{d,1},v_2^{d,1},v_3^{d,2})\in\mathcal{C}^\infty(\Omega_d^\sharp;\mathcal{C}^\infty_\sharp(\Omega_d^1))^3$ for $d\in\{2,3\}$, where $D^{x^0}_{ij}$, $S^{x^0}_{ij}$ and $K^{x^0}_{ij}$ are operators defined by: for $\forall u\in H^2(\Omega_d^\sharp)$, $\mathbf{v}\in H^1(\Omega_d^\sharp)^2$ and $w\in H^1(\Omega_d^\sharp)$,

$$
\begin{aligned}
D^{x^0}_{ij}(u) &= \chi^{(i)}_{\{1,2\}}\chi^{(j)}_{\{1,2\}}\partial^2_{x_i^0x_j^0}u,\ S^{x^0}_{ij}(\mathbf{v})=\chi^{(i)}_{\{1,2\}}\chi^{(j)}_{\{1,2\}}s^{x^0}_{ij}(\widetilde{\mathbf{u}}),\\
K^{x^0}_{ij}(w) &= \delta_{i3}\chi^{(j)}_{\{1,2\}}\partial_{x_j^0}w+\delta_{j3}\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}w.
\end{aligned}
\tag{3.38}
$$

Proof. **a.1-Source term**. Equation (3.34)-(c). We choose test functions $v^{E,0}\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp)$, $v^1\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp,C^\infty_\sharp(\Omega^1_{\mathrm{Pt}}))$.

- **Step a.1-1** Posing $v^{E,\varepsilon}=B(v^{E,0}+\varepsilon v^{E,1})$ in (3.34)-(c), Assumption 165 and Proposition 140 $\Longrightarrow Bv\in\mathcal{C}^\infty_{\partial\Omega_{\mathrm{Pt}}}(\Omega_{\mathrm{Pt}})$ and

$$
\kappa^0\int_{\Omega_{\mathrm{Pt}}}(1+\lambda\theta^\varepsilon)^{-1}a^{ref}_{ij}\partial_{x_j}\varphi^\varepsilon\partial_{x_i}B(v^{E,0}+\varepsilon v^{E,1})\,dx=\kappa^0\int_{\Gamma_{01}}j^\varepsilon B(v^{E,0}+\varepsilon v^{E,1})\,dx.
$$

- **Substep a.1-1-1** Equivalent transformation $\kappa^0 \int_A dz = \kappa^0 |A| \fint_A dz$, $\Longrightarrow$

$$\oint_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref} \partial_{x_j}\varphi^\varepsilon \partial_{x_i} B(v^{E,0}+\varepsilon v^{E,1})\, dx = \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}} j^\varepsilon B(v^{E,0}+\varepsilon v^{E,1})\, dx.$$

- **Step a.1-2** Propositions 141 $\Longrightarrow$

$$\begin{aligned}&\oint_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref} \partial_{x_j}\varphi^\varepsilon B\left(\chi_{\{1,2\}}(i)\partial_{x_i^0} v^{E,0} + \partial_{x_i^1} v^{E,1}\right)\, dx \\ &= \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}} j^\varepsilon B(v^{E,0})\, dx + O(\varepsilon).\end{aligned}$$

  Proposition 142 $\Longrightarrow$

$$\begin{aligned}&\oint_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref,\varepsilon} \partial_{x_j}\varphi^\varepsilon T^*\left(\chi_{\{1,2\}}(i)\partial_{x_i^0} v^{E,0} + \partial_{x_i^1} v^{E,1}\right)\, dx \\ &= \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}} j^\varepsilon T^*(v^{E,0})\, dx + O(\varepsilon).\end{aligned}$$

- **Step a.1-3** Definition 138 and Proposition 132 $\Longrightarrow$

$$\begin{aligned}&\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Pt}}^1} T((1+\lambda\theta^\varepsilon)^{-1}) T(a_{ij}^{ref}) T(\partial_{x_j}\varphi^\varepsilon)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0} v^{E,0} + \partial_{x_i^1} v^{E,1}\right)\, dx^0 dx^1 \\ &= \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}^\sharp\times\Gamma_{01}^1} T(j^\varepsilon)\, v^{E,0}\, dx^0 dx^1 + O(\varepsilon).\end{aligned} \tag{3.39}$$

  The boundary Γ_{01}^1 is one face of Ω_{Pt}^1 with the same out normal vector as $\Gamma_{01}^\sharp$.

- **Step a.1-4** Assumption 165 and Proposition 153, passing to the limit when $\varepsilon \to 0$ $\Longrightarrow$

$$\begin{aligned}&\oint_{\Omega_3^\sharp\times\Omega_{\mathrm{Pt}}^1} (1+\lambda\theta^0)^{-1} a_{ij}^0 \left(\chi_{\{1,2\}}(j)\partial_{x_j^0}\varphi^0 + \partial_{x_j^1}\varphi^1\right)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0} v^{E,0} + \partial_{x_i^1} v^{E,1}\right)\, dx^0 dx^1 \\ &= \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma_{01}^\sharp\times\Gamma_{01}^1} j^0 v^{E,0}\, dx^0 dx^1\end{aligned}$$

  which is the expected result.

a.2-Source term. Equation (3.34)-(b).

- **Step a.2-1** Property 116 $\Longrightarrow$

$$\kappa^0 \int_{\Omega_2^{\mathrm{Si}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_2^{\mathrm{SiO2}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$+\kappa^0 \int_{\Omega_3^{\mathrm{Si}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_3^{\mathrm{SiO2}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_{\mathrm{Pt}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$= \kappa^0 \int_{\Omega_{\mathrm{Pt}}} a_{ij}^\varepsilon \partial_{x_j}\varphi^\varepsilon \partial_{x_i}\varphi^\varepsilon\ v^{H,\varepsilon}\, dx$$

- **Substep a.2-1-1** Proposition 127 on the right side $\Longrightarrow$

$$\kappa^0 \int_{\Omega_2^{\mathrm{Si}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_2^{\mathrm{SiO2}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_3^{\mathrm{Si}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$+\kappa^0 \int_{\Omega_3^{\mathrm{SiO2}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_{\mathrm{Pt}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$= -\kappa^0 \int_{\Omega_{\mathrm{Pt}}} \partial_{x_i}\left(a_{ij}^\varepsilon \partial_{x_j}\varphi^\varepsilon\right)\varphi^\varepsilon\ v^{H,\varepsilon}\, dx - \kappa^0 \int_{\Omega_{\mathrm{Pt}}} a_{ij}^\varepsilon \partial_{x_j}\varphi^\varepsilon \varphi^\varepsilon\ \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$+\kappa^0 \int_{\partial\Omega_{\mathrm{Pt}}} a_{ij}^\varepsilon \varphi^\varepsilon \partial_{x_i}\varphi^\varepsilon n_{x_j} v^{H,\varepsilon} dx$$

- **Substep a.2-1-2** Applying Equation (3.1) $\Longrightarrow$

$$\kappa^0 \int_{\Omega_2^{\mathrm{Si}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_2^{\mathrm{SiO2}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$+\kappa^0 \int_{\Omega_3^{\mathrm{Si}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_3^{\mathrm{SiO2}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_{\mathrm{Pt}}} k_{ij}^\varepsilon \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$= -\kappa^0 \int_{\Omega_{\mathrm{Pt}}} a_{ij}^\varepsilon \partial_{x_j}\varphi^\varepsilon \varphi^\varepsilon\ \partial_{x_i} v^{H,\varepsilon}\, dx$$

- **Substep a.2-1-3** Assumption 165 $\Longrightarrow$

$$\kappa^0 \int_{\Omega_2^{\mathrm{Si}}} k_{ij} \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_2^{\mathrm{SiO2}}} \varepsilon^2 k_{ij} \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$+\kappa^0 \int_{\Omega_3^{\mathrm{Si}}} k_{ij} \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_{\mathrm{Pt}}} k_{ij} \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx + \kappa^0 \int_{\Omega_3^{\mathrm{SiO2}}} \varepsilon^2 k_{ij} \partial_{x_j}\theta^\varepsilon \partial_{x_i} v^{H,\varepsilon}\, dx$$
$$= -\kappa^0 \int_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref} \partial_{x_j}\varphi^\varepsilon \varphi^\varepsilon\ \partial_{x_i} v^{H,\varepsilon}\, dx$$

- **Substep a.2-1-4** Choose test functions $v_2^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp}(\Omega_2^\sharp, C^\infty(\Omega^1_{\mathrm{SiO2}}))$, $v_2^{H,1} \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp}(\Omega_2^\sharp, C^\infty_\sharp(\Omega_2^1))$, $v_3^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp, C^\infty(\Omega^1_{\mathrm{SiO2}}))$, $v_3^{H,1} \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp, C^\infty_\sharp(\Omega_3^1))$ and pose $v^{H,\varepsilon} = B(v_2^{H,0} + \varepsilon v_2^{H,1})$ in Ω_2, $v^{H,\varepsilon} = B(v_3^{H,0} + \varepsilon v_3^{H,1})$ in Ω_3, Proposition 140 $\Longrightarrow$

$$B(v_2^{H,0}) \in \mathcal{C}^\infty_{\partial\Omega_2}(\Omega_2),\ B(v_3^{H,0}) \in \mathcal{C}^\infty_{\partial\Omega_3}(\Omega_3)$$

and

$$\begin{aligned}
&\kappa^0 \int_{\Omega_2^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_2^{H,0} + \varepsilon v_2^{H,1})\ dx + \kappa^0 \int_{\Omega_2^{\mathrm{SiO2}}} \varepsilon^2 k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_2^{H,0} + \varepsilon v_2^{H,1})\ dx \\
&+\kappa^0 \int_{\Omega_3^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx + \kappa^0 \int_{\Omega_{\mathrm{Pt}}} k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx \\
&+\kappa^0 \int_{\Omega_3^{\mathrm{SiO2}}} \varepsilon^2 k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx \\
&= -\kappa^0 \int_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref} \partial_{x_j}\varphi^\varepsilon \varphi^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx
\end{aligned}$$

- **Substep a.2-1-3** Equivalent transformation $\kappa^0 \int_A dz = \kappa^0 |A| \fint_A dz$, $\Longrightarrow$

$$\begin{aligned}
&r_2^{\mathrm{Si}} \fint_{\Omega_2^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_2^{H,0} + \varepsilon v_2^{H,1})\ dx + r_2^{\mathrm{SiO2}} \fint_{\Omega_2^{\mathrm{SiO2}}} \varepsilon^2 k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_2^{H,0} + \varepsilon v_2^{H,1})\ dx \\
&+r_3^{\mathrm{Si}} \fint_{\Omega_3^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx + r^{\mathrm{Pt}} \fint_{\Omega_{\mathrm{Pt}}} k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx \\
&+r_3^{\mathrm{SiO2}} \fint_{\Omega_3^{\mathrm{SiO2}}} \varepsilon^2 k_{ij}\partial_{x_j}\theta^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx \\
&= -r^{\mathrm{Pt}} \fint_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref} \partial_{x_j}\varphi^\varepsilon \varphi^\varepsilon \partial_{x_i} B(v_3^{H,0} + \varepsilon v_3^{H,1})\ dx
\end{aligned}$$

- **Step a.2-2** Propositions 141 $\Longrightarrow$

$$\begin{aligned}
&r_2^{\mathrm{Si}} \fint_{\Omega_2^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon B\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0} v_2^{H,0} + \partial_{x_i^1} v_2^{H,1}\right)\ dx + r_2^{\mathrm{SiO2}} \fint_{\Omega_2^{\mathrm{SiO2}}} k_{ij}(\varepsilon\partial_{x_j}\theta^\varepsilon) B\left(\partial_{x_i^1} v_2^{H,0}\right)\ dx \\
&+r_3^{\mathrm{Si}} \fint_{\Omega_3^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon B\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0} v_3^{H,0} + \partial_{x_i^1} v_3^{H,1}\right)\ dx \\
&+r^{\mathrm{Pt}} \fint_{\Omega_{\mathrm{Pt}}} k_{ij}\partial_{x_j}\theta^\varepsilon B\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0} v_3^{H,0} + \partial_{x_i^1} v_3^{H,1}\right)\ dx + r_3^{\mathrm{SiO2}} \fint_{\Omega_3^{\mathrm{SiO2}}} k_{ij}(\varepsilon\partial_{x_j}\theta^\varepsilon) B\left(\partial_{x_i^1} v_3^{H,0}\right)\ dx \\
&= -r^{\mathrm{Pt}} \fint_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1} a_{ij}^{ref} \partial_{x_j}\varphi^\varepsilon \varphi^\varepsilon B\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0} v_3^{H,0} + \partial_{x_i^1} v_3^{H,1}\right)\ dx + O(\varepsilon)
\end{aligned}$$

Proposition 142 $\Longrightarrow$

$$
\begin{aligned}
r_2^{\mathrm{Si}} \oint_{\Omega_2^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon T^*\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_2^{H,0}+\partial_{x_i^1}v_2^{H,1}\right)\,dx + r_2^{\mathrm{SiO2}} \oint_{\Omega_2^{\mathrm{SiO2}}} k_{ij}(\varepsilon\partial_{x_j}\theta^\varepsilon)T^*\left(\partial_{x_i^1}v_2^{H,0}\right)\,dx \\
+r_3^{\mathrm{Si}} \oint_{\Omega_3^{\mathrm{Si}}} k_{ij}\partial_{x_j}\theta^\varepsilon T^*\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx \\
+r^{\mathrm{Pt}} \oint_{\Omega_{\mathrm{Pt}}} k_{ij}\partial_{x_j}\theta^\varepsilon T^*\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx + r_3^{\mathrm{SiO2}} \oint_{\Omega_3^{\mathrm{SiO2}}} k_{ij}(\varepsilon\partial_{x_j}\theta^\varepsilon)T^*\left(\partial_{x_i^1}v_3^{H,0}\right)\,dx \\
= -r^{\mathrm{Pt}} \oint_{\Omega_{\mathrm{Pt}}} (1+\lambda\theta^\varepsilon)^{-1}a_{ij}^{ref}\partial_{x_j}\varphi^\varepsilon\varphi^\varepsilon T^*\left(\chi_{\{1,2\}}(i)\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx + O(\varepsilon).
\end{aligned}
$$

- **Step a.2-3** Definition 138 and Proposition 132 $\Longrightarrow$

$$
\begin{aligned}
r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}} T\left(k_{ij}\right)T\left(\partial_{x_j}\theta^\varepsilon\right)\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_2^{H,0}+\partial_{x_i^1}v_2^{H,1}\right)\,dx^0dx^1 \\
+r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp\times\Omega^1_{\mathrm{SiO2}}} T\left(k_{ij}\right)T(\varepsilon\partial_{x_j}\theta^\varepsilon)\left(\partial_{x_i^1}v_2^{H,0}\right)\,dx^0dx^1 \\
+r_3^{\mathrm{Si}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} T\left(k_{ij}\right)T\left(\partial_{x_j}\theta^\varepsilon\right)\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx^0dx^1 \\
+r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} T\left(k_{ij}\right)T\left(\partial_{x_j}\theta^\varepsilon\right)\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx^0dx^1 \\
+r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{SiO2}}} T\left(k_{ij}\right)T(\varepsilon\partial_{x_j}\theta^\varepsilon)\left(\partial_{x_i^1}v_3^{H,0}\right)\,dx^0dx^1 \\
= -r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} T(\frac{1}{1+\lambda\theta^\varepsilon})T\left(a_{ij}^{ref}\right)T\left(\varphi^\varepsilon\right)T\left(\partial_{x_j}\varphi^\varepsilon\right)\left(\chi^{(i)}_{\{1,2\}}\partial_{x_i^0}v_3^{H,0}+\partial_{x_i^1}v_3^{H,1}\right)\,dx^0dx^1 \\
+O(\varepsilon).
\end{aligned}
$$

- **Step a.2-4** Assumption 165, Assumption 164, Proposition 153 and Propo-

sition 160, passing to the limit when $\varepsilon \to 0 \Longrightarrow$

$$
\begin{aligned}
& r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} k^0_{ij} \left(\chi^{(j)}_{\{1,2\}} \partial_{x^0_j} \theta^0 + \partial_{x^1_j} \theta^1 \right) \left(\chi^{(i)}_{\{1,2\}} \partial_{x^0_i} v_2^{H,0} + \partial_{x^1_i} v_2^{H,1} \right) \, dx^0 dx^1 \\
& + r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} k^0_{ij} \partial_{x^1_j} \theta^0 \partial_{x^1_i} v_2^{H,0} \, dx^0 dx^1 \\
& + r_3^{\mathrm{Si}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}} k^0_{ij} \left(\chi^{(j)}_{\{1,2\}} \partial_{x^0_j} \theta^0 + \partial_{x^1_j} \theta^1 \right) \left(\chi^{(i)}_{\{1,2\}} \partial_{x^0_i} v_3^{H,0} + \partial_{x^1_i} v_3^{H,1} \right) \, dx^0 dx^1 \\
& + r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} k^0_{ij} \left(\chi^{(j)}_{\{1,2\}} \partial_{x^0_j} \theta^0 + \partial_{x^1_j} \theta^1 \right) \left(\chi^{(i)}_{\{1,2\}} \partial_{x^0_i} v_3^{H,0} + \partial_{x^1_i} v_3^{H,1} \right) \, dx^0 dx^1 \\
& + r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{SiO2}}} k^0_{ij} \partial_{x^1_j} \theta^0 \partial_{x^1_i} v_3^{H,0} \, dx^0 dx^1 \\
& = -r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} \frac{a^0_{ij}}{1 + \lambda \theta^0} \varphi^0 \left(\chi^{(j)}_{\{1,2\}} \partial_{x^0_j} \varphi^0 + \partial_{x^1_j} \varphi^1 \right) \left(\chi^{(i)}_{\{1,2\}} \partial_{x^0_i} v_3^{H,0} + \partial_{x^1_i} v_3^{H,1} \right) \, dx^0 dx^1
\end{aligned}
$$

which is expected.

b-Source term Equation (3.34)-(a).

- **Step b-1.** Property 116 $\Longrightarrow$

$$
\begin{aligned}
\kappa^0 \int_{\Omega_2} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij} \theta^\varepsilon) s^x_{ij}(\mathbf{v}^{M,\varepsilon}) \, dx + \kappa^0 \int_{\Omega_3} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij} \theta^\varepsilon) s^x_{ij}(\mathbf{v}^{M,\varepsilon}) \, dx \\
= \kappa^0 \int_{\Omega_2} f_i^{M,\varepsilon} v_i^{M,\varepsilon} \, dx + \kappa^0 \int_{\Omega_3} f_i^{M,\varepsilon} v_i^{M,\varepsilon} \, dx
\end{aligned}
$$

- **Substep b-1-1** Assumption 165 $\Longrightarrow$

$$
\begin{aligned}
& \kappa^0 \int_{\Omega_2} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij} \theta^\varepsilon) s^x_{ij}(\mathbf{v}^{M,\varepsilon}) \, dx + \kappa^0 \int_{\Omega_3} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij} \theta^\varepsilon) s^x_{ij}(\mathbf{v}^{M,\varepsilon}) \, dx \\
& = \kappa^0 \int_{\Omega_2} f_\alpha^{M,\varepsilon} v_\alpha^{M,\varepsilon} \, dx + \kappa^0 \int_{\Omega_2} \varepsilon f_3^{M,\varepsilon} v_3^{M,\varepsilon} \, dx + \kappa^0 \int_{\Omega_3} f_\alpha^{M,\varepsilon} v_\alpha^{M,\varepsilon} \, dx + \kappa^0 \int_{\Omega_3} \varepsilon f_3^{M,\varepsilon} v_3^{M,\varepsilon} \, dx
\end{aligned}
$$

- **Step b-2** For $d \in \{2,3\}$, we choose test functions $\widetilde{v}^{d,0}_\alpha, v^{d,0}_3, v^{d,1}_3 \in \mathcal{C}^\infty(\Omega_d^\sharp)$, $(v^{d,0}_\alpha)_{\alpha \in \{1,2\}} = -x^1_3 \partial_{x^0_\alpha} v^{d,0}_3 + \widetilde{v}^{d,0}_\alpha$, $(v^{d,1}_\alpha)_{\alpha \in \{1,2\}} \in \mathcal{C}^\infty(\Omega_d^\sharp; \mathcal{C}^\infty_\sharp(\Omega^1_d))$, so that

$$
v^{M,\varepsilon}_\alpha = B(v^{d,0}_\alpha + \varepsilon v^{d,1}_\alpha), \, \varepsilon v^{M,\varepsilon}_3 = B(v^{d,0}_3 + \varepsilon v^{d,1}_3 + \varepsilon^2 v^{d,2}_3) \text{ in } \Omega_d.
$$

We denote by $\mathbf{w}^{d,1} = (v^{d,1}_1, v^{d,1}_2, v^{d,2}_3)$, use notation (3.38), we have

$$
s^x_{ij}(\mathbf{v}^{M,\varepsilon}) = B\left(-x^1_3 D^{x^0}_{ij}(v^{d,0}_3) + S^{x^0}_{ij}(\widetilde{\mathbf{v}}^{d,0}) + K^{x^0}_{ij}(\mathbf{v}^{d,1}) + s^{x^1}_{ij}(\mathbf{w}^{d,1}) \right) \text{ in } \Omega_d
$$

$\Longrightarrow$

$$\sum_d \kappa^0 \int_{\Omega_d} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij}\theta^\varepsilon) B \left(-x_3^1 D^{x^0}_{ij}(v_3^{d,0}) + S^{x^0}_{ij}(\widetilde{\mathbf{v}}^{d,0}) + K^{x^0}_{ij}(\mathbf{v}^{d,1})\right)\, dx$$
$$+ \sum_d \kappa^0 \int_{\Omega_d} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij}\theta^\varepsilon) B \left(s^{x^1}_{ij}(\mathbf{w}^{d,1})\right)\, dx$$
$$= \sum_d \kappa^0 \int_{\Omega_d} f^{M,\varepsilon}_\alpha B \left(-x_3^1 \partial_{x^0_\alpha} v_3^{d,0} + \widetilde{v}_\alpha^{d,0}\right) + f_3^{M,\varepsilon} B \left(v_3^{d,0}\right)\, dx$$

- **Substep b-2-1** Equivalent transformation $\kappa^0 \int_A dz = \kappa^0 |A| \fint_A dz \Longrightarrow$

$$\sum_d r_d \fint_{\Omega_d} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij}\theta^\varepsilon) B \left(-x_3^1 D^{x^0}_{ij}(v_3^{d,0}) + S^{x^0}_{ij}(\widetilde{\mathbf{v}}^{d,0}) + K^{x^0}_{ij}(\mathbf{v}^{d,1})\right)\, dx$$
$$+ \sum_d r_d \fint_{\Omega_d} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij}\theta^\varepsilon) B \left(s^{x^1}_{ij}(\mathbf{w}^{d,1})\right)\, dx$$
$$= \sum_d r_d \fint_{\Omega_d} f^{M,\varepsilon}_\alpha B \left(-x_3^1 \partial_{x^0_\alpha} v_3^{2,0} + \widetilde{v}_\alpha^{2,0}\right) + f_3^{M,\varepsilon} B \left(v_3^{d,0}\right)\, dx$$

- **Step b-2-2.** Proposition 142 $\Longrightarrow$

$$\sum_d r_d \fint_{\Omega_d} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij}\theta^\varepsilon) T^* \left(-x_3^1 D^{x^0}_{ij}(v_3^{d,0}) + S^{x^0}_{ij}(\widetilde{\mathbf{v}}^{d,0}) + K^{x^0}_{ij}(\mathbf{v}^{d,1})\right)\, dx$$
$$+ \sum_d r_d \fint_{\Omega_d} (C^\varepsilon_{ijhk} s^x_{hk}(\mathbf{u}^\varepsilon) + M^\varepsilon_{ij}\theta^\varepsilon) T^* \left(s^{x^1}_{ij}(\mathbf{w}^{d,1})\right)\, dx$$
$$= \sum_d r_d \fint_{\Omega_d} f^{M,\varepsilon}_\alpha T^* \left(-x_3^1 \partial_{x^0_\alpha} v_3^{d,0} + \widetilde{v}_\alpha^{d,0}\right) + f_3^{M,\varepsilon} T^* \left(v_3^{d,0}\right)\, dx$$

- **Step b-3** Definition 138 and Proposition 132 $\Longrightarrow$

$$\sum_d r_d \fint_{\Omega_d^\sharp \times \Omega_d^1} T(C^\varepsilon_{ijhk}(s^x_{hk}\mathbf{u}^\varepsilon + M^\varepsilon_{ij}\theta^\varepsilon)) \left(-x_3^1 D^{x^0}_{ij}(v_3^{d,0}) + S^{x^0}_{ij}(\widetilde{\mathbf{v}}^{d,0}) + K^{x^0}_{ij}(\mathbf{v}^{d,1})\right)\, dx^0 dx^1$$
$$+ \sum_d r_d \fint_{\Omega_d^\sharp \times \Omega_d^1} T(C^\varepsilon_{ijhk}(s^x_{hk}\mathbf{u}^\varepsilon + M^\varepsilon_{ij}\theta^\varepsilon)) s^{x^1}_{ij}(\mathbf{w}^{d,1})\, dx^0 dx^1$$
$$= \sum_d r_d \fint_{\Omega_d^\sharp \times \Omega_d^1} T\left(f^{M,\varepsilon}_\alpha\right) \left(-x_3^1 \partial_{x^0_\alpha} v_3^{d,0} + \widetilde{v}_\alpha^{d,0}\right) + T\left(f_3^{M,\varepsilon}\right) v_3^{d,0}\, dx^0 dx^1$$

- **Step c-4** Denoting by $\boldsymbol{\varsigma}^1 = (u_1^1, u_2^1, u_3^2)$, Assumption 165, Proposition 153, Proposition 160 and Property 165 $\Longrightarrow$

$$\begin{aligned}\sum_d r_d \oint_{\Omega_d^\sharp \times \Omega_d^1} \left(C_{ijhk}^0 \left(-x_3^1 D_{hk}^{x^0}(u_3^0) + S_{hk}^{x^0}(\widetilde{\mathbf{u}}^0) + K_{hk}^{x^0}(\mathbf{u}^1) + s_{hk}^{x^1}(\boldsymbol{\varsigma}^1) \right) + M_{ij}\theta^0 \right) \cdot \\ \left(-x_3^1 D_{ij}^{x^0}(v_3^{d,0}) + S_{ij}^{x^0}(\widetilde{\mathbf{v}}^{d,0}) + K_{ij}^{x^0}(\mathbf{v}^{d,1}) + s_{ij}^{x^1}(\mathbf{w}^{d,1}) \right) \, dx^0 dx^1 \\ = \sum_d r_d \oint_{\Omega_d^\sharp \times \Omega_d^1} f_\alpha^{M,0} \left(-x_3^1 \partial_{x_\alpha^0} v_3^{d,0} + \widetilde{v}_\alpha^{d,0} \right) + f_3^{M,0} v_3^{d,0} \, dx^0 dx^1\end{aligned}$$

■

Lemma 170 ***[Sixth Block: Microscopic Problem:E]***

(a) φ^1 *is solution to (3.15) with* $\mu_\alpha = \partial_{x_\alpha^0}\varphi^0$, $c_{ij}^0 = a_{ij}^0$ *and* $\Omega^1 = \Omega_{\mathrm{Pt}}^1$, *then*

$$\partial_{x_j^1}\varphi^1 = \sum_{\alpha=1}^{2} \partial_{x_\alpha^0}\varphi^0 \partial_{x_j^1}\xi_\alpha^{1,\mathrm{Pt}}.$$

(b) θ^1 *is solution to (3.15) with* $\mu_\alpha = \partial_{x_\alpha^\sharp}\theta^0$, $c_{ij}^0 = k^0_{ij|\Omega_2^\sharp \times \Omega_{\mathrm{Si}}^1}$ *and* $\Omega^1 = \Omega_{\mathrm{Si}}^1$, *then*

$$\partial_{x_j^1}\theta^1 = \sum_{\alpha=1}^{2} \partial_{x_\alpha^0}\theta^0 \partial_{x_j^1}\zeta_\alpha^{1,\mathrm{Si}} \text{ in } \Omega_2^\sharp \times \Omega_{\mathrm{Si}}^1.$$

(c) θ^1 *is solution to (3.15) with* $\mu_\alpha = \partial_{x_\alpha^0}\theta^0$, $c_{ij}^0 = k^0_{ij|\Omega_3^\sharp \times \Omega_{\mathrm{Si}}^1}$ *and* $\Omega^1 = \Omega_{\mathrm{Si}}^1$, *then*

$$\partial_{x_j^1}\theta^1 = \sum_{\alpha=1}^{2} \partial_{x_\alpha^0}\theta^0 \partial_{x_j^1}\zeta_\alpha^{1,\mathrm{Si}} \text{ in } \Omega_3^\sharp \times \Omega_{\mathrm{Si}}^1.$$

(d) θ^1 *is solution to (3.15) with* $\mu_\alpha = \partial_{x_\alpha^0}\theta^0$, $c_{ij}^0 = k^0_{ij|\Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1}$ *and* $\Omega^1 = \Omega_{\mathrm{Pt}}^1$, *then*

$$\partial_{x_j^1}\theta^1 = \sum_{\alpha=1}^{2} \partial_{x_\alpha^0}\theta^0 \partial_{x_j^1}\zeta_\alpha^{1,\mathrm{Pt}} \text{ in } \Omega_3^\sharp \times \Omega_{\mathrm{Pt}}^1.$$

(e) $-\sum_{i,j} \partial_{x_j^1}(k_{ij}^0 \partial_{x_i^1}\theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}}) = 0$ *and* $\theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} = \theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}}$.

(f) $-\sum_{i,j} \partial_{x_j^1}(k_{ij}^0 \partial_{x_i^1}\theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{SiO2}}}) = 0$ *and* $\theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{SiO2}}} = \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}}\theta^- + \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}}\theta^+$, *where* θ^+ *and* θ^- *are solutions of Equation (3.20) and Equation (3.21).*

(g) Let $\boldsymbol{\varsigma}^1 = \boldsymbol{\varsigma}^{1,D} + \boldsymbol{\varsigma}^{1,S} + \boldsymbol{\varsigma}^{1,K} + \boldsymbol{\varsigma}^{1,\theta}$, *then* $\boldsymbol{\varsigma}^{1,D}$, $\boldsymbol{\varsigma}^{1,S}$, $\boldsymbol{\varsigma}^{1,K}$ *and* $\boldsymbol{\varsigma}^{1,\theta}$ *are solutions to Equation (3.18) for* $\mu_{hk} = D_{hk}^{x^0}(u_3^0)$, $\mu_{hk} = S_{hk}^{x^0}(\widetilde{\mathbf{u}}^0)$, $\mu_{hk} = K_{hk}^{x^0}(\mathbf{u}^1)$ *and for* $c_{ijhk}^0 = M_{ij}\delta_{ih}\delta_{jk}$ *and* $\mu_{hk} = 1$. *We have*

$$\begin{array}{l} s_{hk}^{x^1}(\boldsymbol{\varsigma}^{1,D}) = \sum_{p'q'} \mathrm{L}^{2,D}_{p'q'hk}(D_{p'q'}^{x^0}(u_3^0)) \\ s_{hk}^{x^1}(\boldsymbol{\varsigma}^{1,S}) = \sum_{p'q'} \mathrm{L}^{2,S}_{p'q'hk}(S_{p'q'}^{x^0}(\widetilde{\mathbf{u}}^0)) \\ s_{hk}^{x^1}(\boldsymbol{\varsigma}^{1,K}) = \sum_\alpha \delta_{h\alpha}\delta_{k3}\partial_{x_\alpha^0}u_3^1 \\ s_{hk}^{x^1}(\boldsymbol{\varsigma}^{1,\theta}) = \mathrm{L}_{hk}^{2,\theta_{\mathrm{Si}}}(\theta^0_{|\Omega_2^\sharp \times \Omega_{\mathrm{Si}}^1}) \end{array} \quad \text{in } \Omega_2^1.$$

(h) Let $\boldsymbol{\varsigma}^1 = \boldsymbol{\varsigma}^{1,D} + \boldsymbol{\varsigma}^{1,S} + \boldsymbol{\varsigma}^{1,K} + \boldsymbol{\varsigma}^{1,\theta_{\rm Si}} + \boldsymbol{\varsigma}^{1,\theta_{\rm Pt}}$, *then* $\boldsymbol{\varsigma}^{1,D}$, $\boldsymbol{\varsigma}^{1,S}$, $\boldsymbol{\varsigma}^{1,K}$ $\boldsymbol{\varsigma}^{1,\theta_{\rm Si}}$ *and* $\boldsymbol{\varsigma}^{1,\theta_{\rm Pt}}$ *are solutions to Equation (3.18) for* $\mu_{hk} = D^{x^0}_{hk}$, $\mu_{hk} = S^{x^0}_{hk}(\widetilde{\mathbf{u}}^0)$, $\mu_{hk} = K^{x^0}_{hk}(\mathbf{u}^1)$, *for* $c^0_{ijhk} = Q^{\rm Si}_{ij}\delta_{ih}\delta_{jk}$ *and* $\mu_{hk} = 1$, *and for* $c^0_{ijhk} = Q^{\rm Pt}_{ij}\delta_{ih}\delta_{jk}$ *and* $\mu_{hk} = 1$ *respectively, where*

$$Q^{\rm Si}_{ij} = \begin{cases} M_{ij} \text{ in } \Omega^1_{\rm Si} \\ M_{ij}\theta^- \text{ in } \Omega^1_{\rm SiO2} \\ 0 \text{ in } \Omega^1_{\rm Pt}, \end{cases} \quad \text{and } Q^{\rm Pt}_{ij} = \begin{cases} 0 \text{ in } \Omega^1_{\rm Si} \\ M_{ij}\theta^+ \text{ in } \Omega^1_{\rm SiO2} \\ M_{ij} \text{ in } \Omega^1_{\rm Pt}, \end{cases}$$

and θ^- *and* θ^+ *are solutions to (3.21) and (3.20). We have*

$$\begin{array}{l} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,D}) = \sum_{p'q'} \mathrm{L}^{2,D}_{p'q'hk}(D^{x^0}_{p'q'}(u^0_3)) \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,S}) = \sum_{p'q'} \mathrm{L}^{2,S}_{p'q'hk}(S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)) \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,K}) = \sum_{\alpha} \delta_{h\alpha}\delta_{k3}\partial_{x^0_\alpha} u^1_3 \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta_{\rm Si}}) = \mathrm{L}^{3,\theta_{\rm Si}}_{hk}(\theta^0_{|\Omega^\sharp_3\times\Omega^1_{\rm Si}}) \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta_{\rm Pt}}) = \mathrm{L}^{3,\theta_{\rm Pt}}_{hk}(\theta^0_{|\Omega^\sharp_3\times\Omega^1_{\rm Pt}}) \end{array}$$

in Ω^1_3.

Proof. a-Source term. We choose $v^{E,0} = 0$ and $v^{E,1}(x^\sharp, x^1) = w(x^1)\psi(x^\sharp)$ in (3.35) with $\psi \in \mathcal{C}^\infty(\Omega^\sharp_3)$ and $w^1 \in \mathcal{C}^\infty_\sharp(\Omega^1_{\rm Pt})$.

- **Step a-1** Proposition 1, Lemma 154, and the linearity of the integral $\Longrightarrow$

$$(1+\lambda\theta^0)^{-1}\oint_{\Omega^1_{\rm Pt}} a^0_{ij}\partial_{x^1_j}\varphi^1\partial_{x^1_i}v^{E,1}\,dx^0dx^1 = -(1+\lambda\theta^0)^{-1}\partial_{x^0_\alpha}\varphi^0\oint_{\Omega^1_{\rm Pt}} a^0_{i\alpha}\partial_{x^1_i}v^{E,1}\,dx^0dx^1 \tag{3.40}$$

- **Step a-1-1** Equivalent transformation $\Longrightarrow$

$$\oint_{\Omega^1_{\rm Pt}} a^0_{ij}\partial_{x^1_j}\varphi^1\partial_{x^1_i}v^{E,1}\,dx^0dx^1 = -\partial_{x^0_\alpha}\varphi^0\oint_{\Omega^1_{\rm Pt}} a^0_{i\alpha}\partial_{x^1_i}v^{E,1}\,dx^0dx^1$$

- **Step a-2** Proposition 143 with $\mu_\alpha = \partial_{x^0_\alpha}\varphi^0$ $\Longrightarrow$

$$\partial_{x^1_j}\varphi^1 = \sum_{\alpha=1}^{2}\partial_{x^0_\alpha}\varphi^0\partial_{x^1_j}\xi^{1,\rm Pt}_\alpha$$

as announced.

b-Source term We choose $v_2^{H,0}=0$, $v_3^{H,0}=0$, $v_3^{H,1}=0$ and $v_2^{H,1}(x^0,x^1)=w(x^1)\psi(x^0)$ in (3.36) with $\psi\in\mathcal{C}^\infty(\Omega_2^\sharp)$ and $w^1\in\mathcal{C}^\infty_\sharp(\Omega^1_{\rm Si})$, the proof is the same as for Step a-1 to Step a-2.

c-Source term We choose $v_2^{H,0}=0$, $v_2^{H,1}=0$, $v_3^{H,0}=0$, $v_3^{H,1}=w(x^1)\psi(x^0)$ in $\Omega_3^\sharp\times\Omega^1_{\rm Pt}$ with $\psi\in\mathcal{C}^\infty(\Omega_3^\sharp)$, $w^1\in\mathcal{C}^\infty_\sharp(\Omega^1_{\rm Pt})$ and $v_3^{H,1}=0$ $\Omega_3^\sharp\times(\Omega^1_{\rm Si}\cup\Omega^1_{\rm SiO2})$ in (3.36), then the proof is the same as for Step a-1 to Step a-2.

d-Source term. We choose $v_2^{H,0}=0$, $v_2^{H,1}=0$, $v_3^{H,0}=0$, $v_3^{H,1}=w(x^1)\psi(x^0)$ in $\Omega_3^\sharp\times\Omega^1_{\rm Si}$ with $\psi\in\mathcal{C}^\infty(\Omega_3^\sharp)$ and $w^1\in\mathcal{C}^\infty_\sharp(\Omega^1_{\rm Si})$ and $v_3^{H,1}=0$ in $\Omega_3^\sharp\times(\Omega^1_{\rm Pt}\cup\Omega^1_{\rm SiO2})$ in (3.36), then the proof is the same as for Step a-1 to Step a-2.

e-Source term. We denote by $\Gamma^{1,\pm}_{\rm SiO2}$ and $\Gamma^{1,Lat}_{\rm SiO2}$ the top/bottom and lateral boundary of $\Omega^1_{\rm SiO2}$. We choose $v_3^{H,0}=0$, $v_2^{H,0}=w(x^1)\psi(x^0)$ in $\Omega_2^\sharp\times\Omega^1_{\rm SiO2}$ with $\psi\in\mathcal{C}^\infty(\Omega_2^\sharp)$, $w\in\mathcal{C}^\infty_{\Gamma^{1,Lat}_{\rm SiO2}\cup\Gamma^{1,+}_{\rm SiO2}}(\Omega^1_{\rm SiO2})$ in (3.36) $\Longrightarrow$

$$\int_{\Omega^1_{\rm SiO2}} k^0_{ij}\partial_{x^1_j}\theta^0\partial_{x^1_i}w^1\ dx^0dx^1=0.$$

- **Step e-1**. Lemma 156-(g) and Proposition 146 $\Longrightarrow$

$$\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm SiO2}}=\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm Si}}.$$

f-Source term. We choose $v_2^{H,0}=0$, $v_3^{H,0}=w(x^1)\psi(x^0)$ in $\Omega_3^\sharp\times\Omega^1_{\rm SiO2}$ with $\psi\in\mathcal{C}^\infty(\Omega_3^\sharp)$, $w\in\mathcal{C}^\infty_{\Gamma^{1,Lat}_{\rm SiO2}}(\Omega^1_{\rm SiO2})$ in (3.36) $\Longrightarrow$

$$\int_{\Omega^1_{\rm SiO2}} k^0_{ij}\partial_{x^1_j}\theta^0\partial_{x^1_i}w^1\ dx^0dx^1=0.$$

- **Step f-1**. Lemma 156-(g) and Proposition 145 $\Longrightarrow$

$$\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm SiO2}}=\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}\theta^+ +\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}\theta^-.$$

- **Step f-2**. Lemma 127 $\Longrightarrow$

$$-\int_{\Omega^1_{\rm SiO2}}\partial_{x^1_i}(k^0_{ij}\partial_{x^1_j}\theta^0)w^1\ dx^0dx^1=0.$$

- **Step f-3.** Lemma 118 $\Longrightarrow$

$$-\partial_{x^1_i}(k^0_{ij}\partial_{x^1_j}\theta^0)=0 \text{ in } \Omega_3^\sharp\times\Omega^1_{\rm SiO2}.$$

g-Source term. Let $\mathbf{w}^{2,1} = \boldsymbol{\psi}^2(x^0)\boldsymbol{\omega}^2(x^1)$ with $\boldsymbol{\psi}^2(x^0) \in \mathcal{C}^\infty_\sharp(\Omega_2^\sharp)^{3\times 3}$, $\boldsymbol{\omega}^2(x^1) \in \mathcal{C}^\infty_\sharp(\Omega_2^1)^3$, and let other test functions equal to 0 in (3.37) $\Longrightarrow$

$$r_2 \oint_{\Omega_2^1} \left(C^0_{ijhk} \left(-x_3^1 D^{x^0}_{hk}(u_3^0) + S^{x^0}_{hk}(\widetilde{\mathbf{u}}^0) + K^{x^0}_{hk}(\mathbf{u}^1) + s^{x^1}_{hk}(\boldsymbol{\varsigma}^1) \right) + M_{ij}\theta^0 \right) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = 0.$$

- **Step g-1** Equivalent transformation $\Longrightarrow$

$$\begin{aligned} \int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^1) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = & \int_{\Omega_2^1} x_3^1 C^0_{ijhk} D^{x^0}_{hk}(u_3^0) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & - \int_{\Omega_2^1} C^0_{ijhk} S^{x^0}_{hk}(\widetilde{\mathbf{u}}^0) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & - \int_{\Omega_2^1} C^0_{ijhk} K^{x^0}_{hk}(\mathbf{u}^1) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & - \int_{\Omega_2^1} M_{ij}\theta^0 S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1. \end{aligned}$$

- **Step g-2** Let $\boldsymbol{\varsigma}^1 = \boldsymbol{\varsigma}^{1,D} + \boldsymbol{\varsigma}^{1,S} + \boldsymbol{\varsigma}^{1,K} + \boldsymbol{\varsigma}^{1,\theta}$ and separate equation $\Longrightarrow$

$$\begin{cases} \int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,D}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = \int_{\Omega_2^1} x_3^1 C^0_{ijhk} D^{x^0}_{hk}(u_3^0) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ \qquad\qquad \boldsymbol{\varsigma}^{1,D} \text{ is } x^1_\alpha\text{-periodic in } \Omega_2^1, \end{cases}$$

$$\begin{cases} \int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,S}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = -\int_{\Omega_2^1} C^0_{ijhk} S^{x^0}_{hk}(\widetilde{\mathbf{u}}^0) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ \qquad\qquad \boldsymbol{\varsigma}^{1,S} \text{ is } x^1_\alpha\text{-periodic in } \Omega_2^1, \end{cases}$$

$$\begin{cases} \int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,K}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = -\int_{\Omega_2^1} C^0_{ijhk} K^{x^0}_{hk}(\mathbf{u}^1) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ \qquad\qquad \boldsymbol{\varsigma}^{1,K} \text{ is } x^1_\alpha\text{-periodic in } \Omega_2^1, \end{cases}$$

and

$$\begin{cases} \int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = -\int_{\Omega_2^1} M_{ij}\theta^0 S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ \qquad\qquad \boldsymbol{\varsigma}^{1,\theta} \text{ is } x^1_\alpha\text{-periodic in } \Omega_2^1. \end{cases} \tag{3.41}$$

- **Substep g-2-1.** Proposition 116 Equation (3.41) $\Longrightarrow$

$$\begin{aligned} \int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = & -\int_{\Omega^1_{\mathrm{Si}}} M_{ij}\theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & - \int_{\Omega^1_{\mathrm{SiO2}}} M_{ij}\theta^0_{|\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \end{aligned}$$

- **Substep g-2-2.** Lemma 170-(e) $\Longrightarrow$

$$\begin{aligned}\int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \;=\; & -\int_{\Omega^1_{\mathrm{Si}}} M_{ij}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & -\int_{\Omega^1_{\mathrm{SiO2}}} M_{ij}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1\end{aligned}$$

- **Substep g-2-3.** Proposition 117 $\Longrightarrow$

$$\int_{\Omega_2^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 = -\int_{\Omega_2^1} M_{ij}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1$$

- **Step g-3** Lemma 154, Proposition 144 $\Longrightarrow$

$$\left.\begin{array}{l} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,D}) = \sum_{p'q'} L^{2,D}_{p'q'hk}(D^{x^0}_{p'q'}(u^0_3)) \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,S}) = \sum_{p'q'} L^{2,S}_{p'q'hk}(S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)) \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,K}) = \sum_{p'q'} L^{2,K}_{p'q'hk}(K^{x^0}_{p'q'}(\mathbf{u}^1)) \\ s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) = L^{2,\theta_{\mathrm{Si}}}_{hk}(\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}}) \end{array}\right. \quad \text{in } \Omega_2^1.$$

h-Source term. Let $\mathbf{w}^{3,1} = \boldsymbol{\psi}^3(x^0)\boldsymbol{\omega}^3(x^1)$ with $\boldsymbol{\psi}^2(x^0) \in \mathcal{C}^\infty_\sharp(\Omega_3^\sharp)^{3\times 3}$, $\boldsymbol{\omega}^3(x^1) \in \mathcal{C}^\infty_\sharp(\Omega_2^1)^3$, and let other test functions equal to 0 in (3.37) $\Longrightarrow$

$$r_3 \oint_{\Omega_3^1} \left(C^0_{ijhk}\left(-x^1_3 D^{x^0}_{hk}(u^0_3) + S^{x^0}_{hk}(\widetilde{\mathbf{u}}^0) + K^{x^0}_{hk}(\mathbf{u}^1) + s^{x^1}_{hk}(\boldsymbol{\varsigma}^1)\right) + M_{ij}\theta^0\right) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 = 0.$$

The proofs of the linear relation for $s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,D})$, $s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,S})$ and $s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,K})$ are the same as in the proof of (g). We detailed the linear relation for $s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta})$ in the following.

We start from the (3.41) and use the same notations for the steps.

- **Step h-2**

$$\left\{\begin{array}{l} \int_{\Omega_3^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 = -\int_{\Omega_3^1} M_{ij}\theta^0 S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \\ \qquad\qquad\qquad\qquad\qquad\qquad \boldsymbol{\varsigma}^{1,\theta} \text{ is } x^1_\alpha\text{-periodic in } \Omega^1_3. \end{array}\right.$$

- **Substep h-2-1.** Proposition 116 Equation (3.41) $\Longrightarrow$

$$\begin{aligned}\int_{\Omega_3^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \;=\; & -\int_{\Omega^1_{\mathrm{Si}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \\ & -\int_{\Omega^1_{\mathrm{SiO2}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{SiO2}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \\ & -\int_{\Omega^1_{\mathrm{Pt}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1\end{aligned}$$

- **Substep h-2-2.** Lemma 170-(f) $\Longrightarrow$

$$\begin{aligned}\int_{\Omega_3^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \;=\; & -\int_{\Omega^1_{\mathrm{Si}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & -\int_{\Omega^1_{\mathrm{SiO2}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}\theta^- S^{x^1}_{ij}(\boldsymbol{\omega}^2)\, dx^1 \\ & -\int_{\Omega^1_{\mathrm{SiO2}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}}\theta^+ S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \\ & -\int_{\Omega^1_{\mathrm{Pt}}} M_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1\end{aligned}$$

- **Substep h-2-3.** Proposition 117 $\Longrightarrow$

$$\int_{\Omega_3^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta}) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 = -\int_{\Omega_3^1} Q^{\mathrm{Si}}_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 - \int_{\Omega_3^1} Q^{\mathrm{Pt}}_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1$$

with

$$Q^{\mathrm{Si}}_{ij} = \begin{cases} M_{ij} \text{ in } \Omega^1_{\mathrm{Si}} \\ M_{ij}\theta^- \text{ in } \Omega^1_{\mathrm{SiO2}} \\ 0 \text{ in } \Omega^1_{\mathrm{Pt}} \end{cases} \text{ and } Q^{\mathrm{Pt}}_{ij} = \begin{cases} 0 \text{ in } \Omega^1_{\mathrm{Si}} \\ M_{ij}\theta^+ \text{ in } \Omega^1_{\mathrm{SiO2}} \\ M_{ij} \text{ in } \Omega^1_{\mathrm{Pt}}. \end{cases}$$

- **Substep h-2-3-1.** Let $\boldsymbol{\varsigma}^{1,\theta} = \boldsymbol{\varsigma}^{1,\theta_{\mathrm{Si}}} + \boldsymbol{\varsigma}^{1,\theta_{\mathrm{Pt}}}$ and separate equation $\Longrightarrow$

$$\begin{cases} \int_{\Omega_3^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta_{\mathrm{Si}}}) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 = -\int_{\Omega_3^1} Q^{\mathrm{Si}}_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \\ \int_{\Omega_3^1} C^0_{ijhk} s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta_{\mathrm{Pt}}}) S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 = -\int_{\Omega_3^1} Q^{\mathrm{Pt}}_{ij}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} S^{x^1}_{ij}(\boldsymbol{\omega}^3)\, dx^1 \end{cases}$$

- **Step h-3** Lemma 154, Proposition 144 $\Longrightarrow$

$$s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta_{\mathrm{Si}}}) = L^{3,\theta_{\mathrm{Si}}}_{hk}(\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}) \text{ and } s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,\theta_{\mathrm{Pt}}}) = L^{3,\theta_{\mathrm{Pt}}}_{hk}(\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}}) \text{ in } \Omega^1_3.$$

■

Lemma 171 $\mathrm{L}_{\alpha 3hk} = -\delta_{h\alpha}\delta_{k3}$ *and* $s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,K}) = \sum_\alpha \delta_{h\alpha}\delta_{k3}\partial_{x^0_\alpha} u^1_3$

Proof. Source term

$$\int_{\Omega^1} c^0_{ijhk} S^{x^1}_{hk}(\boldsymbol{\zeta}^{pq,1}) S^{x^1}_{ij}(\mathbf{w})\, dx^1 = -\int_{\Omega^1} c^0_{ijpq} S^{x^1}_{ij}(\mathbf{w})\, dx^1 \text{ for all } \mathbf{w} \in \mathcal{C}^\infty_\sharp(\Omega^1)^n.$$

- **Step 1.** Equivalent transformation $\Longrightarrow$

$$\int_{\Omega^1} c^0_{ijhk}\partial_{x^1_h}\boldsymbol{\zeta}^{pq,1}_k \partial_{x^1_i} w_j\, dx^1 = -\int_{\Omega^1} c^0_{ijpq}\partial_{x^1_i} w_j\, dx^1.$$

- **Step 2.** Choose $p = \alpha$, $q = 3 \Longrightarrow$

$$\int_{\Omega^1} c^0_{ijhk} \partial_{x^1_h} \boldsymbol{\zeta}^{\alpha 3,1}_k \partial_{x^1_i} w_j \; dx^1 = - \int_{\Omega^1} c^0_{ij\alpha 3} \partial_{x^1_i} w_j \; dx^1.$$

- **Step 3.** Proposition 128 and factoring $\Longrightarrow$

$$\int_{\Omega^1} c^0_{ijhk} \left(\partial_{x^1_h} \boldsymbol{\zeta}^{\alpha 3,1}_k + \delta_{h\alpha}\delta_{k3} \right) \partial_{x^1_i} w_j \; dx^1 = 0.$$

- **Step 4.** Let $(\tau_i)_{i=1,2,3}$ to be the solution of $\partial_{x^1_h} \tau_k = \delta_{h\alpha}\delta_{k3}$, factoring $\Longrightarrow$

$$\int_{\Omega^1} c^0_{ijhk} \partial_{x^1_h} \left(\boldsymbol{\zeta}^{\alpha 3,1}_k + \tau_k \right) \partial_{x^1_i} w_j \; dx^1 = 0.$$

- **Step 5.** Proposition 147 and Proposition 148 $\Longrightarrow$

$$\lambda_k = x^1_3 \delta_{h\alpha}\delta_{k3} \text{ and } \boldsymbol{\zeta}^{\alpha 3,1}_k + \tau_k = 0.$$

- **Step 6.** Equivalent transformation $\Longrightarrow$

$$\boldsymbol{\zeta}^{\alpha 3,1}_k = -x^1_3 \delta_{h\alpha}\delta_{k3}.$$

- **Step 7.** Proposition 144 $\Longrightarrow$

$$L_{\alpha 3hk} = -\delta_{h\alpha}\delta_{k3} \text{ and } s^{x^1}_{hk}(\boldsymbol{\varsigma}^{1,K}) = -\sum_{\alpha} \delta_{h\alpha}\delta_{k3} \partial_{x^0_\alpha} u^1_3$$

■

Lemma 172 ***[Seventh Block: Macroscopic Problem]***

(a) φ^0 *and* $\theta^0_{|\Omega^\sharp_3 \times \Omega^1_{\mathrm{Pt}}}$ *are solutions to the coupled weak equations:*

(a.1)

$$\oint_{\Omega^\sharp_3} \frac{a^H_{\alpha\beta}}{1 + \lambda\theta^0} \partial_{x^0_\beta} \varphi^0 \partial_{x^0_\alpha} v^{E,0} \; dx^0 = \frac{|\Gamma_{01}|}{|\Omega_{\mathrm{Pt}}|} \oint_{\Gamma^\sharp_{01}} j^0 v^{E,0} \; dx^0,$$

(a.2)

$$r^{\mathrm{Pt}} \oint_{\Omega^\sharp_3} k^{3,\mathrm{Pt}}_{\alpha\beta} \partial_{x^0_\beta} \theta^0_{|\Omega^\sharp_3 \times \Omega^1_{\mathrm{Pt}}} \partial_{x^0_\alpha} v^{H,0}_3 \; dx^0 + r^{\mathrm{SiO2}}_3 \oint_{\Omega^\sharp_3} \theta^0_{|\Omega^\sharp_3 \times \Omega^1_{\mathrm{Pt}}} \left(\oint_{\Omega^1_{\mathrm{SiO2}}} k^{\mathrm{SiO2},+}_3 \; dx^1 \right) v^{H,0}_3 \; dx^0$$

$$= r^{\mathrm{Pt}} \oint_{\Omega^\sharp_3} \frac{a^0_{ij}}{1 + \lambda\theta^0_{|\Omega^\sharp_3 \times \Omega^1_{\mathrm{Pt}}}} \left(\oint_{\Omega^1_{\mathrm{Pt}}} (\delta_{j\beta} + \partial_{x^1_j} \xi^{1,\mathrm{Pt}}_\beta)(\delta_{i\alpha} + \partial_{x^1_i} \xi^{1,\mathrm{Pt}}_\alpha) \; dx^1 \right) \partial_{x^0_\beta} \varphi^0 \varphi^0 \partial_{x^0_\alpha} v^{H,0}_3 \; dx^0$$

(b) $\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm Si}}$ *is the solution to*

$$r_2^{\rm Si}\oint_{\Omega_2^\sharp} k^{2,{\rm Si}}_{\alpha\beta}\partial_{x^0_\beta}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm Si}}\partial_{x^0_\alpha}v_2^{H,0}\ dx^0=0$$

(c) $\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}$ *is the solution to*

$$r_3^{\rm Si}\int_{\Omega_3^\sharp} k^{3,{\rm Si}}_{\alpha\beta}\partial_{x^0_\beta}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}\partial_{x^0_\alpha}v_3^{H,0}\ dx^0-r_3^{\rm SiO2}\oint_{\Omega_3^\sharp}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}\Big(\oint_{\Omega^1_{\rm SiO2}} k_3^{{\rm SiO2},^-}\ dx^1\Big)\ v_3^{H,0}\ dx^0=0$$

(d) $(\widetilde{u}_\alpha)_{\alpha=1,2}$ *and* u_3^0 *are the solutions to*

$$\begin{aligned}
&\int_{\Omega_2^\sharp}\Big(C^{H,DD}_{p'q'pq}D^{x^0}_{p'q'}(u_3^0)+C^{H,SD}_{p'q'pq}S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)+M^{2,D}_{pq}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm Si}}\Big)\cdot D^{x^0}_{pq}(v_3^0)\ dx^0\\
&+\int_{\Omega_2^\sharp}\Big(C^{H,SD}_{p'q'pq}D^{x^0}_{p'q'}(u_3^0)+C^{H,SS}_{p'q'pq}S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)+M^{2,S}_{pq}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\rm Si}}\Big)\cdot S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\ dx^0\\
+\int_{\Omega_3^\sharp}&\Big(C^{H,DD}_{p'q'pq}D^{x^0}_{p'q'}(u_3^0)+C^{H,SD}_{p'q'pq}S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)+M^{3,D,{\rm Pt}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}+M^{3,D,{\rm Si}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}\Big)\cdot D^{x^0}_{pq}(v_3^0)\ dx^0\\
+\int_{\Omega_3^\sharp}&\Big(C^{H,SD}_{p'q'pq}D^{x^0}_{p'q'}(u_3^0)+C^{H,SS}_{p'q'pq}S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)+M^{3,S,{\rm Pt}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Pt}}+M^{3,S,{\rm Si}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\rm Si}}\Big)\cdot S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\ dx^0\\
&=\int_{\Omega^\sharp}-q^0_\alpha\partial_{x^0_\alpha}v_3^0+f_3^0v_3^0+f^0_\alpha\widetilde{v}^0_\alpha\ dx^0,
\end{aligned}$$

Proof. a.1-Source term. We choose $v^{E,0}\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp)$ and $v^{E,1}=\partial_{x^0_\alpha}v^{E,0}\theta^{1,{\rm Pt}}_\alpha\in\mathcal{C}^\infty(\Omega_3^\sharp,C^\infty_\sharp(\Omega^1_{\rm Pt}))$ in (3.35).

- **Step a.1-1** Lemma 170 $\Longrightarrow$

$$\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}}\frac{a^0_{ij}}{1+\lambda\theta^0}\Big(\chi^{(j)}_{\{1,2\}}\partial_{x^0_j}\varphi^0+\partial_{x^0_\beta}\varphi^0\partial_{x^1_j}\xi^{1,{\rm Pt}}_\beta\Big)\Big(\chi^{(i)}_{\{1,2\}}\partial_{x^0_i}v^{E,0}+\partial_{x^0_\alpha}v^{E,0}\partial_{x^1_i}\xi^{1,{\rm Pt}}_\alpha\Big)\ dx^0dx^1 \tag{3.42}$$
$$=\frac{|\Gamma_{01}|}{|\Omega_{\rm Pt}|}\oint_{\Gamma^\sharp_{01}\times\Gamma^1_{01}}j^0v^{E,0}dx^0dx^1$$

- **Step a.1-2** Proposition 128

$$\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}}\frac{a^0_{ij}}{1+\lambda\theta^0}(\delta_{j\beta}+\partial_{x^1_j}\xi^{1,{\rm Pt}}_\beta)(\delta_{i\alpha}+\partial_{x^1_i}\xi^{1,{\rm Pt}}_\alpha)\partial_{x^0_\alpha}\varphi^0\partial_{x^0_\beta}v^{E,0}\ dx^0dx^1$$
$$=\frac{|\Gamma_{01}|}{|\Omega_{\rm Pt}|}\oint_{\Gamma^\sharp_{01}\times\Gamma^1_{01}}j^0v^{E,0}\ dx^0dx^1$$

- **Step a.1-3** Factoring and definitions (166) $\Longrightarrow$

$$\oint_{\Omega_3^\sharp} \frac{a^H_{\alpha\beta}}{1+\lambda\theta^0}\partial_{x^0_\beta}\varphi^0\partial_{x^0_\alpha}v^{E,0}\ dx^0dx^1\ dx^0 = \frac{|\Gamma_{01}|}{|\Omega_{\rm Pt}|}\oint_{\Gamma_{01}^\sharp} j^0 v^{E,0}\ dx^0dx^1,$$

with $a^H_{\alpha\beta} = \oint_{\Omega^1_{\rm Pt}} a^0_{ij}(\delta_{j\beta}+\partial_{x^1_j}\xi^{1,{\rm Pt}}_\beta)(\delta_{i\alpha}+\partial_{x^1_i}\xi^{1,{\rm Pt}}_\alpha)\ dx^1$.

a.2-Source term. Choose $v_2^{H,0}=0$, $v_2^{H,1}=0$, $v_3^{H,0}\in\mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp;\mathcal{C}^\infty_{\Gamma^{1,Lat}_{\rm SiO2}}(\Omega^1_{\rm SiO2}))$ and $v_3^{H,1}=\partial_{x^0_\alpha}v^{H,0}_{3\alpha}\zeta^{1,{\rm Pt}}_\alpha$ in $\Omega_3^\sharp\times\Omega^1_{\rm Pt}$ in (3.36), where $\Gamma^{1,Lat}_{\rm SiO2}$ is the lateral boundary of $\Omega^1_{\rm SiO2}$.

- **Step a.2-1.** Lemma 170(f) $\Longrightarrow$

$$\begin{aligned}
& r^{\rm Pt}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}} k^0_{ij}\left(\chi^{(j)}_{\{1,2\}}\partial_{x^0_j}\theta^0+\partial_{x^0_\beta}\theta^0\partial_{x^1_j}\zeta^{1,{\rm Pt}}_\beta\right)\left(\chi^{(i)}_{\{1,2\}}\partial_{x^0_i}v_3^{H,0}+\partial_{x^0_\alpha}v_3^{H,0}\partial_{x^1_i}\zeta^{1,{\rm Pt}}_\alpha\right)\ dx^0dx^1 \\
& \qquad + r_3^{\rm SiO2}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm SiO2}} k^0_{ij}\partial_{x^1_j}\theta^0\partial_{x^1_i}v^{H,0}\ dx^0dx^1 \\
= \ & -r^{\rm Pt}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}} \frac{a^0_{ij}\varphi^0}{1+\lambda\theta^0}\left(\chi^{(j)}_{\{1,2\}}\partial_{x^0_j}\varphi^0+\partial_{x^0_\beta}\varphi^0\partial_{x^1_j}\zeta^{1,{\rm Pt}}_\beta\right)\left(\chi^{(i)}_{\{1,2\}}\partial_{x^0_i}v_3^{H,0}+\partial_{x^0_\alpha}v_3^{H,0}\partial_{x^1_i}\zeta^{1,{\rm Pt}}_\alpha\right)\ dx^0dx^1
\end{aligned}$$

- **Step a.2-2**. Proposition 128 $\Longrightarrow$

$$\begin{aligned}
& r^{\rm Pt}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}} k^0_{ij}(\delta_{j\beta}+\partial_{x^1_j}\zeta^{1,{\rm Pt}}_\beta)(\delta_{i\alpha}+\partial_{x^1_i}\zeta^{1,{\rm Pt}}_\alpha)\partial_{x^0_\alpha}\theta^0\partial_{x^0_\beta}v_3^{H,0}\ dx^0dx^1 \\
& + r_3^{\rm SiO2}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm SiO2}} k^0_{ij}\partial_{x^1_j}\theta^0\partial_{x^1_i}v_3^{H,0}\ dx^0dx^1 \\
= \ & r^{\rm Pt}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}} \frac{a^0_{ij}\varphi^0}{1+\lambda\theta^0}(\delta_{j\beta}+\partial_{x^1_j}\xi^{1,{\rm Pt}}_\beta)(\delta_{i\alpha}+\partial_{x^1_i}\xi^{1,{\rm Pt}}_\alpha)\partial_{x^0_\beta}\varphi^0\partial_{x^0_\alpha}v^{H,0}_{3\alpha}\ dx^0dx^1
\end{aligned}$$

- **Substep a.2-2-1.** Lemma 127 $\Longrightarrow$

$$\begin{aligned}
& r^{\rm Pt}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}} k^0_{ij}(\delta_{j\beta}+\partial_{x^1_j}\zeta^{1,{\rm Pt}}_\beta)(\delta_{i\alpha}+\partial_{x^1_i}\zeta^{1,{\rm Pt}}_\alpha)\partial_{x^0_\alpha}\theta^0\partial_{x^0_\beta}v_3^{H,0}\ dx^0dx^1 \\
& -r_2^{\rm SiO2}\oint_{\Omega_2^\sharp\times\Omega^1_{\rm SiO2}} \partial_{x^1_i}\left(k^0_{ij}\partial_{x^1_j}\theta^0\right)v_3^{H,0}\ dx^0dx^1 + r_3^{\rm SiO2}\oint_{\Omega_3^\sharp\times\Gamma^{1,\pm}_{\rm SiO2}} k^0_{ij}\partial_{x^1_j}\theta^0 n_{x^1_3}v_3^{H,0}\ dx^0dx^1 \\
& = r^{\rm Pt}\oint_{\Omega_3^\sharp\times\Omega^1_{\rm Pt}} \frac{a^0_{ij}}{1+\lambda\theta^0}(\delta_{j\beta}+\partial_{x^1_j}\xi^{1,{\rm Pt}}_\beta)(\delta_{i\alpha}+\partial_{x^1_i}\xi^{1,{\rm Pt}}_\alpha)\partial_{x^0_\beta}\varphi^0\varphi^0\partial_{x^0_\alpha}v^{H,0}_{3\alpha}\ dx^0dx^1
\end{aligned}$$

- **Substep a.2-2-2.** Lemma 170(f) $\Longrightarrow$

$$r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} k^0_{ij}(\delta_{j\beta} + \partial_{x_j^1}\zeta^{1,\mathrm{Pt}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\zeta^{1,\mathrm{Pt}}_\alpha)\partial_{x^0_\beta}\theta^0 \partial_{x^0_\alpha} v_3^{H,0}\, dx^0 dx^1$$
$$+ r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp \times \Gamma^{1,+}_{\mathrm{SiO2}}} \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} k^0_{3j}\partial_{x_j^1}\theta^+ v_3^{H,0}\, dx^0 dx^1$$
$$= r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} \frac{a^0_{ij}\varphi^0}{1+\lambda\theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}}}(\delta_{j\beta} + \partial_{x_j^1}\xi^{1,\mathrm{Pt}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\xi^{1,\mathrm{Pt}}_\alpha)\partial_{x^0_\beta}\varphi^0 \partial_{x^0_\alpha} v_{3\alpha}^{H,0}\, dx^0 dx^1$$

- **Step a.2-3.** Choose $v_3^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp)$ and factoring $\Longrightarrow$

$$r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp} k^{3,\mathrm{Pt}}_{\alpha\beta}\partial_{x^0_\beta}\theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}}\partial_{x^0_\alpha} v_3^{H,0}\, dx^0 + r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp} \theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} k_3^{\mathrm{SiO2},+} v_3^{H,0}\, dx^0$$
$$= r^{\mathrm{Pt}} \oint_{\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}} \frac{a^0_{ij}}{1+\lambda\theta^0_{|\Omega_3^\sharp \times \Omega^1_{\mathrm{Pt}}}}(\delta_{j\beta} + \partial_{x_j^1}\xi^{1,\mathrm{Pt}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\xi^{1,\mathrm{Pt}}_\alpha)\partial_{x^0_\beta}\varphi^0\varphi^0 \partial_{x^0_\alpha} v_{3\alpha}^{H,0}\, dx^0 dx^1$$

with

$$k^{3,\mathrm{Pt}}_{\alpha\beta} = \oint_{\Omega^1_{\mathrm{Pt}}} k^0_{ij}(\delta_{j\beta}+\partial_{x_j^1}\zeta^{1,\mathrm{Pt}}_\beta)(\delta_{i\alpha}+\partial_{x_i^1}\zeta^{1,\mathrm{Pt}}_\alpha)\, dx^1 \text{ and } k_3^{\mathrm{SiO2},+} = \oint_{\Gamma^{1,+}_{\mathrm{SiO2}}} k^0_{3j}\partial_{x_j^1}\theta^+\, dx^1.$$

b-Source term. Choose $v_3^{H,0} = 0$, $v_3^{H,1} = 0$, $v_2^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp}(\Omega_2^\sharp; \mathcal{C}^\infty_{\Gamma^{1,Lat}_{\mathrm{SiO2}}}(\Omega^1_{\mathrm{SiO2}}))$ and $v_2^{H,1} = \partial_{x^0_\alpha} v_2^{H,0}\zeta^{1,\mathrm{Si}}_\alpha$ in $\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}$ in (3.36), where $\Gamma^{1,Lat}_{\mathrm{SiO2}}$ is the lateral boundary of Ω^1_{SiO2}.

- **Step b-1** Lemma 170 $\Longrightarrow$

$$r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} k^0_{ij}\left(\chi_{\{1,2\}}(j)\partial_{x_j^0}\theta^0 + \partial_{x^0_\beta}\theta^0\partial_{x_j^1}\zeta^{1,\mathrm{Si}}_\beta\right)\left(\chi_{\{1,2\}}(i)\partial_{x_i^0} v_2^{H,0} + \partial_{x^0_\alpha} v_2^{H,0}\partial_{x_i^1}\zeta^{1,\mathrm{Si}}_\alpha\right)\, dx^0 dx^1$$
$$+ r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} k^0_{ij}\partial_{x_j^1}\theta^0\partial_{x_i^1} v_2^{H,0}\, dx^0 dx^1 = 0$$

- **Step b-2.** Proposition 128 $\Longrightarrow$

$$r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} k^0_{ij}(\delta_{j\beta} + \partial_{x_j^1}\zeta^{1,\mathrm{Si}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\zeta^{1,\mathrm{Si}}_\alpha)\partial_{x^0_\alpha}\theta^0\partial_{x^0_\beta} v_2^{H,0}\, dx^0 dx^1$$
$$+ r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} k^0_{ij}\partial_{x_j^1}\theta^0\partial_{x_i^1} v_2^{H,0}\, dx^0 dx^1 = 0$$

- **Substep b-2-1.** Lemma 127 $\Longrightarrow$

$$r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} k^0_{ij}(\delta_{j\beta} + \partial_{x_j^1}\zeta^{1,\mathrm{Si}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\zeta^{1,\mathrm{Si}}_\alpha)\partial_{x^0_\alpha}\theta^0\partial_{x^0_\beta}v_2^{H,0}\ dx^0dx^1$$
$$-r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{SiO2}}} \partial_{x_i^1}\left(k^0_{ij}\partial_{x_j^1}\theta^0\right) v_2^{H,0}\ dx^0dx^1$$
$$+r_2^{\mathrm{SiO2}} \oint_{\Omega_2^\sharp \times \Gamma^{1,\pm}_{\mathrm{SiO2}}} n_{x_3^1}\left(k^0_{3j}\partial_{x_j^1}\theta^0\right) v_2^{H,0}\ dx^0dx^1 = 0$$

- **Substep b-2-2.** Lemma 170(e) $\Longrightarrow$

$$r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp \times \Omega^1_{\mathrm{Si}}} k^0_{ij}(\delta_{j\beta} + \partial_{x_j^1}\zeta^{1,\mathrm{Si}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\zeta^{1,\mathrm{Si}}_\alpha)\partial_{x^0_\alpha}\theta^0\partial_{x^0_\beta}v_2^{H,0}\ dx^0dx^1 = 0$$

- **Step b-3.** Choose $v_2^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_2^\sharp}(\Omega_2^\sharp)$ and factoring $\Longrightarrow$

$$r_2^{\mathrm{Si}} \oint_{\Omega_2^\sharp} k^{2,\mathrm{Si}}_{\alpha\beta}\partial_{x^0_\beta}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}}\partial_{x^0_\alpha}v_2^{H,0}\ dx^0 = 0$$

with

$$k^{2,\mathrm{Si}}_{\alpha\beta} = \oint_{\Omega^1_{\mathrm{Si}}} k^0_{ij}(\delta_{j\beta} + \partial_{x_j^1}\zeta^{1,\mathrm{Si}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\zeta^{1,\mathrm{Si}}_\alpha)\ dx^1.$$

c-Source term. Choose $v_2^{H,0} = 0$, $v_2^{H,1} = 0$, $v_3^{H,0} \in \mathcal{C}^\infty_{\partial\Omega_3^\sharp}(\Omega_3^\sharp; \mathcal{C}^\infty_{\Gamma^{1,Lat}_{\mathrm{SiO2}}}(\Omega^1_{\mathrm{SiO2}}))$ and $v_3^{H,1} = \partial_{x^0_\alpha}v_3^{H,0}\zeta^{1,\mathrm{Si}}_\alpha$ in $\Omega_3^\sharp \times \Omega^1_{\mathrm{Si}}$ in (3.36). Follow the same steps as the proof for (c), we get the conclusion

$$r_3^{\mathrm{Si}} \int_{\Omega_3^\sharp} k^{3,\mathrm{Si}}_{\alpha\beta}\partial_{x^0_\beta}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}\partial_{x^0_\alpha}v_3^{H,0}\ dx^0 - r_3^{\mathrm{SiO2}} \oint_{\Omega_3^\sharp} \theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}} k_3^{\mathrm{SiO2},-}v_3^{H,0}\ dx^0dx^1 = 0$$

with

$$k^{3,\mathrm{Si}}_{\alpha\beta} = \oint_{\Omega^1_{\mathrm{Si}}} k^0_{ij}(\delta_{j\beta} + \partial_{x_j^1}\zeta^{1,\mathrm{Si}}_\beta)(\delta_{i\alpha} + \partial_{x_i^1}\zeta^{1,\mathrm{Si}}_\alpha)\ dx^1 \text{ and } k_3^{\mathrm{SiO2},-} = \oint_{\Gamma^{1,-}_{\mathrm{SiO2}}} k^0_{3j}\partial_{x_j^1}\theta^-\ dx^1.$$

d-Source term. We choose $\widetilde{v}^0_\alpha, v^0_3, v^1_3 \in \mathcal{C}^\infty(\Omega^\sharp)$, for $d \in \{2,3\}$, let

$$s^{x^1}_{ij}(\mathbf{w}^{d,1}) = \widetilde{L}^{d,D}_{pqij}D^{x^0}_{pq}(v^0_3) + \widetilde{L}^{d,S}_{pqij}S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0) + \sum_\beta \delta_{i\beta}\delta_{j3}\partial_{x^0_\alpha}v^1_3 \text{ in } \Omega_d^\sharp \times \Omega^1_d$$

in (3.37).

- **Step d-1.** Lemma 170, Proposition 128 and Lemma 171 $\Longrightarrow$

$$
\begin{aligned}
r_2 \oint_{\Omega_2^\sharp\times\Omega_2^1} \left(C^0_{ijhk}\left(\widetilde{L}^{2,D}_{p'q'hk} D^{x^0}_{p'q'}(u_3^0) + \widetilde{L}^{2,S}_{p'q'hk} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + L^{2,\theta_{\mathrm{Si}}}_{hk}(\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}})\right) + M_{ij}\theta^0\right)\cdot \\
\left(\widetilde{L}^{2,D}_{pqij} D^{x^0}_{pq}(v_3^0) + \widetilde{L}^{2,S}_{pqij} S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\right)\ dx^0dx^1 \\
+r_3 \oint_{\Omega_3^\sharp\times\Omega_3^1} \left(C^0_{ijhk}\left(\widetilde{L}^{3,D}_{p'q'hk} D^{x^0}_{p'q'}(u_3^0) + \widetilde{L}^{3,S}_{p'q'hk} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0)\right) + M_{ij}\theta^0\right)\cdot \\
\left(\widetilde{L}^{3,D}_{pqij} D^{x^0}_{pq}(v_3^0) + \widetilde{L}^{3,S}_{pqij} S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\right)\ dx^0dx^1 \\
+r_3 \oint_{\Omega_3^\sharp\times\Omega_3^1} \left(C^0_{ijhk}\left(L^{3,\theta_{\mathrm{Si}}}_{hk}(\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}) + L^{3,\theta_{\mathrm{Pt}}}_{hk}(\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}})\right) + M_{ij}\theta^0\right)\cdot \\
\left(\widetilde{L}^{3,D}_{pqij} D^{x^0}_{pq}(v_3^0) + \widetilde{L}^{3,S}_{pqij} S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\right)\ dx^0dx^1 \\
= \sum_d r_d \oint_{\Omega_d^\sharp\times\Omega_d^1} f^{M,0}_\alpha\left(-x_3^1\partial_{x^0_\alpha} v_3^0 + \widetilde{v}^0_\alpha\right) + f^{M,0}_3 v_3^0\ dx^0dx^1
\end{aligned}
$$

- **Step d-2.** Lemma 170(e) and (f), factoring and definitions 166 $\Longrightarrow$

$$
\begin{aligned}
&\int_{\Omega_2^\sharp}\left(C^{H,DD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SD}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{2,D}_{pq}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}}\right)\cdot D^{x^0}_{pq}(v_3^0)\ dx^0 \\
&+\int_{\Omega_2^\sharp}\left(C^{H,SD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SS}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{2,S}_{pq}\theta^0_{|\Omega_2^\sharp\times\Omega^1_{\mathrm{Si}}}\right)\cdot S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\ dx^0 \\
&+\int_{\Omega_3^\sharp}\left(C^{H,DD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SD}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{3,D,\mathrm{Pt}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} + M^{3,D,\mathrm{Si}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}\right)\cdot D^{x^0}_{pq}(v_3^0)\ dx \\
&+\int_{\Omega_3^\sharp}\left(C^{H,SD}_{p'q'pq} D^{x^0}_{p'q'}(u_3^0) + C^{H,SS}_{p'q'pq} S^{x^0}_{p'q'}(\widetilde{\mathbf{u}}^0) + M^{3,S,\mathrm{Pt}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Pt}}} + M^{3,S,\mathrm{Si}}_{pq}\theta^0_{|\Omega_3^\sharp\times\Omega^1_{\mathrm{Si}}}\right)\cdot S^{x^0}_{pq}(\widetilde{\mathbf{v}}^0)\ dx^0 \\
&=\int_{\Omega^\sharp} -q^0_\alpha\partial_{x^0_\alpha} v_3^0 + f_3^0 v_3^0 + f^0_\alpha\widetilde{v}^0_\alpha\ dx^0,
\end{aligned}
$$

for $a,b\in\{D,S\}$ and $m\in\{\mathrm{Si},\mathrm{Pt}\}$ the homogenized coefficients are defined by $C^{H,ab}_{p'q'pq} = \chi_{(\Omega_d^\sharp)}(x^0)\oint_{\Omega_d^1} C^0_{ijhk}\widetilde{L}^{d,a}_{p'q'hk}\widetilde{L}^{d,b}_{pqij}dx^1$, $M^{2,D}_{pq} = \oint_{\Omega_2^1}\left(C^0_{ijhk}L^{2,\theta_{\mathrm{Si}}}_{hk} + M_{ij}\right)\widetilde{L}^{2,D}_{pqij}dx^1$, $M^{2,S}_{pq} = \oint_{\Omega_2^1}\left(C^0_{ijhk}L^{2,\theta_{\mathrm{Si}}}_{hk} + M_{ij}\right)\widetilde{L}^{2,S}_{pqij}dx^1$ and $M^{3,b,m}_{pq} = \oint_{\Omega_3^1}\left(C^0_{ijhk}L^{3,\theta_m}_{hk} + Q^m_{ij}\right)\widetilde{L}^{3,b}_{pqij}dx^1$, the homogenized force loads are $q^0_\alpha = \chi_{(\Omega_d^\sharp)}(x^0)\oint_{\Omega_d^1} x_3^1 f^{M,0}_\alpha\,dx^1$, $f^0_\alpha = \chi_{(\Omega_d^\sharp)}(x^0)\oint_{\Omega_d^1} f^{M,0}_\alpha\,dx^1$ and $f^0_3 = \chi_{(\Omega_d^\sharp)}(x^0)\oint_{\Omega_d^1} f^{M,0}_3\,dx^1$.

■

3.4 Appendix I: The Reference Proof

This chapter follows the same reference proof as introduced in chapter 1 Section 1.3 with some modifications corresponding to the new approach. In the previous approach, the weak expansion of two-scale transform i.e $T(u^\varepsilon) = u^0 + \varepsilon u^1$ is applied. The difficulty of this approach is that εu^1 is non-periodic. In this approach, Assumption (152) which allows a periodic εu^1 is applied. This reduces much of the proof.

Only different proof steps between this approach and the previous one is discussed here.

Assumption 173 ***[Two-scale approximation of*** u***]*** *There exist* u^0, $u^1 \in L^2(\Omega^\sharp \times \Omega^1)$ *such that*

$$\kappa^0 \int_\Omega u^\varepsilon \; Bv \; dx - \kappa^1 \int_{\Omega^\sharp \times \Omega^1} u^0 \; v \; dx^0 dx^1 = O(\varepsilon) \text{ for all } v \in \mathcal{C}^\infty(\Omega^\sharp \times \Omega^1) \quad (3.43)$$

$$\text{and } \kappa^0 \int_\Omega u^\varepsilon \; Bv \; dx - \kappa^1 \int_{\Omega^\sharp \times \Omega^1} (u^0 + \varepsilon u^1) v \; dx^0 dx^1 = \varepsilon O(\varepsilon) \text{ for all } v \in \mathcal{D}(\Omega^\sharp; \mathcal{C}^\infty_\sharp(\Omega^1)). \quad (3.44)$$

In this assumption, we can prove that u^1 is periodic.

Proposition 174 ***[Two-scale Limit of a Derivative]*** *If* u^ε *is a sequence bounded as in (1.15) and satisfying (3.44), then* u^0 *is independent of* x^1 *and*

$$\kappa^0 \int_\Omega \partial_x u^\varepsilon Bv \; dx - \kappa^1 \int_{\Omega^\sharp \times \Omega^1} \eta v \; dx^0 dx^1 = O(\varepsilon) \text{ for all } v \in \mathcal{C}^\infty(\Omega^\sharp \times \Omega^1)$$

where

$$\eta = \frac{\partial u^0}{\partial x^\sharp} + \frac{\partial u^1}{\partial x^1}. \quad (3.45)$$

Moreover, if $u^\varepsilon = 0$ *on* Γ *then* $u^0 = 0$ *on* $\Gamma^\sharp$.

The proof is split into four Lemmas.

Lemma 175 ***[First Block: Constraint on*** u^0***]*** u^0 *is independent of* x^1.

The proof is the same as for that of Lemma 22. In step 2, instead of using operator T^*, we use two-scale approximation (3.43) directly. The other part of the proof keeps the same.

Lemma 176 ***[Second Block: Two-Scale Limit of the Derivative]*** $\eta = \frac{\partial u^0}{\partial x^\sharp} + \frac{\partial u^1}{\partial x^1}$.

Proof. This proof starts from the source term

$$\Psi = \kappa^0 \int_\Omega \frac{du^\varepsilon}{dx} B v dx \tag{3.46}$$

with $v \in \mathcal{C}^\infty_{\Gamma^\sharp}(\Omega^\sharp; \mathcal{C}^\infty_{\Gamma^1}(\Omega^1))$.

- **Step 1.** Green formula (1.12), Proposition 16 and the linearity of integrals $\Longrightarrow$

$$\Psi = -\kappa^0 \int_\Omega u^\varepsilon B(\frac{\partial v}{\partial x^\sharp})\ dx - \frac{\kappa^0}{\varepsilon} \int_\Omega u^\varepsilon B(\frac{\partial v}{\partial x^1})\ dx + O(\varepsilon).$$

- **Step 2.** Assumption (3.43) in the first term and (3.44) in the second one $\Longrightarrow$

$$\Psi = -\kappa^1 \int_{\Omega^\sharp \times \Omega^1} u^0 \frac{\partial v}{\partial x^\sharp}\ dx^0 dx^1 - \frac{\kappa^1}{\varepsilon} \int_{\Omega^\sharp \times \Omega^1} u^0 \frac{\partial v}{\partial x^1}\ dx^0 dx^1 - \kappa^1 \int_{\Omega^\sharp \times \Omega^1} u^1 \frac{\partial v}{\partial x^1}\ dx^0 dx^1 + O(\varepsilon).$$

- The following steps are the same as Step 4 to Step 6 of proof of Lemma 3.46, we get

$$\eta = \frac{\partial u^0}{\partial x^\sharp} + \frac{\partial u^1}{\partial x^1}.$$

■

Lemma 177 ***[Third Block: Microscopic Boundary Condition]*** *u^1 is Ω^1-periodic.*

Proof. **Source term.** In (3.46), we choose $v \in \mathcal{C}^\infty_{\Gamma^\sharp}(\Omega^\sharp; \mathcal{C}^\infty_\sharp(\Omega^1))$.

- **Step 1.** The steps 1-3 of the second block $\Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp \times \Omega^1} \eta v\ dx^0 dx^1 - \kappa^1 \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^0}{\partial x^\sharp} v\ dx^0 dx^1 - \frac{\kappa^1}{\varepsilon} \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^0}{\partial x^1} v\ dx^0 dx^1$$
$$-\kappa^1 \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^1}{\partial x^1} v\ dx^0 dx^1 - \kappa^1 \int_{\Omega^\sharp \times \Gamma^1} u^1 v\ n_{\Gamma^1}\ dx^0 dx^1 + O(\varepsilon).$$

- **Step 2.** Lemma 175, and passing to the limit when $\varepsilon \to 0$ and Lemma 176 $\Longrightarrow$

$$\int_{\Omega^\sharp \times \Gamma^1} u^1 v\ n_{\Gamma^1}\ dx^0 ds(x^1) = O(\varepsilon). \tag{3.47}$$

- **Step 3.** Proposition 2 $\Longrightarrow$

$$u^1 \text{ is } \Omega^1\text{-periodic.} \tag{3.48}$$

■

Lemma 178 ***[Fourth Block: Macroscopic Boundary Condition]*** *u^0 vanishes on $\Gamma^\sharp$.*

Proof. **Source term.** In (3.46), we choose $v \in \mathcal{C}^\infty(\Omega^\sharp; \mathcal{C}^\infty_{\Gamma^1}(\Omega^1))$,

- **Step 1.** The steps 1-3 of the second block and $u^\varepsilon = 0$ on $\Gamma \Longrightarrow$

$$\kappa^1 \int_{\Omega^\sharp \times \Omega^1} \eta\ v\ dx^0 dx^1 = \kappa^1 \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^0}{\partial x^\sharp} v\ dx^0 dx^1 + \frac{\kappa^1}{\varepsilon} \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^0}{\partial x^1} v\ dx^0 dx^1$$
$$+\kappa^1 \int_{\Omega^\sharp \times \Omega^1} \frac{\partial u^1}{\partial x^1} v\ dx^0 dx^1 - \kappa^1 \int_{\Gamma^\sharp \times \Omega^1} u^0 v n_{x^\sharp}\ ds(x^\sharp) dx^1 + O(\varepsilon).$$

- **Step 2.** Lemma 175, passing to the limit when $\varepsilon \to 0$, and using Lemma 176 $\Longrightarrow$

$$\kappa^1 \int_{\Gamma^\sharp \times \Omega^1} u^0 v n_{x^\sharp}\ ds(x^\sharp) dx^1 = 0.$$

- **Step 3.** Proposition 1 $\Longrightarrow$

$$u^0 = 0 \text{ on } \Gamma^\sharp.$$

■

Chapter 4

Optimization for the SThM probe

Abstract. *In this chapter we introduce an optimization tool and discuss its application to the optimization of SThM probe developed in the NANOHEAT project. This tool combines the house-made optimization software package SIMBAD with COMSOL-MATLAB simulation. The parametrization of the probe and the simulation conditions are given first. Then the contribution of each parameters are analyzed independently and some influential ones are selected. In this step, the optimization principles which could be used in the similar design are summarized. Next, the optimization of parameters for the identified tradeoffs are implemented and the results are shown by the pareto front plot.*

4.1 Introduction

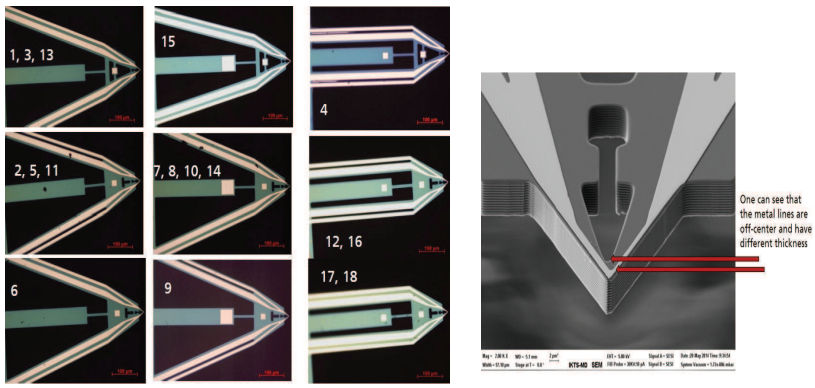
This chapter is devoted to design an optimization tool for the application of the model from *MEMSLab*. Since this part of work is supported by the NANOHEAT project, this tool is applied for the optimization of the SThM probe developed in this project. This tool is a combination of the house made optimization software package SIMBAD and the COMSOL-MATLAB simulation. The application of this tool for the optimization of the SThM probe contributes in two aspects. The first one is the general optimization principle for the design and the second one is obtaining an optimal design which improved much the performance than the original design. The first contribution comes from the general analysis for each parameter and the second one comes from the trade-off optimization for the influential parameters.

4.1.1 Organization of the Chapter

This chapter is organized as follows: In Section 4.2, the optimization problem for the SThM probe is described. It includes the description of the probe structure, the physical functioning of each component, critical phenomena should be considered in the design and the design goal of the probe. In addition, the limitation of the optimization without using a specialised tool is illustrated. In Section 4.3, the parametrization of the SThM probe has been done but only the figure and values are reported. In Section 4.4, a single simulation used in the optimization loop and some useful features are discussed. In Section 4.5, The house-made software package Simbad is briefly illustrated. Then in Section 4.6.1, the discussion of the influences of each parameter is detailed and design rules are summarized. In the Section 4.6.2, trade-offs of some influential parameters are found by SIMBAD and an optimal design is reported.

4.2 Statement of the design problem

The SThM probes used in NANOHEAT project, see [43], as shown in Figure 4.1, are designed as three-layered structures. A thick Silicon cantilever is at the bottom layer to support the whole structure and a SiO2 layer is deposited on it to serve as an electric insulator layer. A thin Platinum trail consisting of four legs and a sharp tip is deposited on the top layer. The internal two legs are used to form a heating circuit and the external ones are for tip voltage sensing. The piezo-resistive sensor which is used to measure the tip displacement under a force is embedded in the silicon layer, covered by the SiO2 layer and located at the bottom of the middle part.



(a) Samples of the SThM probe (b) Tip

Figure 4.1: Samples of SThM probes

Two critical phenomena are considered in the design. They are bimetallic due to the differences of the thermal expansion coefficients in each layer and dependence of the tip-sample interface resistance on the contact pressure, see [36][40] and [54].

In view of the application, the following design objectives should be achieved. First, a flexible cantilever is needed to prevent the damage of the the fragile tip when the tip-sample contact force exceeds some limit. Second, the tip displacement caused by the bimetallic effect should be reduced. Third, a high efficient resistive tip is needed. Last, the piezo-resistive sensor should be sensitive to the tip displacement at least for the photographic measurement. These design goals are characterized by some features in the simulation which will be introduced later.

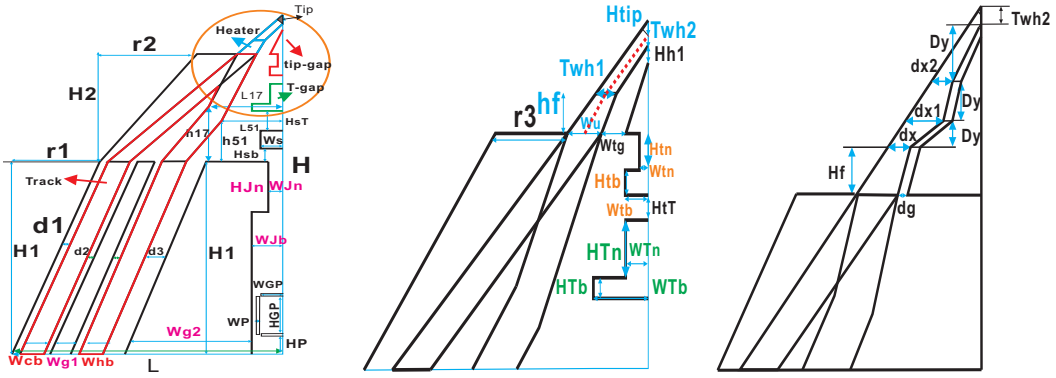
Some efforts has been tried for optimization of this probe by trial and error method. As shown in Figure 4.1(a), a lot of samples are designed and fabricated, then the best one will be selected according to their experimental performances. It is time consuming and expensive. In addition, they could not understand the main optimization rules which might be useful for future works. On the other hand, the objective features could be predicted by numerical simulations which is much faster and cheaper than experiments. The simulation could be used by optimization software packages to find the design rules.

We observe that each sample in Figure 4.1(a) contains a Platinum trail, a small tip, see Figure 4.1(b), some gaps near the tip and some gaps at the bottom. So instead of studying these samples one by one, we introduce a parametrization which more or less can covers all these samples and the analysis is done for this abstract probe.

4.3 Parametrization of the probe

The parametrization of the geometry is the first step for optimization. It includes the parameterized diagram, the initial values and limits of each parameter and the geometry constraints between them. In this part, the discussion of the complex constraints are not reported.

The parameterized figure of the probe is shown in Figure 4.2(a) and the detailed figure of the tip is shown in Figure 4.2(b). The red dotted line shows the watching points in the heater and these points are indexed increasingly from bottom to the top An additional parametrization of the tip is done for studying the influence of a non-regular shaped tip. Its graphical expression is shown in Figure 4.2(c). The initial values and limitations of parameters is reported in Table 4.1. The parameters SiTh, SiO2Th, PtTh and PiezoTh correspond to the silicon, SiO2 and Platinum layer thicknesses and the piezoresistive sensor thickness.



(a) Cantilever (b) Tip (c) Test Tip

Figure 4.2: Parametrization of the first probe design

4.4 Simulation

This section is focused on the implementation of the simulation which is used in the optimization. First we describe the boundary conditions. Then we explain the COMSOL-MATLAB modules used in the simulation and objective features that are used in the optimization presented in the following section. The simulation is written in a COMSOL-MATLAB script so that to be combined with SIMBAD. This work takes a long time and we close this section by illustrating the difficulties met during its development.

The simulation is done for the left-half part of the probe thanks to its symmetry property. A symmetric boundary condition is thus imposed on the symmetric axis. The probe is clamped at its bottom where a 300K room temperature is imposed.

Two COMSOL modules are applied independently to extract the needed objective features. Joule-heating thermoelasticity module is the first one used to simulate the Joule-heating and the bimetallic effects. An electric source is imposed on the inner leg of the metal trail and the right end of the tip is grounded. Six objective features are extracted from this module: the maximum absolute value W of displacements generated by bimetallic effect; the maximum temperature T of the tip; the heat flux $Flux$ crossing the interface between the heater and the trail; the difference Td between the mean temperature in the tip and that in the heater; the voltage drop SV on the sensing leg when a -5μW heat flux load is imposed to the tip; the heat distribution in heater is another objective feature, it can only be expressed through a graph.

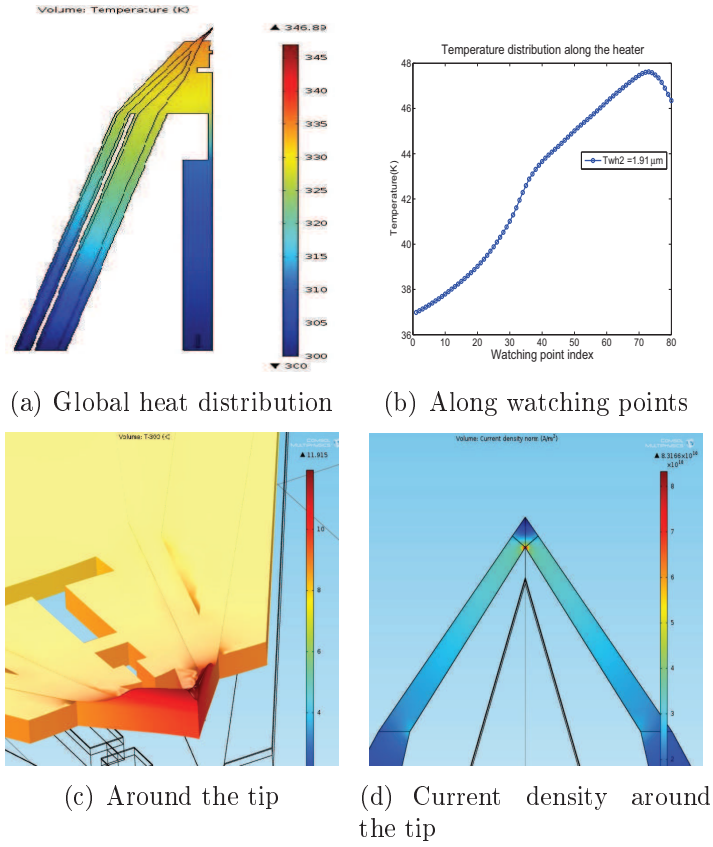
The second module is a solid mechanic which are used twice with two different loads to extract two objective features: the maximum absolute value D of displacements for a 1μN force imposed to the tip; the mean value S of Von-Mises

Name	L	H1	r1	H2	r2	r3	H	d2
Initial	203	407	103	125	71.5	11.5	555	3
Limit	-	-	-	-	-	-	-	-
Name	d1	Wcb	Wu	hf	Whb	Wg1	d3	Wg2
Initial	3	10	5.87	9.4	20	5	9	150
Limit	-	2~10	2~5.87	2~14	2~20	2.5~10	-	128~160
Name	WJb	HJn	WJn	Hsb	Ws	HsT	HTb	HTn
Initial	30	80	5	30	10	21	8.5	24
Limit	15~75	30~80	5 ~30	-	-	10~21	-	-
Name	WTn	WTb	HtT	Htb	Wtb	Wtn	Htn	Wtg
Initial	4	16	5	8.5	4	1.5	8.5	4.57
Limit	4~14	16~21	-	-	4~8	-	-	2~4.57
Name	Twh1	Hh1	L51	h51	L17	h17	Htip	SiTh
Initial	1.91	1.91	28.5	62.27	31.08	72.5	0.04	5
Limit	0.1~1.91	1~1.91	-	-	-	-	-	3~5
Name	SiO2Th	PtTh	WGP	WP	HGP	HP	PiezoTh	Twh2
Initial	0.2	0.1	11.25	2.5	22.5	1.7	1.5	1.91
Limit	0.2~0.5	0.05~0.15	-	-	-	-	-	0.1~1.91

Table 4.1: Initial value and limit of parameters

stress in the piezo-resistive sensor for an imposed 1μm tip displacement. Feature D indirectly expresses the probe stiffness.

An simulation is done with the parameters in Table 4.1 for a 0.5V voltage source. The curve in Figure 4.3(b) shows the temperature along the watching points introduced in Section 4.3. It decreases to the end of the tip. This phenomenon is made more visible in Figure 4.3(c) where the temperature variations are represented by color and also by deformation of the volume. Figure 4.3(d) shows the current density distribution, it provides a good explanation for this phenomenon. Because of the low current density in the upper end of the tip, that part can not be self-heated. The singularity of the current density at the corner comes from the property of Laplace equation which governs the electric equation. The other objective features in this simulation are $D = 0.5248\mu$m, $W = -0.09915\mu$m, $T = 45.76$K, $SV = 23\mu V$, $S = 2.13M$Pa, $Flux = 11.65$W/m^2, $Td = 0.4863$K. It



(a) Global heat distribution (b) Along watching points

(c) Around the tip (d) Current density around the tip

Figure 4.3: Temperature and current density distribution of the probe

takes 130 seconds and 6000 elements are used.

Work History

This report is simple but the process was difficult. This work has been started with the 3.5a version of COMSOL that offers poor possibilities of script programming. The scrip was not established until the adopting of COMSOL 4.2b. It accelerates significantly the work because the standard MATLAB functions can be used. This makes the programming easier and clearer. However, we found bugs that block the process of the work. Precisely, the system cannot scale the equations correctly when the non-standard geometry unit is used and the meshing function cannot work for some small geometries. We derived the scaled equations expressed in µm unit and identified the limits of each small parameters which allows meshing. We fixed all these bugs when the more powerful version of COMSOL 4.3b appeared. In this version, equation scaling problem is solved and the meshing function is much improved. So a robust script including material property setting, equation setting, meshing and objective feature extraction is created. This rendered the scaled equa-

tion no more necessary.

4.5 Simbad

The software package SIMBAD provides a generic simulation-based design tool for investigating the behaviour of complex modeled systems. A MATLAB link has been set between COMSOL and SIMBAD so that COMSOL models may be used as an input for a design under SIMBAD. It includes the definition of the optimization problem including initial value of parameters, parameter relative ranges, objective features, constraints for geometry and objective features. It serves to transmit current parameters between the two software packages. Finally, the results are visualized and reported.The following driver functions are available:

- Design sensitivity and effects analysis

  Used to quantify the impact of design variable modifications on the design objective of interest. This general allows the design space to be reduced to the subset of influential variables.

- Mono-objective performance optimization

Used to minimize a scalar function of the design objectives while satisfying design constraints.

- Multi-objective performance optimization

Used to obtain an approximation of the Pareto front for the different design objectives. This provides the analyst with a useful indicator for weighing the trade-offs between the objectives of interest.

- Reliability analysis under aleatory uncertainty

Used to evaluate system reliability for one or more failure criteria with random uncertainty a set of design variables.

- Model validation and uncertainty quantification

Used to quantify the impact of both aleatory and epistemic (lack of knowledge) uncertainties in the design variables and system environment on the design objectives and constraints.

- Info-gap robustness of design decisions to lack of knowledge

Used to investigate the impact of lack of knowledge in design variables on system performance.

Three toolboxes were used is this work. The design sensitivity and effects analysis toolbox is used to quantify the impact of design variable modifications on the design objective of interest. This allows the design space to be reduced to the subset of influential variables. Then, the multi-objective performance optimization toolbox is used to obtain an approximation of the Pareto front for the different design objectives. This provides the analyst with a useful indicator for weighting the trade-offs between the objectives of interest. Finally, the model validation and uncertainty quantification is used to quantify the impact of both aleatory and epistemic (lack of knowledge) uncertainties in the design variables and system environment on the design objectives and constraints.

4.6 Optimization

This subsection discusses a multi-objective optimization for the SThM probe introduced in Section 4.2. The varying of some parameters may improve some design properties but worsen the others. For example, the increase of the silicon layer thickness reduces the bimetallic effect but increases. In this case, the optimization requires a trade-off between the two requirements. To the contrary, an optimization of other parameters could be obtained directly from the clear understanding of their contributions.

This subsection contains two parts. The first one is dedicated to study each parameter and to identify those whose optimization requires tradeoffs. The second one focuses on the optimization of parameters for the identified tradeoffs. A set of solutions are reported in the pareto plot which facilitates the selection of optimal designs.

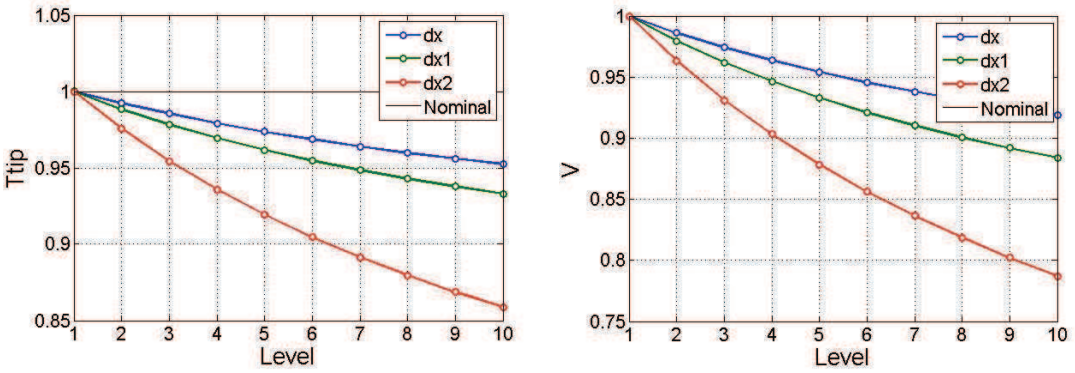
4.6.1 Analysis by subset of parameters

The influence of each parameter is analyzed separately, but the analyses are presented for small groups to make the presentation easy. Precisely, the variables are grouped into heater dimensions, T-shaped and tip-gap dimensions, layer thicknesses, trail widths and cantilever dimensions. They are marked by blue, green and red letters in Figure 4.2(b), and by red and pink letters in Figure 4.2(a).

To make the result presentation easier, a special kind of chart, see Figure 4.4 as an example, is used. For a parameter v with initial value v^0 and varies in $[av^0, bv^0]$, then the current variable v^n of v at level n is computed by $v^n = (a + \frac{n}{10}(b-a))v^0$, for an objective feature w corresponds to v with w^0 and w^n correspond to v^0 and

v^n, the x-axis represents the values of n and the y-axis represents the ratio w^n/w^0 corresponding to the variation of the objective feature.

Optimization for heater dimension The shape of the heater affects the tip temperature and sensing voltage directly. It affects also the bimetallic effect through the heat distribution in metal trail. First, we discuss the influence of a polyline shaped heater, see Figure 4.2(c), on the tip temperature and on the sensing voltage. This shows that the straight heater yields a higher sensing voltage and a higher tip temperature. It also exhibits their linear relation. So in the following, the subsequent results are only for straight shaped heater.



(a) (b)

Figure 4.4: Sensitivity analysis for varying tip width

In Figure 4.4, the platinum layer is heated by a 0.5V voltage source and the sensing voltage is measured for a 10μW heat flux load to the tip. The increase of width of any heater segment yields decrease of both tip temperature and sensing voltage. We conclude that a straight heater with a small width allows a better performance for these two features. In addition, the voltage-temperature curve of each sample shown in Figure 4.5 exhibits the linear relation between them.

In the following, we discuss the heat distribution in the straight shaped heater for several values of parameters shown in Figure 4.2(c). In Figure 4.6,

we use the kind of chart as in Figure 4.3(b). It shows the concentration of the heat distribution in the straight heater. The effects of the width $Thw2$ of the tip, the height Hf and the width Wu of the bottom part of the heater are discussed.

In Figure 4.6(a), the blue line with solid circles marks the curve of the highest temperature concentration. It corresponds to the minimal allowable value of $Twh2$. Figure 4.6(b) reports the influence of Hf where $Twh2$ is fixed to its minimum and a 0.2V heating voltage is imposed. The reduce of the heating voltage is to keep the

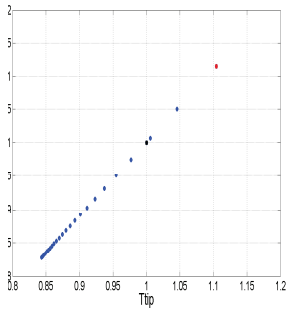
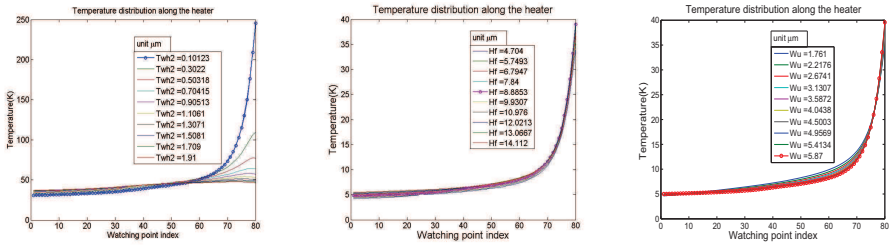


Figure 4.5: Sensing Voltage VS tip temperature



(a) (b) (c)

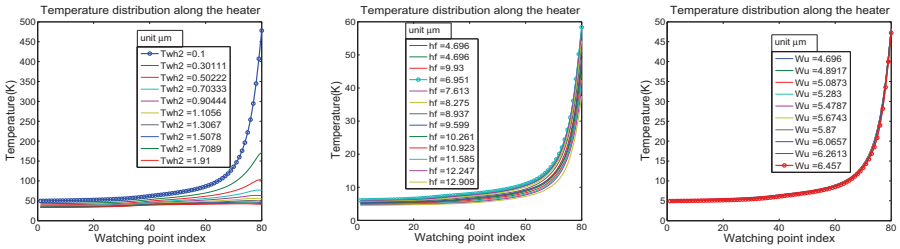
Figure 4.6: Heat distribution in the heater for a voltage source

tip temperature in a reasonable range. The differences of curvatures between each curves are small which means that Hf is uninfluential to the heat distribution. But we still mark the curve of the highest temperature concentration in Figure 4.6(b) by a bold pink line where Hf equal to 8.885μm. At last, we study the influence of Wu where both of $Twh2$ and Hf are fixed. The best curve is marked by bold red circled line in Figure 4.6(c) corresponding to the upper limit of Wu.

The heat distributions in the straight heater for current sources are shown in Figure 4.7. Figure 4.7(a) shows the temperature distribution for a $8m$A current source, and Figure 4.7(b) and 4.7(c) show it for a $2.6m$A current source. The conclusion is same as for the voltage source that Hf is uninfluential, the optimal value of $Twh2$ and Wu should be taken their minimal allowable value and maximal allowable value.

The optimization of the parameters in this group does no require any tradeoffs between the objective features. In conclusion, the optimal heater should have a wide bottom and a sharp tip.

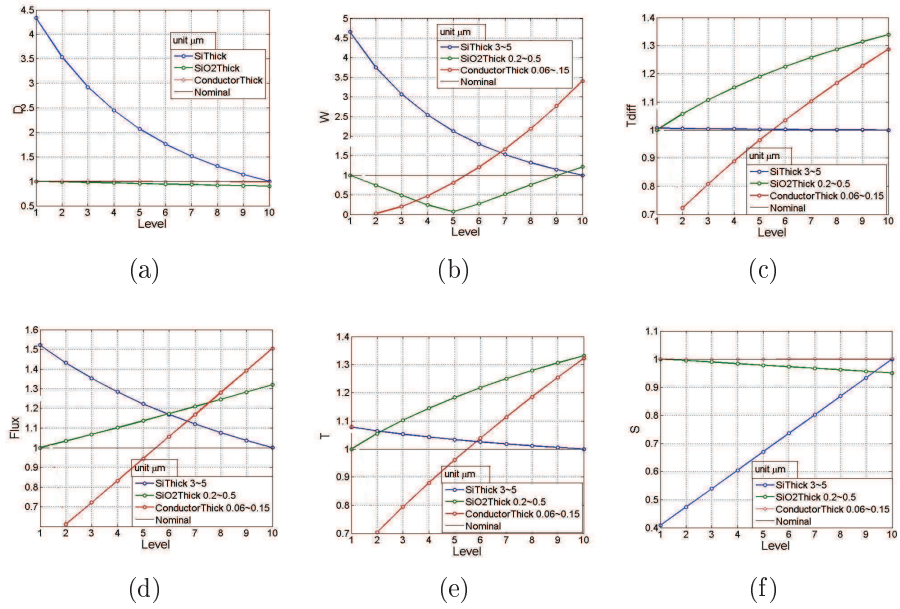
Optimization for layer thickness We discuss the optimization of thicknesses. Six objective features D, W, T, S, $Flux$ and Td are considered. Figure 4.8 shows



(a) (b) (c)

Figure 4.7: Heat distribution in the heater for a current source

the influences of the layer thicknesses on these objective features.



(a) (b) (c)

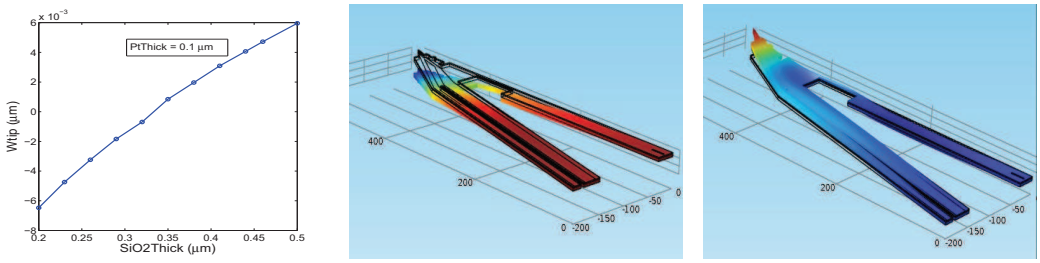
(d) (e) (f)

Figure 4.8: Sensitivity of objective features to Layer thicknesses

Figure 4.8(d) and Figure 4.8(e) show that T and $Flux$ increase with the SiO2 layer thickness. The increase of the Platinum layer thickness causes the reduction of the electric resistance and so increases the heating power in the case of a voltage source. The thickness of the SiO2 layer determines the thermal resistance between platinum layer and silicon layer. The SiO2 layer blocks the propagation of the heat from the platinum layer to the silicon layer. When it becomes thicker, the temperature as well as the heat flux in the platinum layer increase.

The inflection point of the green curve in Figure 4.8(b) corresponds to the thermal bending tendency change. This change is discussed in the following.

Figure 4.9(a) shows the variation of tip displacement with the SiO2 layer thickness when the Platinum layer thickness is fixed to 100nm and the tip temperature is fixed to 350K. The temperature is controlled by the heating voltage. The SiO2 layer thickness varies from 0.2μm to 0.5μm. Two colored and deformed volumes are used to detail the displacements when the probe is equipped with a 0.2μm and a 0.5μm SiO2 layer, see Figure 4.9(b) and Figure 4.9(c).



(a) W-SiO2 curve for 100nm Pt layer (b) Deformation for 200nm SiO2 (c) Deformation for 500nm SiO2

Figure 4.9: Tip displacements for different SiO2 layer thickness

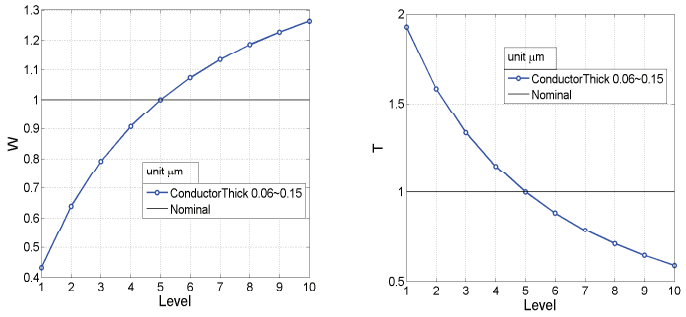
In Figure 4.9(a), the tip displacement W starts from a negative value until to be positive when the SiO2 layer thickness varies from 0.2μm to 0.5μm. The zero displacement happens when SiO2Thick reaches 0.3˜0.35μm which corresponds to the inflection point in Figure 4.8(b) as explained in the following.

As shown in Figure 4.9(c), the deformation of the left of the two cantilever legs are upward, but the deformation of the cantilever under the T-shaped gap is downward. This comes from the heat distribution. On the other hand, this dented shape under the T-shaped gap causes the upward displacement of the tip. A thick SiO2 layer increases the dented shape and so increases the tip displacement. To keep the probe smooth during its application, the SiO2 layer should be taken as thin as possible.

Since the influences of the SiO2 layer and silicon layer are not related to the kind of electric source, the discussion for the current source is only focused on the platinum layer. Figure 4.10 shows the influence of the Platinum layer on the tip temperature and on the tip displacement.

The increase of the platinum thickness increases the tip displacement and decreases the tip temperature at the same time. So its optimization does not require the trade-off between these two features.

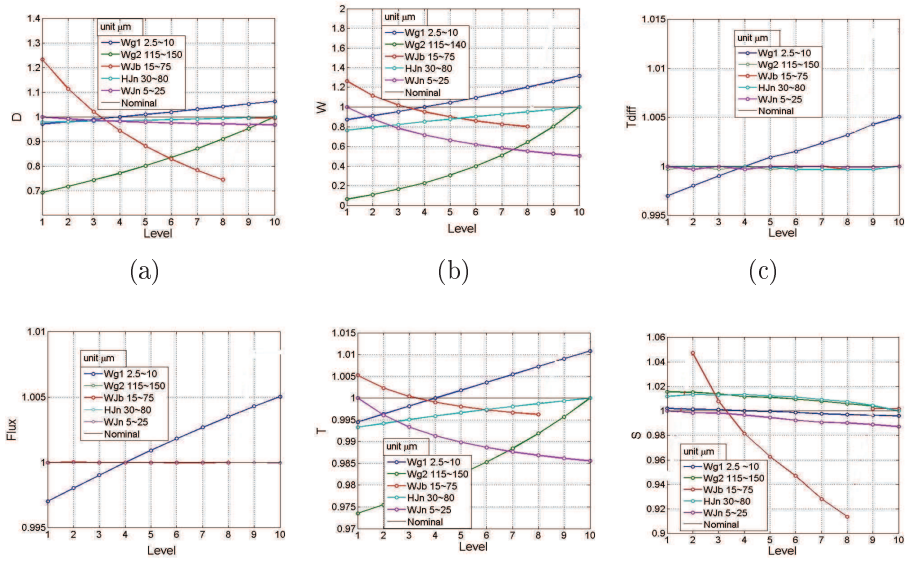
In conclusion, the thicknesses of the silicon layer and the SiO2 layer should be taken their to lower limit to keep the probe flexible and flat. For a voltage source, the platinum layer thickness could be used to optimize the tip displacement, but in the case of a current source, the platinum layer should be taken as thin as possible.



(a) (b)

Figure 4.10: Influence of Pt layer thickness for current source

Optimization for cantilever dimensions The optimizations of the middle leg and of the two gaps around the legs of the cantilever are discussed. Figure 4.11 exhibits the influences of the parameters in this group.



(a) (b) (c)

(d) (e) (f)

Figure 4.11: Sensitivity of objective features to the cantilever dimension

It shows that the parameters in this group influence mainly the probe stiffness. Figure 4.11(a) shows that a wide middle leg and a narrow gap around it yields a stiff cantilever. The pink curves in Figure 4.11(a) and in Figure 4.11(b) show that the increase of WJn only decreases the tip displacement.

In conclusion, the middle leg of the cantilever should have a uniform width, the optimizations of WJb and $Wg2$ require the trade-off between the tip displacement and the tip deflection.

Optimization for tip gap and T-shaped gap dimensions The influences of the tip gap and the T-shaped gap are discussed. In fact, these two gaps are influential to the tip temperature for the original design. In that design, the probe is equipped with a wide tip and a large area of the cantilever is heated, see Figure 4.3. But when the tip becomes sharp, their contribution becomes little. Figure 4.12 shows the influences of the tip gap when a probe is equipped with a $100n$m wide tip.

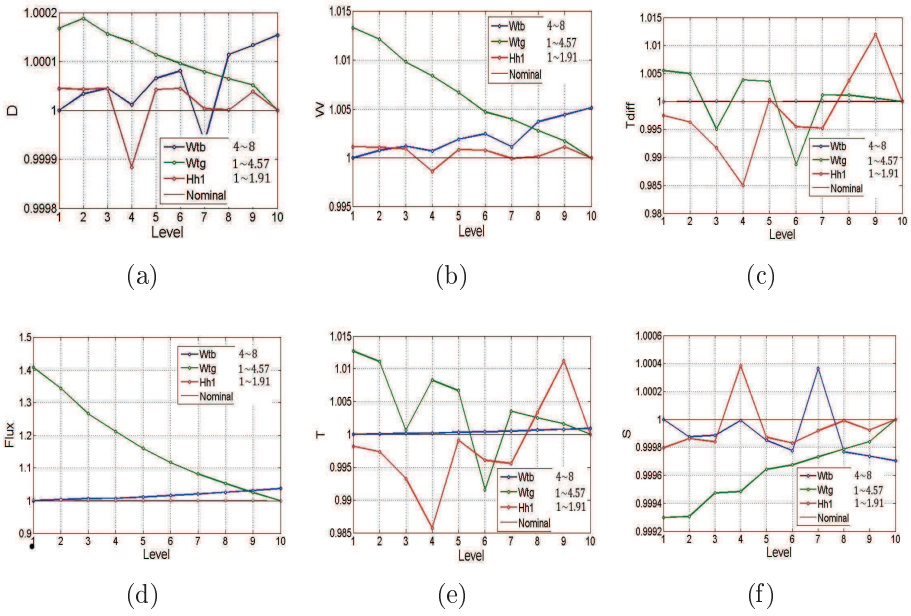


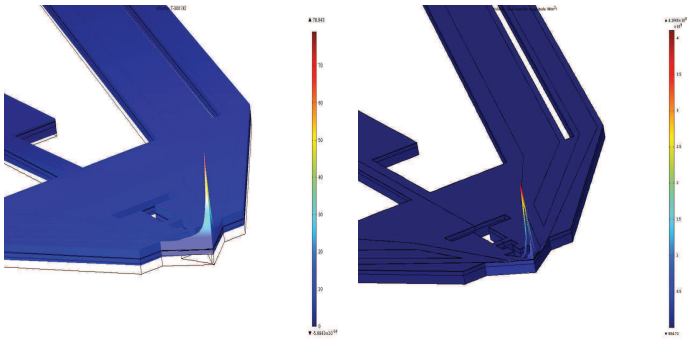
Figure 4.12: Sensitivity of objective features to Layer thicknesses

The heat and the heat flux magnitude distribution of the probe is shown in Figure 4.13.

It is clear that the temperature elevation is restricted in a little vicinity of the tip and very little heat flux goes through the tip gap. The discussion of the T-shaped gap is the same.

We conclude that these two gaps are not useful for the probe with a sharp tip.

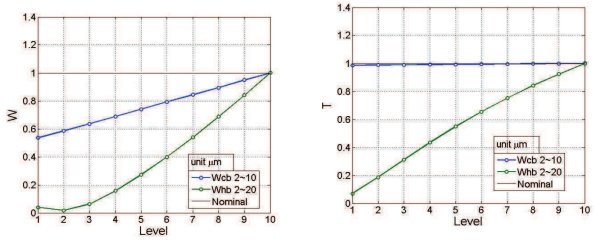
Optimization for Trail dimensions The optimization of widths of the sensing trail and the heating trail are discussed. Since they influence mainly the tip



(a) Heat distribution (b) Heat flux distribution

Figure 4.13: Heat and Heat flux distribution around the optimized tip

temperature and the tip displacement, Figure 4.14 only reports their influences on these two features.



(a) (b)

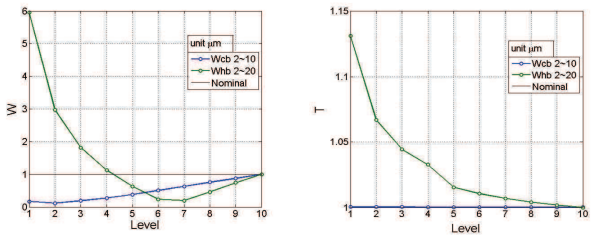
Figure 4.14: Sensitivity of objective features to the track dimension

It shows that the increase of the sensing trail width does not increase the tip temperature but only increases the tip displacement, the increase of the heating circuit width increases both of them.

The same analysis is done for the current source and Figure 4.15 reports the result.

The influence of the sensing circuit is the same but the influence of the heating circuit is different. Both of the tip temperature and the tip displacement decreases as the increase of the heating circuit width.

This yields the conclusion that the sensing trail should be as narrow as possible and the optimization of the heating trail width requires a trade-off.



(a) (b)

Figure 4.15: Sensitivity analysis of track dimension for current source

4.6.2 Trade-off optimization

In this section, we find tradeoffs between different objective features for parameters WJb, $Wg2$, Whb and $PtThick$ which are identified in the previous section and a pre-optimized geometry is used. The tip width is fixed to $100nm$ and the heater bottom width is fixed to 5.87μm, the sensing trail is fixed to 2μm, the width of the middle leg is set to be uniform, the silicon layer thickness is fixed to 3.5μm and the SiO2 thickness is fixed to 0.2μm. In the optimization, a $0.2V$ voltage source is imposed to the heating circuit.

The optimization is implemented by SIMBAD together with COMSOL-MATLAB simulation. It takes about 19 hours and 522 samples are computed. In the graphical representation, see Figure 4.16, only four sensitive ones are selected because of the limitation of graphical representation method. In Figure 4.16, each point corresponds to a sample, their position is determined by their tip deflection, tip displacement and tip temperature, and the color is determined by their sensor stresses.

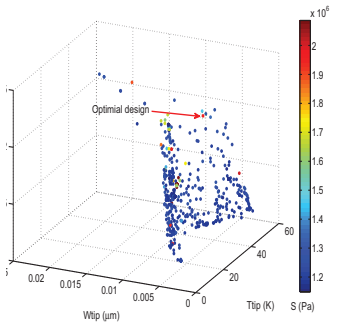


Figure 4.16: Pareto plot for four objective optimization

We compare the performances of the optimal design and the original one under the condition that they have the same tip temperature. So a $0.24V$ voltage source

is imposed to the optimal design to obtain the same tip temperature as the original one. Table 4.2 reports the comparison.

Feature	Original design	Optimal design	Relative change
D	0.5248μm	2.26μm	+330.64%
W	-99.15nm	4.66nm	-95.30%
T	45.76K	45.09K	-1.46%
S	2.13MPa	1.26MPa	-40.85%
Flux	11.65W/m^2	1.54W/m^2	-86.78%
Tdiff	0.48K	34.82K	7154%
SV	23μV	125μV	443%

Table 4.2: Report of one optimal design

Table 4.2 shows that the optimal probe is more flexible, the heat distribution around the tip is more concentrated, the bimetallic effect is much reduced and the sensing voltage is much increased. The cantilever flexibility comes from the thin silicon layer and the wide gap around the middle leg. The drawback is then the lower stress in the piezo-resistive sensor, but this could be remedied by applying signal amplifier in the stress measuring circuit. The concentrated heat distribution around the tip and the higher sensing voltage are due to the sharp tip. The sharp tip together with the narrower sensing trail and the heating trail significantly reduce the bimetallic effect. This section is closed by Table 4.3 which reports the parameters of the selected optimal design.

Name	L	H1	r1	H2	r2	r3	H	d2	d1	Wcb
Value	203	407	103	125	71.5	11.5	555	3	3	2
Name	Wu	hf	Whb	Wg1	d3	Wg2	WJb	HJn	WJn	Hsb
Value	5.87	9.93	11.65	5	9	164.7	16.45	80	5	30
Name	Ws	Twh1	L51	h51	L17	h17	Htip	SiTh	SiO2Th	PtTh
Value	10	1.91	28.5	62.27	31.08	72.5	0.1	3.5	0.2	0.0853
Name	WGP	WP	HGP	HP	PiezoTh	Twh2				
Value	11.25	2.5	22.5	1.7	1.5	0.1				

Table 4.3: Parameters of the selected sample

In the end of this section, we summarize optimization rules obtained before.

- A straight line shaped heater maximizes the tip temperature and the sensing voltage.
- The heater with a wide bottom and a sharp tip concentrates the heat distribution and reduces the bimetallic effects.
- The sensing track should be taken as narrow as possible to reduce the bimetallic effect.
- The T-shaped gap and the tip-gap are not useful when the tip is sharp.
- The increase of the heating trail width decreases the electric resistance, so it increases the temperature for a voltage source but decreases the temperature for a current source. By anyway, its optimization needs trade-off between the tip temperature and the tip displacement.
- The middle leg should be designed with a uniform width and its optimization requires the trade-off between the probe stiffness and the bimetallic effect.
- The width of the gap around the middle leg is influential to the probe stiffness and to the bimetallic effect, the trade-off between these two features should be considered in its optimization.
- The silicon layer should be taken as thin as possible to have a flexible cantilever. The SiO2 layer causes the dented shape and it forces the upper part of the probe to bend upward. To keep the probe flat during its application, the SiO2 layer should be thin. The increase of the platinum thickness decreases the electric resistance, so it increases the temperature for a voltage source but increases the temperature of a current source. This could be used to optimize the bimetallic effect.
- The sensor stress is only sensitive to the thickness of the silicon layer.

4.7 Conclusion

The connection between SIMBAD and COMSOL-MATLAB has been established and a complete optimization loop has been tested. In addition, the COMSOL-MATLAB script based programming has been studied and the experience could be used in other problems. Through the detailed discussion regarding the influences of each variable, the parameters needing tradeoffs have been identified and optimization rule for the others have been established. Finally, the pareto plot of samples for tradeoffs features has been presented.

Chapter 5

CONCLUSIONS AND PERSPECTIVES

A methodology for the kernel of an asymptotic model derivation software package MEMSALab has been proposed. The contribution of this thesis comes from three aspects.

In computer science part, the rewriting technique is firstly used for the asymptotic model derivation. A grammar which allows an symbolic expression for abstract mathematical objects has been proposed and has been successfully applied in the symbolic model derivation. In the symbolic model derivation, an approach named "*by extension-combination*" which facilitates to work with families of models has been first proposed. In this approach, the model derivation is based on extensions and their combinations. Each extension covers a specific feature comparing with the reference proof. The new proof is generated by transforming the reference proof through extensions. Since the transformation is more or less similar for a family of equations, this approach facilitates much for programming of the symbolic model derivation.

For a fluent combination of extensions, a theoretical framework for extension combination has been proposed. Concepts of *Semantic conservation transformation* and *Parametrization* and their implementation tools *Outward growth* and *Parameterized meta strategy* are introduced to decompose one extension to make sure that the final result is correct. The theories for combination of outward growths and parameterizations are introduced to solve the problem of combination of generalizations. Their implementation by rewriting strategies and some application have also been discussed.

In mathematical part, an homogenization model of the electrothermoelastic equation defined in a multi-layered thin domain has been derived. New features ie multi-dimension, thin-domain,sub-domains with different physics, vector valued solutions and multi-physics are taken into account.In the model derivation, the

proofs of the reference model derivation are followed with using extended mathematical rules and some extended steps, so that it has a good comparison with the reference one. This benefits the preparation of the design of related extensions for its inclusion in MEMSALab.

Last, an optimization tool which is a combination of a house-made optimization software package SIMBAD and COMSOL-MATLAB simulation has been developed. As an example, it has been applied for optimization of a SThM probe used in the NANOHEAT project. The general optimization principles for the similar SThM probe designs have been summarized and a set of optimal designs corresponding to different compromise of objective features have be obtained.

In this thesis, only a few aspects in the solution based on MEMSALab have been discussed. Currently, only a skeleton of the kernel of the software is proposed, the kernel itself is still very weak. There are a lot of work to do to enhance the kernel to make it applicable. In the following, we discuss the work to do in future and perspectives of our work.

Future work:

- Rewrite the rewriting strategies of the reference proof in a term rewriting language *Caml*.
- Implement the extension combination theories by rewriting strategies.
- Design elementary extensions to cover the Joule-heating thermoelastic thin plate model and implement its derivation by *Caml*.
- Implement the missed interfaces in the solution based on MEMSALab.
- Derive new models following the reference proof.
- Calibrate simulation parameters and compare with experimental result.

Perspectives

- An extension strategy library.
- A good extension combination strategy.
- A complete loop of the solution based on MEMSALab.

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Abstract:

This thesis is dedicated to develop a kernel of a symbolic asymptotic modeling software package *MEMSALab* which will be used for automatic generation of asymptotic models for arrays of micro and nanosystems. Unlike traditional software packages aimed at numerical simulations by using pre-built models, the purpose of *MEMSALab* is to derive asymptotic models for input equations by taking into account their own features. An approach called "*by extension-combination*" for the asymptotic modeling which allows an incremental model construction is firstly proposed for the homogenization model derivation. It relies on a combination of the asymptotic method used in the field of partial differential equations with term rewriting techniques coming from computer science. This approach focuses on the model derivation for family of PDEs instead of each of them. An homogenization model of the electrothermoelastic equation defined in a multi-layered thin domain has been derived by applying the mathematical method used in this approach. At last, an optimization tool has been developed by combining a house-made optimization software package SIMBAD and COMSOL-MATLAB simulation and it has been applied for optimization of a SThM probe.

Keywords: Multi-scale, Arrays, Nanosystem, Asymptotic model, Rewriting technique, extension-combination, Elementary model, Thin-domain, Feature, Optimization

Résumé :

Cette thèse est consacrée au développement d'un noyau du logiciel MEMSALab de modélisation par calcul symbolique qui sera utilis é pour la génération automatique de modèles asymptotiques pour des matrices de micro et nanosystèmes. Contrairement à des logiciels traditionnels réalisant des simulations numériques utilisant des modèles prédéfinis, le principe de fonctionnement de MEMSALab est de construire des modèles asymptotiques qui transforment des équations aux dérivées partielles en tenant compte de leurs caractéristiques. Une méthode appelée "par extension-combinaison" pour la modélisation asymptotique, qui permet la construction de modèle de façon incrémentale de sorte que les caractéristiques désirées soient incluses étape par étape est tout d'abord proposé pour le modèle d'homogénisation dérivation. Il repose sur une combinaison de méthodes asymptotiques issues de la théorie des équations aux dérivés partielles et de techniques de réécriture issues de l'informatique. Cette méthode concentre sur la dérivation de modèle pour les familles de PDEs au lieu de chacune d'entre elles. Un modèle d'homogénéisation de l'électro thermoélastique équation définie dans un domaine mince multicouche est dérivé par utiliser la méthode mathématique dans cette approche. Pour finir, un outil d'optimisation a été développé en combinant SIMBAD, une boite à outils logicielle pour l'optimisation et développée en interne, et COMSOL-MATLAB. Il a été appliqué pour étudier la conception optimale d'une classe de sondes de microscopie atomique thermique et a permis d'établir des règles générale pour leurs conception.

Mots-clés : Multi-échelle, réseau, nanosystèmes, modèle asymptotique, technique de réécriture, extension-combinaison, modèle primaire, mince-domaine, caractéristique, Optimisation

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