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Analytical continuum mechanics à la Hamilton-Piola: least action principle for second gradient continua and capillary fluids

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“On ne trouvera point de Figures dans cet Ouvrage. Les méthodes que j’y expose ne demandent ni constructions, ni raisonnemens géométriques ou mécaniques, mais seulement des opérations algébriques, assujetties à une marche régulière et uniforme. Ceux qui aiment l’Analyse, verront avec plaisir la Méchanique en devenir une nouvelle branche, et me sauront gré d’en avoir étendu ainsi le domaine.”

From the *Avertissement of the Méchanique Analitique* by Lagrange [85]

1 Abstract

In this paper a *stationary action principle* is proven to hold for capillary fluids, i.e. fluids for which the deformation energy has the form suggested, starting from molecular arguments, for instance by Cahn and Hilliard [14, 15]. Remark that these fluids are sometimes also called Korteweg-de Vries or Cahn-Allen. In general continua whose deformation energy depend on the second gradient of placement are called *second gradient* (or *Piola-Toupin* or *Mindlin* or *Green-Rivlin* or *Germain* or *second gradient*) continua. In the present paper, a material description for second gradient continua is formulated. A Lagrangian action is introduced in both material and spatial description and the corresponding Euler-Lagrange bulk and boundary conditions are found. These conditions are formulated in terms of an objective deformation energy volume density in two cases: when this energy is assumed to depend on either C and ∇C or on C^{-1} and ∇C^{-1} , where C is the Cauchy-Green deformation tensor. When particularized to energies which characterize fluid materials, the capillary fluid evolution conditions (see e.g. Casal [24] or Seppecher [139, 142] for an alternative deduction based on thermodynamic arguments) are recovered. A version of Bernoulli law valid for capillary fluids is found and, in the Appendix B, useful kinematic formulas for the present variational formulation are proposed. Historical comments about Gabrio Piola’s contribution to continuum analytical mechanics are also presented. In this context the reader is also referred to Capecchi and Ruta [16].

Part I

Introduction

Since its first formulation, which can be attributed to D’Alembert and Lagrange, continuum mechanics has been founded on the *principle of virtual works*. Moreover, since the early modern¹ studies on equilibrium and motion of fluids, the concept of continuous body was considered suitable to model macroscopic mechanical phenomena. At the opposite Poisson [121, 122, 123] preferred, instead, a treatment based on an atomistic or molecular point of view. As the actual configuration of a continuous system is characterized by a placement function (see Piola [116, 117, 119] for one of the first precise presentation of the analytical concepts involved in this statement) one can clearly see the main mathematical difference between discrete and continuous models: the configuration space is finite dimensional in the first case and infinite dimensional in the second one. Indeed a configuration is characterized as a n – *tuple* of real variables (Lagrange parameters) when introducing discrete models or as a set of fields, defined

¹It is well known that Archimedes could formulate a precise theory of the equilibrium of fluids (see e.g. Rorres [129]) and there are serious hints that a form of Bernoulli law for fluid flow was known to Hellenistic scientists (see e.g. Vailati [167] or Russo [130]).

in suitably fixed domains, when introducing continuous models. Of course the comparison of the two modeling approaches has to be based on the different relevant physical aspects of the considered phenomena. The reader is referred to the vivid discussion of this point already presented by Piola (see *infra* in the following subsections and in particular his discussion about the reality as perceived by the *animaletti infusorj* (i.e. micro-organisms)). It appeared clear already to Euler, D'Alembert and Lagrange [85] that, in order to formulate an effective model to describe a large class of physical phenomena occurring in deformable bodies, it can be more convenient to introduce a set of space-time partial differential equations for a small number of fields (i.e. functions defined in suitably regular subsets of \mathbb{R}^3) instead of a set of ordinary differential equations in which the set of unknown functions outnumbers any imaginable cardinality.

The fundamental conceptual tool used in continuous models is the definition of the so-called Lagrangian configuration, in which any material particle of the considered continuous body is labeled by three real variables, the material (or Lagrangian) coordinates of the considered particle. As a consequence the motion of a continuous system is characterized by the time dependence of the chosen set of fields. For both discrete and continuous models the obvious problem arises, once the space of configurations is fixed and the set of admissible motions chosen, how to determine the equations of the motion? In other words: how to model the external interactions between the external world, the considered body and the internal interactions in order to get some evolution equations which, once solved, supply a reliable prevision of the body behavior?

There are different postulation schemes which, during the centuries, have been proposed to that aim. All of these schemes have their merits and their defects: with a somehow inappropriate simplification we have classified them into two subgroups (see a subsection *infra*) gathered under the collective names *analytical continuum mechanics* and *continuum thermodynamics*. It has to be underlined that some remarkable results were obtained by inbreeding the two approaches: in the present context one has to cite the works by Seppecher [139, 142]. In these papers the author obtained the evolution equations for capillary fluids by combining the principle of virtual works in the Eulerian description with the first principle of thermodynamics (also in the case of isothermal motions). This shows that it can be sometimes useful to use an heuristic procedure in which the principle of virtual powers is reinforced by additionally requiring also the validity of the balance of mechanical energy. Also interesting in this context are the results presented in Casal [24], Gavrilyuk and Gouin [66].

In the opinion of the authors the methods of analytical continuum mechanics are the most effective ones (see also [98]), at least when formulating models for mechanical phenomena involving multiple time and length scales. The reader is invited to consider, with respect to this particular class of phenomena, the difficulties which are to be confronted when using continuum thermodynamics, for instance, to describe interfacial phenomena in phase transition (see e.g. dell'Isola and Romano [39, 40, 41] and dell'Isola and Kosinski [42], or in poroelasticity see e.g. dell'Isola and Hutter [46]). These difficulties are elegantly overcome when accepting to use as a fundamental tool the principle of virtual works (as done in Casal and Gouin [25], Seppecher [141] and dell'Isola et al. [53]). Very relevant phenomena occur during the flow of bubbles surrounded by their liquid phase: it could be interesting to apply the homogenization techniques presented in Boutin and Auriault [11] to the equations for capillary fluids presented here.

1.1 It is possible to deduce the evolution equations for capillary fluids and second gradient solids by using the principle of least action

In the present paper we show that it is possible to deduce from the principle of least action, and without any further assumption, the whole set of evolution equations (i.e. bulk equations and boundary conditions) for capillary fluids both in the Lagrangian and Eulerian descriptions. These equations can be seen as the Euler-Lagrange conditions corresponding to a precisely given action functional. The obtained variational principle will be useful at least when formulating numerical schemes for studying a large class of flows of capillary fluids. Also a form of Bernoulli law valid for capillary fluids is here recognized to hold. Moreover we find the complete Lagrangian form of the evolution equations for second gradient solids when the deformation energy is assumed to depend on the deformation measure $C := F^T F$ (where F is the placement gradient with respect to Lagrangian referential coordinates) or, alternatively, C^{-1} . The obtained equations are valid in the general case of large deformations and large deformation gradients. The appropriate boundary conditions which complete the set of bulk equations are also supplied². The main computational tool that we use is the Levi-Civita tensor calculus, also applied to embedded submanifolds. It has to be remarked that the works of Piola, although correct and rigorous, are encumbered by heavy component-wise notation which made their understanding difficult. Piola's works are really modern in spirit, except in what concerns

²Some of the found equations are a possible regularization of those proposed e.g. in Yermeyev et al. [56, 172] for phase transitions in solids and may give an insight into some of the results presented in Yermeyev and Lebedev [59].

their difficulty in treating tensorial quantities: the reader will appreciate the enormous economy of thought which is gained by the use of Levi-Civita formalism.

The same Piola was aware of the difficulties which are to be confronted when formulating new theories, he claims (see [119], page 1):

“It happens not so seldom that new achievements -by means of which a branch of applied mathematics was augmented- do not appear immediately, in the concept and in the exposition, free from lengthiness and superfluities. The complication of analytical procedures can reach such a level that it could seem impossible to proceed: indeed it is in this moment instead that sometimes a more general point of view can be discovered, many particularities are concentrated, and a compendious theory is formed which is so well-grounded that it can infuse vigor for further progresses.”

We conclude by citing a part of the Introduction of Piola [119] page 5 which is suitable to conclude also the present one³, when decontextualizing the references to previous works and replacing the word *fluids* by *capillary fluids*:

“While with the present memoir I will aim again to the goal now devised⁴ I will manage to reach also other ones. [Indeed] it is rigorously proven in many places the general equation of mechanics, written with the notation of calculus of variations, in the case of a whatsoever discrete system of bodies regarded as points in which different concentrated masses are subjected to external active forces and to internal active and passive forces. However, to start from this last equation [i.e. the equation for a discrete system of points] and to obtain the formulas relative to equilibrium and motion of bodies with three dimensional extensions [i.e. deformable bodies], it indeed is a step very difficult for those who are willing to see things clearly and who are not happy to get an incomplete understanding. One among my first efforts in this subject can be recognized in my Memoir "On the principles of Analytical mechanics by Lagrange". Published in Milan already in the year 1825, where I presented in this regard some correct ideas but with many specific technical details either too complex or indeed superfluous. I came back to this point in the memoir published in T. XXI of these Atti and I believed to have obtained a remarkable improvement by introducing not negligible abbreviations and simplifications: but thereafter I perceived the possibility of further improvements which I introduced in the present one. Indeed great advantage can always be obtained when having the care of clarifying appropriately the ideas concerning the nature of different analytical quantities and the spirit of the methods: [to establish] if also from this point of view something has been left to be done, I will leave the judgment to intelligent readers. The scholar will perceive that I propose myself also other aims with the present work, having established here various formulas, which can serve as a starting point for further investigations. I will not omit to mention one of these aims and precisely that one which consists in demonstrating anew (Capo V), by adopting the ideas better founded which are provided by modern Physics about fluids, the fundamental equations of their motions. In as much as I treated longly in other my works the problems of hydrodynamics (See the first two volumes of Memoirs of I. R. Istituto Lombardo) it was objected that my deduction could be defective, considered what stated by Poisson about the equations of ordinary Hydrodynamics. Now I believed to be able to prove that the considerations of the French Geometer in this circumstance were pushed too far ahead, and that notwithstanding his objections the fundamental theory of the motions of fluids is well grounded as established by D'Alembert and Euler, and exactly as it was reproduced by Fourier himself with the addition of another equation deduced with the theory of heat, [equation] to which, however, it is not necessary to refer in the most obvious questions concerning the science of waters. For what concerns the motion of fluids, the present Memoir is intended to support and complement the aforementioned ones.”

In the Appendix B the reader will find various kinematic formulas, which in our opinion will be useful in further developments of analytical continuum mechanics. The reader should also explicitly remark that already Piola has stated that the heat equation does not need to be considered when purely mechanical phenomena are involved.

1.2 What we mean with the expressions *second gradient continua* and *capillary fluids*

Following Germain [67] we will call second gradient continua those whose Lagrangian volumic deformation energy depends both on the first and second gradients of the placement field. When using the expression *capillary fluids* we will refer to those continua whose Eulerian volumic deformation energy density depends both on their Eulerian mass density ρ and its gradient $\nabla\rho$. Of course the aforementioned dependences must be independent of the observer (this requirement was already demanded by Piola [117]). We prefer to avoid to name the introduced class of fluids after Cahn and Hilliard or Korteweg and de Vries, as done sometimes in the literature (See e.g. Seppecher [139, 142, 143, 144, 145], Casal and Gouin [25, 26]). This is done in order to avoid ambiguities: Cahn and Hilliard,

³The translation from the original italian text tries to reproduce the English style of the famous works by Maxwell [103], which are nearly contemporary with Piola's ones.

⁴Piola refers here to his intention of deducing all the evolution equations of continuum mechanics from the principle of virtual works.

for instance, intended the equations which were subsequently named after them to be valid for the concentration of a solute in motion with respect to a stationary solvent, and deduced them with *molecular* arguments (and missed some thermodynamically relevant terms, see Casal and Gouin [25]). On the other hands the Korteweg-de Vries equations [78] were originally deduced for a completely different class of phenomena: waves on shallow water surfaces. Later it was discovered that they can also be deduced with an *atomistic* argument, since the so-called Fermi-Pasta-Ulam [61] discrete system has Korteweg-De Vries equations as *continuum limit*. Only in a later paper (Korteweg [80]) a connection with capillarity phenomena has been established.

The nomenclature capillary fluids is suggestive of many of the most fundamental phenomena which may be described by the model discussed here: wettability, the formation of interfacial boundary layers, the formation of liquid or gaseous films close to walls, the formation and the motion of drops or bubbles inside another fluid phase or the formation of drops pending from or laying on a horizontal plane and many others (see e.g. the papers by Seppecher [139, 142], dell’Isola et al. [43], Gouin and Casal [25]). Finally, remark that second gradient theories are strictly related to continuum theories with microstructure (see e.g. Green, Rivlin [70, 71, 72, 73], Mindlin [104, 105, 106], Kroner [81] and Toupin [162, 163]) as clarified in the note by Bleustein [9] and in the papers by Forest [63, 62].

2 An interlude: some (apparent?) dichotomies

2.1 Analytical continuum mechanics and continuum thermodynamics

It is natural here to refer to the original sources of analytical continuum mechanics. Some of them are relatively close in time and, very often, their spirit has been somehow misjudged. Sometimes they were forgotten or considered by some authors not general enough to found *modern* mechanics. This is not our opinion. However, instead of looking for new words to support this point of view, we will continue to cite a champion of analytical mechanics: the Italian mathematical-physicist Gabrio Piola. Despite his being one of the founders of modern continuum mechanics, his contribution to it has been most likely underestimated. To our knowledge the appropriate expression *analytical continuum mechanics* has not been considered frequently up to now. In Maugin [97] the following statement can be found

“The road to the analytical continuum mechanics was explored in particular by P.Germain [69], but not in a variational framework.”

The concept underlying analytical continuum mechanics has to be opposed to those of continuum thermodynamics. Actually continuum thermodynamics is based on a postulation process which can be summarized as follows (see e.g. Noll and Truesdell [115], Noll [114]):

- find a set of kinematic fields of relevance in the formulation of the considered continuum model which is sufficient to describe considered phenomena;
- postulate a suitable number of balance laws having the structure of conservation laws. Specify *the physical* meaning of each conserved quantity and introduce for each a *flux*, a *source* and a *volume density*;
- postulate a suitable number of constitutive equations in order to *close* the formulated mathematical problems: that is to have enough equations to determine the evolution of the kinematic fields, once suitable initial and boundary data are assigned;
- as the possible choices of constitutive equations are too large, and many of them are unphysical, choose a particular balance law, i.e. the balance of entropy, and assume that its source is underdetermined and always positive. The physically acceptable constitutive equations are those for which all possible motions produce a positive entropy.

Everybody who has carefully considered the performances of such an approach may agree that:

- when one wants to formulate new models it is difficult to use it as a heuristic tool;
- it is somehow involved and often requires many *ad-hoc* assumptions.

A clear and elegant⁵comparative analysis of the advantages obtained by using instead the principle of virtual works (or the principle of least action) is found in Hellinger [75]. Actually even a more elegant discussion of this point can be found in Piola (Memoir [119] page 1) where one can read the following words:

⁵and also relatively old: but older does not mean always worse! (see [130])

“[By means of the concepts of Analytical mechanics] a compendious theory is formed which is so well-grounded that it can infuse vigor for further progresses. It should be desirable that this could happen also for the last additions made by the modern Geometers to Rational mechanics: and in my opinion I should say that the true method suitable to succeed we have in our own hands: it has to be seen if others will be willing to share my opinion. I wrote many times that it does not seem to me needed to create a new mechanics, departing from the luminous method of Lagrange’s Analytical mechanics, if one wants to describe the internal phenomena occurring in the motion of bodies: [indeed it is my opinion that] it is possible to adapt those methods to all needs of modern Mathematical physics : [and that] this is, nay, the true route to follow because, being well grounded in its principles, it leads to reliable consequences and it promises ulterior and grandiose achievements. However I had -and still nowadays I have- as opposers well respectable authorities, in front of which I should concede the point, if the validity of a scientific opinion had to be based on an argument concerning the scientific value of its supporter. Nevertheless, as I cannot renounce to my persuasion, I believed it was suitable to try another effort, gathering in this memoir my thoughts about the subject and having care to expose them with the accuracy needed to assure to them the due attention of Geometers. [...] Even more than for its elegance and the grandiosity of its analytical processes, the true reason for which I prefer to all the other methods in mechanics those methods due to Lagrange is that I see in them the expression of that wise philosophy thought to us by Newton, which starts from the facts to rise up to the laws and then [starting from established laws] goes down again to the explanation of other facts.”

Indeed, analytical continuum mechanics has a much simpler postulation process since one has to

- postulate the form of a suitable action functional;
- postulate the form of a suitable dissipation Hamilton-Rayleigh functional, and calculate its first variation with respect to velocity fields;
- assume that in conservative motions the action is stationary, and to determine these motions calculate the first variation of action and equate it to zero for every infinitesimal variation of motion;
- equate, for non-conservative motions, the first variation of action functional (on the infinitesimal variations of motion) to the first variation of Hamilton-Rayleigh functional with respect to Lagrangian velocities (estimated on the same infinitesimal variations of motion).

The true difficulty in analytical continuum mechanics is that it strongly relies on the methods and on the ideas of the calculus of variations. Most likely it is for avoiding the mathematical abstraction required by the calculus of variations that many opposers reject Lagrangian mechanics. Again we give voice to Piola ([119] page 4):

“Somebody could here object that this [i.e. the variational foundations of Analytical mechanics] is a very old knowledge, which does not deserve to be newly promulgated by me: however [it seems that my efforts are needed] as my beautiful theories [after being published] are then criticized, because Poisson has assured (*Mémoires Institut de France T. VIII. pag. 326, 400; Journal Ecole polyt. cah. XX. pag 2*) that the Lagrangian method used for writing the effects of the forces by means of constrains equations (method which is proclaimed here as the only one really idoneous to take into accounts facts instead of causes) is too abstract; that it is necessary to develop a Science closer to the reality of things; that such analysis [the Lagrangian one] extended to the real bodies must be rejected as insufficient. I respond that I also recognize the difficult question to be in these considerations. If it is well founded or not the statement that the Lagrangian methods are sufficient to the description of all mechanical Phenomena, and are so powerful that they are suitable for all further possible researches, this is what will be decided later, and before rebutting my point of view, it will be fair to leave me to expose all arguments which I have gathered to defend my point of view. I hope to clarify in the following Memoir that the only reason for which the Analytical mechanics seemed to be insufficient in the solution of some problems, is that Lagrange, while writing the conditions for equilibrium and motion of a three dimensional body, did not detailed his model by assigning the equations relative to every material point belonging to it. If he had done this, and he could very well do it without departing from the methods imparted in his book, he would have obtained easily the same equations at which the French Geometers of our times arrived very painfully, [equations] which now are the foundation of new theories. However those results which Lagrange could not obtain, because death subtracted him to sciences before he could complete his great oeuvre, those results can be obtained by others.”

2.2 Least (or stationary) action principle and the principle of virtual works

Let consider a physical system denoted \mathcal{S} , the set of the possible states this system is mathematically described by a space of configurations \mathcal{C} . The time evolution of \mathcal{S} is modeled by a suitably regular function of the time variable whose values belong to \mathcal{C} . In the following this function will be called motion function (or shortly motion).

Therefore a well-posed mathematical model for \mathcal{S} can be specified only by starting with the choice of a space of configurations and a set of conditions which determine the motions.

Least action principle:

The motions in a time interval $[t_0, t_1]$ can be characterized as those motion functions which minimize (or which are stationary for) a suitably defined action functional in a specified set of admissible motions.

Indeed it is very important, in order to have a well-posed minimization (or stationarity) problem, to precisely specify the set of *admissible* motions among which these minimizers have to be searched. Following Lagrange it is generally assumed that the set of admissible motions is included in the set of isochronous motions between the instants t_0 and t_1 , i.e. motions which start from a given configuration at instant t_0 and arrive to another given configuration at the instant t_1 . When differential calculus is applicable to the action functional, the first variation of this functional (in the sense of Taylor series) can be estimated. This first variation is a linear continuous functional defined on the set of isochronous infinitesimal variations of motion. In this case, the stationarity condition can be formulated by a differential equation. This equation requires that the first variation vanishes for every infinitesimal variation of motion.

Lagrange studied a particular class of action functionals and gave a method for calculating their first variation under suitable regularity conditions on the action functional and the searched motions. The resulting equations of motion are sufficient conditions for the stationarity of a given action. This method allows for the consideration of both finite and infinite dimensional configuration spaces, hence the action principle can be formulated in both cases. Lagrangian action functionals are given in terms of a suitable Lagrange function, whose integration in time (and also in space if the configuration space is constituted by spatial fields) is required for calculating the action relative to a given motion. The form of such a function can be regarded as a conjectural choice, whose validity has to be experimentally tested. One can say that a *constitutive* choice is implicit in the choice of a Lagrange function.

However, given a configuration space \mathcal{C} , one can postulate, instead of a least action principle, a principle of virtual works. This principle states that the motion of the considered system is characterized by assuming that for every (admissible) variation the sum of three linear continuous functionals is vanishing. These functionals are, respectively, the *internal work*, the *external work* and the *inertial work*. Their choice has a nature similar to the one which leads to choose a Lagrange function and is also conjectural in nature. As previously, the validity of these *constitutive* equations has to be experimentally tested. It has to be remarked that if a Lagrange action functional can be split into three addends, i.e. into the sum of inertial, internal and external terms, the stationarity of action implies the validity of a virtual work principle. However it is clear that, in general, a linear continuous functional of infinitesimal variations of motions is not the first variation of a functional whatsoever. In this sense the principle of virtual works is more general than the principle of least action. The principle of virtual works include the principle of least action as modified by Hamilton and Rayleigh.

Therefore, and contrary to what is sometimes stated, both the principle of least action and the principle of virtual works depend on fundamental constitutive assumptions: those which lead to the choice of, respectively, either the three work functionals or the Lagrange function. The principle of virtual works is, once the configuration space is fixed, able to produce a wider class of motions. In particular it seems to be able to describe a wider class of dissipative phenomena (see e.g. Santilli [131]). However, it has to be remarked that

i) there are dissipative systems which are governed by a least action principle (see e.g. Moiseiwitsch [111] or Vujanovic and Jones [168]);

ii) it is conceivable, by a suitable embedding into a larger space of configuration, to find Lagrangian forms for systems which are initially not Lagrangian (see again Santilli [131] or Carcaterra and Akay [21, 22]).

The physical insight gained using the principle of least action (or the principle of virtual works) cannot be underestimated. For a deeper discussion of this point we limit ourselves to cite here, among the vast literature, the textbooks Landau and Lifshitz [83], Lanczos [84], Soper [146], Bedford [7], Kupershmidt [82], Kravchuk and Neittaanmaki [79], Lemons D.S. [88] and the methodological essay by Edwards [54]. Some results of interest in continuum mechanics and structural engineering are gathered in Leipholz [87], Lippmann [89], while in Luongo and Romeo [91], Luongo et al. [90, 92], are presented some interesting results in nonlinear dynamics of some structural members.

2.3 Discrete and continuous models

In many works (see e.g. Truesdell [164]) it is stated that the principle of least action is suitable to derive the evolution equations for finite dimensional systems only. Moreover, in some *époques* and some cultural environments,

the atomistic vision prevailed in physics to the point that continuum models were considered inappropriate simply for philosophical reasons. Indeed already Poisson bitterly criticized the first works of Piola (see e.g. the introduction of [119]) in which the foundations of modern continuum mechanics are laid based on the principle of virtual works. Actually in Poisson's opinion the true physical reality was *atomistic* and the most fundamental concept in mechanics was the concept of force, whose balance was bound to lead to the evolution equations of every mechanical systems. As a consequence and in order to respond to the objections of Poisson, even if Piola was aware that a variational deduction of the searched evolution equations for continuous systems was possible, in the first half of XIX century he decided to found the continuum theory as the limit of a discrete system. It is interesting to remark that, only few years later, a similar controversy arose between Mach and Boltzmann, based on Mach's rejection of atomistic point of view in thermodynamics. We prefer to leave Piola ([119] page 2) explain his (and our) point of view:

“In my opinion it is not safe enough to found the primordial formulas [of a theory] upon hypotheses which, even being very well-thought, do not receive support if not for a far correspondence with some observed phenomena, correspondence obtained particularizing general statements, [in my opinion] this should be as coming back in a certain sense to the philosophy of Descartes and Gassendi: indeed the magisterium of nature [the experimental evidence] at the very small scale in which we try to conceive the effect of molecular actions will perhaps actually be very different from what we can mentally realize by means of the images impressed in our senses when experiencing their effects in a larger scale. Even let us assume that this difference be very small: a deviation quite insensitive in the fundamental constituents [of matter] -which one needs to consider as multiplied by millions and by billions before one can reach sensible dimensions- can be the ultimate source of notable errors. On the contrary, by using Lagrangian methods, one does not consider in the calculations the actions of internal forces but [only] their effects, which are well-known and are not at all influenced by the incertitude about the effects of prime causes, [so that] no doubt can arise regarding the exactitude of the results. It is true that our imagination may be less satisfied, as [with Lagrangian methods] we do not allow to it to trace the very fundamental origins of the internal motions in bodies: does it really matters? A very large compensation for this deprivation can be found in the certitude of deductions. I could here repeat, if they were not very well-known, the wise documents with which Newton summoned to the science of facts those philosophers who before him had left a too free leap to their imagination. It has to be remarked that I do not intend for this reason to proscribe the dictation of modern Physics about the internal constitution of bodies and the molecular interactions; I think, nay, to render to them the greater of services. When the equations of equilibrium and motion will be established firmly upon indisputable principles, because one has calculated certain effects rather than hypothetical expression of forces, I believe to be licit to try to reconstruct anew these equations by means of [suitable] assumptions about such molecular interactions: and if we manage in this way to get results which are identical to those we already know to be true, I believe that these hypotheses will acquire such a high degree of likeliness which one could never hope to get with other methods. Then the molecular Physics will be encouraged to continue with its deductions, under the condition that, being aware of the aberrations of some bald ancient thinkers, it will always mind to look carefully in the experimental observation those hints [coming by the application of Lagrangian macroscopic methods] which are explicit warnings left there to indicate every eventual deviations.”

Regarding the concept of characteristic scale lengths relevant in physical phenomena Piola had crystal clear ideas, expressed by him with such an elegance that even nowadays his words can be used (Piola [119] page 13):

“Scholium. The admissibility of the principle [i.e. the principle which assume the existence of a characteristic length σ determining the average distance among the molecules microscopically constituting the considered continuum] refers to the true condition of the human being, placed, as said by Pascal in his Thoughts (Part I. Art.IV) at immense distances both from infinity and the zero: distances in which one can imagine many orders of magnitude, of which one [order of magnitude] can be regarded as the whole when compared with the one which is preceding it, and nearly nothing when compared with [the order of magnitude] which follows it. Therefore it results that the same quantities which are asserted to be negligible for us without being afraid of being wrong, could be great and not at all negligible quantities for beings which could be, for instance, capable to perceive the proportions which are relevant for the structure of micro-organisms . For those beings those bodies which appear to us to be continuous could appear as bunches of sacks: water, which for us is a true liquid, could appear as for us [appears] millet or a flowing bunch of lead pellets. But also for these beings there would exist true fluids, relative to which for them the same consequences which we deduce relatively to water should be considered as true. There are therefore quantities which are null absolutely for all orders of beings, as the analytical elements used in the Integral Calculus, and there are quantities which are null only for beings of a certain order, and these quantities would not be null for other beings, as some elements which are considered in mechanics. As I was educated by Brunacci to the school of Lagrange, I always opposed to the metaphysical infinitesimal, as I believe that for the analysis and the geometry (if one wants to achieve clear ideas) it has to be replaced by the indeterminately small when it is needed: however I accept the

physical infinitesimal, of which the idea is very clear. It is not an absolute zero, it is nay a magnitude which for other beings could be appreciable, but it is a zero relatively to our senses, for which everything which is below them is exactly as if it were not existing.

The reader should remark that the original formulations which lead to the Cahn-Hilliard equations [14, 15] and to capillary fluid equations (see e.g. van Kampen [166], Evans [55], De Gennes [38]) were based on atomistic arguments. However these arguments may lead sometimes to equations (see for more details Casal and Gouin [25]) which are thermodynamically inconsistent. This circumstance was already clear to Piola, who suggests to use macroscopic theories (based on the principle of virtual works) to *drive* and *confirm* the correct deductions from atomistic arguments. This good scientific practice is nowadays generally accepted. Many efforts have been dedicated to deduce from an *atomistic* scale discrete model the *macroscopic* form of the deformation energies which depend on first or higher gradients of deformation starting from the works of Piola [119]. The reader is referred to Esposito and Pulvirenti [60] for an extensive review about the results available for fluids. It is suggestive to conjecture that the macro-models for fluid flows discussed e.g. in [6, 27, 76], which involve some micro-macro identification procedure and more than one length scale, may be framed in the general scheme which is put forward here. In solid mechanics also, multiscale models have attracting the interest of many authors: we may refer, for instance, to Sunyk and Steinmann [148], Alibert et al. [1], Steinmann et al. [159], Rinaldi et al. [128], Misra and Chang [107], Yang and Misra [169][170], Yang et al. [171], Misra and Singh [109], Misra and Ching [110] for some other interesting results concerning granular solids. In the same context the results presented in Boutin and Hans [13], Auriault et al. [3], Chesnais et al. [29, 28], Soubestre [147] and Boutin [12, 11] have also to be cited. In these papers the authors, although starting in their procedure from balance laws valid at a microscopic level, proceed in a spirit very similar to the one found in the pioneering works by Piola.

Part II

Deduction of evolution equations for continuous systems using the least action principle

In this part, starting from the least action principle, we present the formal deduction of the evolution equations which govern the motion of i) first gradient continua, in particular Euler fluids, and of ii) second gradient continua, in particular capillary fluids. Although the content of the following subsection is well-know (even if more or less consciously ignored in some literature) it was written pursuing a twofold aim: i) to prepare the notation and calculation tools to be used in the subsequent sections; ii) to rephrase there, in a modern notation, the results of Piola [116, 120]. It has to be remarked that in the literature the least action principle in continuum mechanics is presented in a very clear way in Berdichevsky [8]. It is evident that the Soviet school (see e.g. Sedov [136, 137], which developed, improved and elaborated it in several aspects), was aware of the content of Piola's contribution to continuum mechanics⁶, even if it is not so clear how the information managed to reach Soviet scientists. To establish the ways in which such connections are established is a scientific problem by itself, whose importance has been underestimated up to now.

3 First gradient continua

In this section we reproduce, by introducing more recent notations and by extensively using Levi-Civita absolute tensor calculus, the arguments used by Piola for founding the classical continuum mechanics. The reader will remark by simple comparison (see Piola [116, 117, 118, 119, 120]) that the use of tensor calculus makes the presentation dramatically shorter. Moreover, as we will see in a subsequent subsection, by means of its use the calculations needed to deal with second gradient fluids become feasible. Another difference with Piola's presentation consists in our use of the least action principle instead of the principle of virtual works (see e.g. dell'Isola and Placidi [52]). However we keep the distinction among inertial, internal and external actions. Notations used in the following are detailed in the Appendices.

⁶To be honest it cannot be excluded logically that Piola could have sources which we could not find. However his works fix a date from which certain concepts start to appear in published-printed form.

3.1 Action functional

Let us introduce the following action functional:

$$\mathcal{A} = \int_{t_o}^{t_1} \int_{\mathcal{B}} \left(\frac{1}{2} \rho_0 v^2 - W(\chi, F, X) \right) dV dt + \int_{t_o}^{t_1} \int_{\partial \mathcal{B}} (-W_S(\chi, X)) dAdt$$

where :

- the field χ denotes the placement field between the referential (or Lagrangian) \mathcal{B} and the spatial (or Eulerian) $\chi(\mathcal{B}) \subset \mathcal{E}$ configurations

$$\chi : \mathcal{B} \rightarrow \mathcal{E}$$

- the field $\rho_0(X)$ refers to the Lagrangian time-independent mass density, so that the Eulerian mass density is given by

$$\rho = \det F^{-1} (\rho_0)_{\overline{(\mathcal{E})}}$$

where the used notation is carefully defined in Appendix A;

- the placement gradient $F = \nabla_X \chi$ is a Lagrangian tensor field, i.e. a tensor field defined in \mathcal{B} ;
- the velocity field $v = \frac{\partial \chi}{\partial t}$, associated to the placement field χ , is a Lagrangian field of Eulerian vectors;
- the potential $W(\chi, F, X)$ is relative to the volumic density of action inside the volume \mathcal{B} ;
- the potential $W_S(\chi, X)$ is relative to the actions externally applied at the boundary $\partial \mathcal{B}$.

The results valid for infinite dimensional Lagrangian models (see e.g. dell'Isola and Placidi [52] and references therein) applied to the introduced action, leads to the following Euler-Lagrange equations (which hold at every internal point of \mathcal{B}):

$$-\frac{\partial}{\partial t} (\rho_0 v_i) + \frac{\partial}{\partial X^A} \left(\frac{\partial W}{\partial F_A^i} \right) - \frac{\partial W}{\partial \chi^i} = 0$$

and, if the boundary $\partial \mathcal{B}$ is suitably smooth, the following boundary conditions⁷

$$-\frac{\partial W}{\partial F_A^i} N_A - \frac{\partial W_S}{\partial \chi^i} = 0.$$

which hold at every point P belonging to the (Lagrangian) surface $\partial \mathcal{B}$ whose normal field is denoted $N(P)$ or, in components, $N_M(P)$. In the former expressions and throughout the paper, Lagrangian indices are written in upper case while Eulerian indices are written in lower case. Furthermore the classical Einstein convention is applied and the summed indices are taken in the beginning of the alphabet.

3.2 Objective deformation energy

We now assume that the energy W can be split into two addends, the first one representing the deformation energy, the second one an external (conservative) action of a bulk load

$$W(\chi, F, X) = W^{\text{def}}(C, X) + U^{\text{ext}}(\chi, X)$$

where $C := F^T F$ is the right Cauchy-Green tensor which, in components, has the following expressions:

$$C_{MN} = g_{NA} F_a^A F_M^a = F_{Na} F_M^a = g_{ab} F_M^b F_N^a,$$

where g_{MN} and g_{ij} denotes, respectively, the metric tensors over \mathcal{B} and \mathcal{E} . The Euler-Lagrange stationarity conditions are the so-called *balance of linear momentum*, or *balance of forces*, represented by the equations

$$-\frac{\partial}{\partial t} (\rho_0 v_i) + \frac{\partial}{\partial X^C} \left(\frac{\partial W^{\text{def}}}{\partial C_{AB}} \frac{\partial C_{AB}}{\partial F_C^i} \right) - \frac{\partial U^{\text{ext}}}{\partial \chi^i} = 0. \quad (1)$$

⁷To avoid any misunderstanding, in the expression W_S it is worth noting that S refers to "Surface" and is not an index.

Remark that the equality concerns Eulerian vectors, but the fields are expressed in terms of the Lagrangian variables, therefore the differential operators are Lagrangian. Let us now observe that as:

$$\frac{\partial C_{MN}}{\partial F_P^i} = g_{ab} \frac{\partial}{\partial F_P^i} (F_M^b F_N^a) = g_{ab} \left(\frac{\partial F_M^b}{\partial F_P^i} F_N^a + F_M^b \frac{\partial F_N^a}{\partial F_P^i} \right) = (\delta_M^P F_{iN} + F_{iM} \delta_N^P)$$

we get

$$\frac{\partial W^{\text{def}}}{\partial C_{AB}} \frac{\partial C_{AB}}{\partial F_P^i} = 2 \frac{\partial W^{\text{def}}}{\partial C_{PA}} F_{iA}$$

and the balance (1) becomes

$$-\rho_0 \frac{\partial v_i}{\partial t} + \frac{\partial}{\partial X^A} \left(2F_{iB} \frac{\partial W^{\text{def}}}{\partial C_{AB}} \right) - \frac{\partial U^{\text{ext}}}{\partial \chi^i} = 0. \quad (2)$$

The tensor

$$P_i^M := 2F_{iA} \frac{\partial W^{\text{def}}}{\partial C_{AB}} g^{BM}$$

is the Piola stress tensor. It appears also in the boundary conditions which are deduced from

$$\frac{\partial W^{\text{def}}}{\partial F_A^i} N_A = - \frac{\partial W_S}{\partial \chi^i} \quad (3)$$

In Piola [119] the requirement of objectivity (i.e. the invariance under changes of observer) of Piola stress is clearly stated and analytically formulated. However, due to the lack of conceptual tools supplied by tensor calculus, in his results he cannot achieve the same clarity allowed by the tensorial formalism.

3.3 The Eulerian form of force balance

Using the Piola transformation (see Appendices), the equations (2), which represent the equations of the motion become

$$-\left(\rho_0 \frac{\partial v_i}{\partial t} \Big|_X \right)^{\overrightarrow{(\mathcal{E})}} + J^{\overrightarrow{(\mathcal{E})}} \frac{\partial}{\partial x^a} \left(2J^{-1} \left(F_{iA} \frac{\partial W^{\text{def}}}{\partial C_{AB}} F_B^a \right)^{\overrightarrow{(\mathcal{E})}} \right) - \left(\frac{\partial U^{\text{ext}}}{\partial \chi^i} \right)^{\overrightarrow{(\mathcal{E})}} = 0.$$

We remark here that $J^{-1} = \det(F^{-1})$, consequently J^{-1} has to be considered as an Eulerian quantity. Multiplying this expression by J^{-1} one gets

$$-J^{-1} \left(\rho_0 \frac{\partial v_i}{\partial t} \Big|_X \right)^{\overrightarrow{(\mathcal{E})}} + \frac{\partial}{\partial x^a} \left(2J^{-1} \left(F_{iA} \frac{\partial W^{\text{def}}}{\partial C_{AB}} F_B^a \right)^{\overrightarrow{(\mathcal{E})}} \right) - J^{-1} \left(\frac{\partial U^{\text{ext}}}{\partial \chi^i} \right)^{\overrightarrow{(\mathcal{E})}} = 0. \quad (4)$$

This is recognized to be the celebrated balance equations of linear momentum of classical continuum mechanics, once one introduces:

1. the Cauchy stress tensor (which is self-adjoint)

$$T_i^j := 2J^{-1} \left(F_{iA} \frac{\partial W^{\text{def}}}{\partial C_{AB}} F_B^j \right)^{\overrightarrow{(\mathcal{E})}} \quad (5)$$

2. the material Eulerian time derivative of a Lagrangian field Φ as

$$\left(\frac{\partial \Phi}{\partial t} \Big|_X \right)^{\overrightarrow{(\mathcal{E})}}$$

3. the field

$$b^{\text{ext}} := -J^{-1} \left(\frac{\partial U^{\text{ext}}}{\partial \chi^i} \right)^{\overrightarrow{(\mathcal{E})}}$$

which can be called the Eulerian volume force density for considered bulk loads.

Finally, in order to transport the boundary conditions (3) into the Eulerian configuration, we introduce the following notations, assumptions and results:

1. The body boundary $\partial\mathcal{B}$, whose unit normal field is denoted N , is mapped by the placement χ onto the Eulerian surface $\chi(\partial\mathcal{B})$ whose unit normal field is denoted n ;
2. Particularizing the relations (43) and (44) provided in the appendix, we obtain that

$$N_M^{\vec{\mathcal{E}}} = \frac{(J^{-1} (F^T)_M^a) n_a}{\left\| \left(J^{-1} (F^T)_A^b \right) n_b \right\|} \quad (6)$$

and that

$$\frac{dA_{\mathcal{E}}}{dA_{\mathcal{B}}} = \left(\left\| \left(J^{-1} (F^T)_A^a \right) n_a \right\|^{-1} \right)^{\vec{\mathcal{B}}} = \left\| \left(J (F^{-T})_a^A \right) N_A \right\| \quad (7)$$

3. The Lagrangian conditions (3) imply

$$2 \frac{\partial W^{\text{def}}}{\partial C_{AB}} F_{iA} N_B = - \frac{\partial W_S}{\partial \chi^i}$$

which, by using (6), become

$$2 F_{iA} \frac{\partial W^{\text{def}}}{\partial C_{AB}} F_B^a (J^{-1} n_a)^{\vec{\mathcal{B}}} = - \frac{\partial W_S}{\partial \chi^i} \left\| \left(J (F^{-T})_a^A \right) N_A \right\|$$

These last equations, by using (5) and (7), allows us to obtain the well-known Eulerian boundary conditions

$$T_i^a n_a = \left(- \frac{dA_{\mathcal{E}}}{dA_{\mathcal{B}}} \frac{\partial W_S}{\partial \chi^i} \right)^{\vec{\mathcal{E}}} \quad (8)$$

3.4 Euler fluids

We now continue to parallel Piola ([119] Capo V pages 111-146). However our treatment differs since we characterize the material symmetry of Euler fluids by assuming the equation (9), while Piola imposes it to the Eulerian transformation of Piola stress. Let us assume that

$$W^{\text{def}}(C) = \Psi(\rho^{\vec{\mathcal{B}}})(C) = W^{\text{eul}}(F) \quad (9)$$

and recall the following relations:

$$\rho^{\vec{\mathcal{B}}} = \rho_0 (\det F)^{-1}; \quad (\det F)^2 = \det(F^T F) = \det(C); \quad \rho^{\vec{\mathcal{B}}} = \rho_0 (\det C)^{-\frac{1}{2}}$$

To particularize (4) we need to determine the particular form assumed by Cauchy tensor for Euler fluids. This is done by using:

1. The equality (47) given in the appendices

$$\frac{\partial \rho^{\vec{\mathcal{B}}}}{\partial C_{MN}} = - \frac{\rho^{\vec{\mathcal{B}}}}{2} (F^{-1})^{Ma} (F^{-1})_a^N$$

2. The equality

$$T_i^j = 2J^{-1} \left(F_{iA} \frac{\partial \Psi}{\partial \rho^{\vec{\mathcal{B}}}} \frac{\partial \rho^{\vec{\mathcal{B}}}}{\partial C_{AB}} F_B^j \right)^{\vec{\mathcal{E}}} = -J^{-1} \rho \frac{\partial \Psi}{\partial \rho} \delta_i^a \delta_a^j = -\rho^2 \frac{\partial \left(\Psi / \rho_0^{\vec{\mathcal{E}}} \right)}{\partial \rho} \delta_i^j \quad (10)$$

3. The definition of the constitutive equation giving the pressure as a function of density

$$p(\rho) := \rho^2 \frac{\partial \left(\Psi / \rho_0^{\vec{\mathcal{E}}} \right)}{\partial \rho} \quad (11)$$

In conclusion, by using (11) and (10), the Eulerian force balance equations assume the form:

$$-\rho_0^{\overrightarrow{\mathcal{E}}} J^{-1} \left(\frac{\partial v_i}{\partial t} \Big|_X \right)^{\overrightarrow{\mathcal{E}}} - \frac{\partial p(\rho)}{\partial x^i} - J^{-1} \left(\frac{\partial U}{\partial \chi^i} \right)^{\overrightarrow{\mathcal{E}}} = 0.$$

By considering the external potential energy per unit mass, the last equation reads

$$-\rho \left(\frac{\partial v_i}{\partial t} \Big|_X \right)^{\overrightarrow{\mathcal{E}}} - \frac{\partial p(\rho)}{\partial x^i} - \rho \left(\frac{\partial (U/\rho_0)}{\partial \chi^i} \right)^{\overrightarrow{\mathcal{E}}} = 0.$$

Finally, using the formula for calculating the material derivative of velocity we obtain

$$-\rho \left(\frac{\partial v_i^{\overrightarrow{\mathcal{E}}}}{\partial t} + \frac{\partial v_i^{\overrightarrow{\mathcal{E}}}}{\partial x^a} (v^a)^{\overrightarrow{\mathcal{E}}} \right) - \frac{\partial p(\rho)}{\partial x^i} - \rho \left(\frac{\partial (U/\rho_0)}{\partial \chi^i} \right)^{\overrightarrow{\mathcal{E}}} = 0.$$

The expression (10) for Cauchy stress, which is valid for Euler fluids, together with the boundary condition (8) implies that:

Not all externally applied actions can be sustained by Euler fluids. Indeed Euler fluids cannot sustain surface tractions (as pressure is always positive) nor surface shear forces.

This statement, which can be already found in Piola [119] (see equation (37) page 136 and the subsequent discussion), implies that:

“The assumptions about the internal deformation energy determine the capability of the considered body to sustain externally applied actions. Therefore: the expression of the internal deformation energy characterizes the class of admissible external actions of a continuous body.”

We will return on this point in the next sections.

4 Second gradient continua

In this section we generalize the expression for deformation energy used up to now to take the second gradient of the displacement field into account. It has to be remarked that in Piola ([119] page 152) a first (and persuasive!) argument supporting the possible importance of dependence of internal work functional on higher gradients of displacement field is put forward. This point deserves a deeper discussion and is postponed to further investigations. To our knowledge Piola is the first author who analyzed such a dependence. Therefore we propose to name after him the obtained generalized continuum theories. It is assumed that second gradient materials have a deformation energy which depends both on the Cauchy-Green tensor and on its first gradient. The more general Lagrangian density function to be considered has the following shape

$$\mathcal{L} = \frac{1}{2} \rho_0 v^2 - (W^I(\chi, F, X) + W^{II}(\chi, F, \nabla F, X)). \quad (12)$$

4.1 Piola-type second gradient deformation energy

The expression (12) will be assumed in the sequel. The term $W^I(\chi, F, X)$ coincides with the first order term previously considered, while $W^{II}(\chi, F, \nabla F, X)$ stands for an additive term in which the first order derivative of the gradient F appears. As a consequence, we need to compute the first variation of the following functional

$$\mathcal{A}^{II} = \int_{\mathcal{B}} -W^{II}(\chi, F, \nabla F, X) dV$$

Paralleling the style of presentation used by Piola, while developing the calculations we comment on the results as soon as they are obtained. Because of the assumed structure of the added deformation energy, we have

$$\begin{aligned} \delta \mathcal{A}^{II} &= \delta_\chi \mathcal{A}^{II} + \delta_F \mathcal{A}^{II} + \delta_{\nabla F} \mathcal{A}^{II} \\ &= \int_{\mathcal{B}} - \left(\frac{\partial W^{II}(\chi, F, \nabla F, X)}{\partial \chi} \delta \chi + \frac{\partial W^{II}(\chi, F, \nabla F, X)}{\partial F} \delta F + \frac{\partial W^{II}(\chi, F, \nabla F, X)}{\partial \nabla F} \delta \nabla F \right) dV \end{aligned}$$

It can be observed that the first two terms can be treated exactly how done for the first gradient action. The following addend in bulk equation will be obtained

$$DIV_X \left(\frac{\partial W^{II}}{\partial F} \right) - \frac{\partial W^{II}}{\partial \chi} \quad (13)$$

together with the following addend to boundary conditions

$$- \frac{\partial W^{II}}{\partial F} \cdot N \quad (14)$$

On the contrary, new difficulties appear when calculating the first variation $\delta_{\nabla F} \mathcal{A}$. However, the techniques developed by Mindlin, Green, Rivlin, Toupin and Germain (see also dell'Isola et al. [53]) allow us to treat this term efficiently and elegantly. Starting from (the comma indicates partial differentiation)

$$\delta_{\nabla F} \mathcal{A}^{II} = \int_{\mathcal{B}} - \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \delta F_{A,B}^a \right) dV$$

we perform a first integration by parts. Indeed remarking that

$$\frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \delta F_A^a \right) = \frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta F_A^a + \frac{\partial W^{II}}{\partial F_{A,B}^a} \delta F_{A,B}^a$$

and applying the divergence theorem (recall that we denote by N_M the components of the unit normal to the surface $\partial \mathcal{B}$), we obtain

$$\begin{aligned} \delta_{\nabla F} \mathcal{A}^{II} &= \int_{\mathcal{B}} - \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \delta F_{A,B}^a \right) dV = - \int_{\mathcal{B}} \frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \delta F_A^a \right) dV + \int_{\mathcal{B}} \left(\frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta F_A^a \right) dV \\ &= - \int_{\partial \mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta F_A^a dA + \int_{\mathcal{B}} \left(\frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta F_A^a \right) dV \end{aligned} \quad (15)$$

Let us observe that the second addend of the previous expression has exactly the same form as the first variation in the case of first gradient action. Therefore this addend becomes

$$\begin{aligned} \int_{\mathcal{B}} \left(\frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta F_A^a \right) dV &= \int_{\mathcal{B}} \frac{\partial}{\partial X^A} \left(\frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta \chi^a \right) dV - \int_{\mathcal{B}} \left(\frac{\partial^2}{\partial X^A \partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta \chi^a \right) dV \\ &= \int_{\partial \mathcal{B}} \left(N_A \frac{\partial}{\partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \right) \delta \chi^a dA - \int_{\mathcal{B}} \left(\frac{\partial^2}{\partial X^A \partial X^B} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} \right) \delta \chi^a \right) dV \end{aligned}$$

which implies that to (13) and (14) the following terms must, respectively, be added to the bulk and surface Euler-Lagrange conditions

$$-DIV_X \left(DIV_X \left(\frac{\partial W^{II}}{\partial \nabla F} \right) \right); \quad DIV_X \left(\frac{\partial W^{II}}{\partial \nabla F} \right) \cdot N$$

4.2 First gradient surface stress

We now have to treat the first addend in (15), performing a surface integration by parts we obtain

$$- \int_{\partial \mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta F_A^a dA. \quad (16)$$

Remark that in dell'Isola et al. [53] the factor

$$\left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right)$$

appearing in a virtual work functional of the kind given in (16) was called first gradient surface stress. To proceed in the calculations we need to use some results from Gaussian differential geometry (see e.g. Appendices for more details). The main tool we use consists in the introduction of two projector fields P and Q in the neighborhood of the surface $\partial\mathcal{B}$. The operator P projects onto its tangent plane, while Q projects on the normal. The used integration-by-parts techniques reached us by means of Seppecher [138]. They are developed in the framework of Levi-Civita absolute tensor calculus, however it is clear that the sources of Berdichevsky [8] systematically employed these techniques. With their help, the expression (16) is transformed in the following way

$$\begin{aligned} - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,A}^a dA &= - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,C}^a \delta_A^C dA = - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,C}^a (Q_A^C + P_A^C) dA \\ &= - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,C}^a Q_D^C Q_A^D dA - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,C}^a P_D^C P_A^D dA \end{aligned} \quad (17)$$

In the following subsections, each elementary term will be processed.

4.3 External and contact surface double forces

Considering that

$$Q_D^C := N^C N_D$$

the first addend in equation (17) is rewritten

$$- \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,C}^a Q_D^C Q_A^D dA = - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi_{,C}^a N^C N_D N^D N_A dA = - \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B N_A \right) (\delta\chi_{,C}^a N^C) dA$$

or, in a more compact form,

$$- \int_{\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial \nabla F} \cdot (N \otimes N) \right) \cdot \left(\frac{\partial \delta\chi}{\partial N} \right) dA. \quad (18)$$

This last expression cannot be reduced anymore, and makes clear the appearance of a new kind of boundary condition. This quantity represents the work expended on the kinematical (independent at the boundary $\partial\mathcal{B}$!) quantity

$$\frac{\partial \delta\chi}{\partial N}$$

by its dual action, which is sometimes called a *double force* (see e.g Germain [67])

$$\frac{\partial W^{II}}{\partial \nabla F} \cdot (N \otimes N).$$

Actually the appearance of the work functional (18) justifies the following statement, which fits in the spirit of Piola [119] and is reaffirmed in Berdichevsky [8]:

Second gradient continua can sustain external surface double forces, i.e. external actions expending work on virtual normal gradient of displacement fields.

As a consequence, in the action functional, one is allowed to add a term of the kind:

$$\mathcal{A}_S^{II} = \int_{t_0}^{t_1} \int_{\partial\mathcal{B}} \left(-W_S^{II}(\chi, \frac{\partial\chi}{\partial N}, X) \right) dA dt$$

where the potential $W_S^{II}(\chi, \frac{\partial\chi}{\partial N}, X)$ can be called *surface external double potential*.

4.4 Edge contact forces

The addend expressing the work expended on virtual displacement fields parallel to the tangent space to $\partial\mathcal{B}$

$$\int_{\partial\mathcal{B}} \delta\chi_{,C}^a P_D^C P_A^D \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) dA$$

can be reduced by means of an integration by parts in the submanifold $\partial\mathcal{B}$

$$\int_{\partial\mathcal{B}} \left(\delta\chi^a_{,C} P_A^D \frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) P_D^C dA = \int_{\partial\mathcal{B}} \frac{\partial}{\partial X^C} \left(P_A^D \frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \delta\chi^a \right) P_D^C dA - \int_{\partial\mathcal{B}} \frac{\partial}{\partial X^C} \left(P_A^D \frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \right) \delta\chi^a P_D^C dA. \quad (19)$$

Surface divergence theorem is then applied to the first addend, resulting in the following equality (see Appendices or dell'Isola et al. [53])

$$\int_{\partial\mathcal{B}} \frac{\partial}{\partial X^C} \left(P_A^D \frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \delta\chi^a \right) P_D^C dA = \int_{\partial\partial\mathcal{B}} \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \delta\chi^a \right) P_A^C \nu_C dL = \int_{\partial\partial\mathcal{B}} \delta\chi^a \left(\frac{\partial W^{II}}{\partial F_{A,B}^a} N_B \nu_A \right) dL \quad (20)$$

When the surface $\partial\mathcal{B}$ is orientable and C^1 , the boundary $\partial\partial\mathcal{B}$ is empty. At the opposite, if $\partial\mathcal{B}$ is piecewise C^1 then $\partial\partial\mathcal{B}$ is the union of the edges of $\partial\mathcal{B}$ and the found expression represents the work expended by contact edge forces on the virtual displacement $\delta\chi$. To the boundary conditions it is therefore necessary to add on $\partial\partial\mathcal{B}$ the following terms, which balance external line forces

$$\frac{\partial W^{II}}{\partial F_{A,B}^i} N_B \nu_A$$

Once again, the appearance of the work functional (20) justifies for the following statement:

Second gradient continua can sustain external line forces, i.e. external actions expending work on virtual displacement fields on the edges of the boundary $\partial\mathcal{B}$.

This means that, in the action functional, one is allowed to add a term of the kind:

$$\mathcal{A}_L^{II} = \int_{t_0}^{t_1} \int_{\partial\partial\mathcal{B}} (-W_L^{II}(\chi, X)) dL dt$$

where the potential $W_L^{II}(\chi, X)$ can be called *line external potential*.

4.5 Contact forces depending on curvature of contact surfaces

The second addend of equation (19) produces a further term to be added to surface boundary conditions, which can be interpreted as a new kind of contact force (as it expends work on virtual displacements). The newly (by Casal, Mindlin, Green, Rivlin and Germain) found contact force does not *obey* to the so-called Cauchy postulate, as it depends not only on the normal of Cauchy cuts but also on their curvature. The surface boundary conditions have to be complemented by the following terms

$$-DIV_{\partial\mathcal{B}} \left(P \left(\frac{\partial W^{II}}{\partial \nabla F} \cdot N \right) \right).$$

which depend explicitly on the curvature of the surface $\partial\mathcal{B}$.

4.6 Resumé of terms to be added to Euler-Lagrange equations for second gradient continua

The Euler-Lagrange conditions found for first gradient action have to be completed by the terms listed below (see [44, 45]):

- terms to be added to bulk equations

$$DIV_X \left(\frac{\partial W^{II}}{\partial F} \right) - \frac{\partial W^{II}}{\partial \chi^i} - DIV_X \left(DIV_X \left(\frac{\partial W^{II}}{\partial \nabla F} \right) \right) \quad (21)$$

- terms to be added to surface boundary conditions

$$-\frac{\partial W^{II}}{\partial F} \cdot N + DIV_X \left(\frac{\partial W^{II}}{\partial \nabla F} \right) \cdot N - DIV_{\partial\mathcal{B}} \left(P \left(\frac{\partial W^{II}}{\partial \nabla F} \cdot N \right) \right) \quad (22)$$

- terms to be added to form new edge boundary conditions

$$\frac{\partial W^{II}}{\partial \nabla F} \cdot (N \otimes \nu) - \frac{\partial W_L^{II}(\chi, X)}{\partial \chi} \quad (23)$$

- terms forming new surface boundary conditions (which may be called *balance of contact double forces*)

$$\frac{\partial W^{II}}{\partial \nabla F} \cdot (N \otimes N) - \frac{\partial W_S^{II}(\chi, \frac{\partial \chi}{\partial N}, X)}{\partial \left(\frac{\partial \chi}{\partial N} \right)} \quad (24)$$

4.7 Objective second gradient energies

Also the added term

$$W^{II}(\chi, F, \nabla F, X)$$

must be invariant under the change of the observer in the Eulerian configuration. The use of the Cauchy-Green deformation tensor ensures that the deformation energy is objective (see e.g. [51]). This requirement is verified by a deformation energy having one of the forms

$$\hat{W}^{II}(C, \nabla C, X); \quad \check{W}^{II}(C^{-1}, \nabla C^{-1}, X)$$

It is interesting to remark that many continuum models of fiber reinforced materials (see e.g Steigmann [149], Atai and Steigmann [2], Nadler and Steigmann [112], Nadler et al. [113], Haseganu and Steigmann [74]) show some peculiarities which can be explained by the introduction of second gradient or even higher gradient models. Therefore, in order to calculate the partial derivatives with respect to F and ∇F appearing in the equations (21), (22), (23) and (24), it is necessary to calculate the derivatives listed in the following formulas (see Appendix B for more details).

- Derivatives of C and ∇C :

$$\begin{aligned} \frac{\partial C_{MN}}{\partial F_P^i} &= \delta_M^P F_{iN} + F_{iM} \delta_N^P \\ \frac{\partial C_{MN,O}}{\partial F_P^i} &= F_{iM,O} \delta_P^N + F_{iN,O} \delta_P^M \\ \frac{\partial C_{MN,O}}{\partial F_{P,Q}^i} &= \left(\delta_M^P \delta_O^Q F_{Ni} + \delta_N^P \delta_O^Q F_{Mi} \right) \end{aligned}$$

- Derivatives of C^{-1} and ∇C^{-1} :

$$\begin{aligned} \frac{\partial C_{MN}^{-1}}{\partial F_P^i} &= - (F^{-1})_{Mi} (F^{-1})_a^P (F^{-1})_N^a - (F^{-1})_{Ni} (F^{-1})^{bP} (F^{-1})_{bM} \\ \frac{\partial C_{MN,O}^{-1}}{\partial F_P^i} &= - (F^{-1})^{aP} \left((F^{-1})_{Ni} (F^{-1})_{Ma,O} + (F^{-1})_{Mi} (F^{-1})_{aN,O} \right) \\ \frac{\partial C_{MN,O}^{-1}}{\partial F_{P,Q}^i} &= - \left[(F^{-1})_{Mi} (F^{-1})^{aP} (F^{-1})_{aN} + (F^{-1})_{Ni} (F^{-1})^{bP} (F^{-1})_{bM} \right] \delta_Q^O \end{aligned}$$

4.8 Capillary fluids

In Poisson [123] pages 5-6: (translated by the authors) one finds the following statements about the region of a fluid in which a phase transition occurs page 5

“But Laplace omitted, in his calculations, a physical circumstance whose consideration is essential: I refer to the rapid variation of density which the liquid experiences in proximity of its free surface and of the tube wall, [variation] without which the capillary phenomena could not occur [...] Actually, in an equilibrium state, each layer infinitely thin of a liquid is compressed equally on both of its faces by the repulsive actions of all close molecules diminished by their attractive force [...] and its level of condensation is determined by the magnitude of the compressive force. At a sensible distance from the surface of the liquid the aforementioned force is exerted by a liquid layer adjacent to the infinitely thin layer, whose thickness is complete and everywhere constant, i.e. equal to the radius of activity

of fluid molecules; and for this reason the internal density of the liquid is also constant [...] But when this distance is less than the radius of molecular activity the thickness of the layer under the layer which we are considering is also smaller than this radius: the compressive force which is exerted by the said upper layer is therefore decreasing very rapidly with the distance from the surface and vanishes at the surface itself, where the infinitesimal thin layer is compressed only by the atmospheric pressure. Consequently, the condensation of the liquid is also decreasing, following an unknown law, when one is approaching its free surface and its density is very different in that surface and at a depth which exceeds a small amount the activity radius of its molecules, which is sufficient for having this density to be equal to the internal density of the liquid. Now it will be proven in the first chapter of this work that if one neglects this rapid variation of density in the thickness of the interfacial layer⁸ then the capillary surface should result to be plane and horizontal and one could not observe neither elevation nor lowering of the liquid level.[...]"

Therefore we can conclude that already Poisson wanted, with some assumptions which probably need to be clarified, to model the interfacial layer as a thin but three-dimensional layer. It is interesting to remark that it is only because of the development of the ideas by Piola (ideas which Poisson violently criticized) that the modern theory of capillary fluids managed to give a precise meaning to the Poisson's intuitions. What Poisson calls *an unknown law* is now explicitly determined by using second gradient continua (see e.g. [23, 139]).

In the spirit of the Piola's works, we now consider the most simple class of second gradient continua, i.e. capillary fluids. We recall here that capillary fluids are continua whose Eulerian volumic deformation energy density depends both on their Eulerian mass density ρ and on its gradient $\nabla\rho$. For capillary fluids an additive extra term in the part of action related to deformation energy has to be considered:

$$\mathcal{A}^{\text{cap}} = \int_{\mathcal{E}} \hat{W}^{\text{cap}}(\rho, \nabla\rho) dv = \int_{\mathcal{B}} J \hat{W}^{\text{cap}}\left(\left(\rho\right)^{\overrightarrow{\mathcal{B}}}, \left(\nabla\rho\right)^{\overrightarrow{\mathcal{B}}}\right) dV$$

The notations $(\cdot)^{\overrightarrow{\mathcal{B}}}$ and $(\cdot)^{\overrightarrow{\mathcal{E}}}$ introduced in the Appendix A, will be omitted occasionally for making readability easier. Obviously the dependence of \hat{W}^{cap} on $\nabla\rho$ must be objective. Therefore (interesting connections can be seen in this context with the considerations developed in Steigmann [151, 150]) we must have

$$\hat{W}^{\text{cap}}(\rho, \nabla\rho) = \check{W}^{\text{cap}}(\rho, \beta) \quad (25)$$

where we introduced the scalar

$$\beta := \nabla\rho \cdot \nabla\rho.$$

A particular case of the energy (25) is given by the one discussed by Cahn and Hilliard

$$\check{W}^{\text{cap}}(\rho, \beta) = \frac{1}{2}\lambda(\rho)\beta = \frac{1}{2}\lambda(\rho)(\nabla\rho \cdot \nabla\rho)$$

where the function $\lambda(\rho)$ has been often considered to be constant.

4.8.1 Lagrangian expression for the deformation energy of capillary fluids

It is therefore needed to calculate the following first variation

$$\delta\mathcal{A}^{\text{cap}} = \delta\left(\int_{\mathcal{B}} J \check{W}^{\text{cap}}\left(\left(\rho\right)^{\overrightarrow{\mathcal{B}}}, \left(\beta\right)^{\overrightarrow{\mathcal{B}}}\right) dV\right)$$

Once we have defined (with an abuse of notation)

$$W^{\text{cap}}(F, \nabla F) := J \check{W}^{\text{cap}}\left(\left(\rho\right)^{\overrightarrow{\mathcal{B}}}, \left(\beta\right)^{\overrightarrow{\mathcal{B}}}\right) = \frac{\rho_0}{\left(\rho\right)^{\overrightarrow{\mathcal{B}}}} \check{W}^{\text{cap}} \quad (26)$$

it is clear that

$$\begin{aligned} \delta(J\check{W}^{\text{cap}}) &= \left(\check{W}^{\text{cap}}\delta J + J \frac{\partial \check{W}^{\text{cap}}}{\partial \left(\rho\right)^{\overrightarrow{\mathcal{B}}}} \delta \left(\rho\right)^{\overrightarrow{\mathcal{B}}} + J \frac{\partial \check{W}^{\text{cap}}}{\partial \left(\beta\right)^{\overrightarrow{\mathcal{B}}}} \delta \left(\beta\right)^{\overrightarrow{\mathcal{B}}} \right) \\ &= \left(\check{W}^{\text{cap}} \frac{\partial J}{\partial F} \delta F + J \frac{\partial \check{W}^{\text{cap}}}{\partial \left(\rho\right)^{\overrightarrow{\mathcal{B}}}} \frac{\partial \left(\rho\right)^{\overrightarrow{\mathcal{B}}}}{\partial F} \delta F \right) + \frac{\partial \check{W}^{\text{cap}}}{\partial \left(\beta\right)^{\overrightarrow{\mathcal{B}}}} J \left(\frac{\partial \left(\beta\right)^{\overrightarrow{\mathcal{B}}}}{\partial F} \delta F + \frac{\partial \left(\beta\right)^{\overrightarrow{\mathcal{B}}}}{\partial \nabla F} \delta \nabla F \right) \end{aligned}$$

⁸This thickness must have a finite value but this value must be absolutely not sensible, because of the hypothesis which was accepted about the extension of molecular activity. This is confirmed by the experience made by M.Gay-Lussac.

As a consequence (with another abuse of notation) we have

$$\frac{\partial W^{\text{cap}}}{\partial F} = \check{W}^{\text{cap}} \frac{\partial J}{\partial F} + J \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \frac{\partial \rho}{\partial F} + J \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial F} \quad (27)$$

$$\frac{\partial W^{\text{cap}}}{\partial \nabla F} = J \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial \nabla F} \quad (28)$$

4.8.2 Eulerian balance equations for capillary fluids

Keeping to follow the original methods introduced by Piola, after having applied the principle of least action or the principle of virtual works in the Lagrangian description, we must transform the obtained stationarity conditions in some other conditions which are valid in the Eulerian description. As previously seen, in Lagrangian description the balance equations for capillary fluids read

$$-\frac{\partial}{\partial t} (\rho_0 v_i) + \text{DIV}_X \left(\frac{\partial W^{\text{eul}}}{\partial F} + \frac{\partial W^{\text{cap}}}{\partial F} \right) - \text{DIV}_X \left(\text{DIV}_X \left(\frac{\partial W^{\text{cap}}}{\partial \nabla F} \right) \right) = 0 \quad (29)$$

where W^{eul} and W^{cap} were defined, respectively, in (9) and (26). The terms in (29), which are specific to capillary fluids, must therefore be estimated. Starting from equation (27) and using the following result (calculated in (B.1.7) and (B.1.2))

$$\frac{\partial J}{\partial F_M^i} = J (F^{-1})_i^M, \quad \frac{\partial \rho}{\partial F_M^i} = -\rho (F^{-1})_i^M, \quad \frac{\partial \beta}{\partial F_M^i} = -2g^{ab} \left(\rho_{,a} \rho_{,i} (F^{-1})_b^M + \rho_{,a} \left(\rho (F^{-1})_i^M \right)_{,b} \right)$$

we obtain (the notation $(\cdot)^{\overrightarrow{\mathcal{B}}}$ has been dropped down for having more readable formulas),

$$\frac{\partial W^{\text{cap}}}{\partial F_M^i} = -\mathcal{P}^{\text{cap}} J (F^{-1})_i^M - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} J \left(g^{ab} \rho_{,a} \rho_{,i} (F^{-1})_b^M + \beta (F^{-1})_i^M + g^{ab} \rho_{,a} \rho (F^{-1})_{i,b}^M \right) \quad (30)$$

where we have introduced

$$\mathcal{P}^{\text{cap}} := \rho \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} - \check{W}^{\text{cap}}$$

4.8.3 Piola stress decomposition

In the remaining part of the paper, different Piola stress tensors will be considered. Therefore, and in order to avoid any misunderstanding, some time will be devoted to properly defined these different stress tensors. This discussion is specific to higher-order continua, since for first gradient continuum these different tensors are either identical or null. As a starting point we define the *bulk Piola* stress for capillary fluids

$$\mathbb{P}_i^M := \frac{\partial W^{\text{eul}}}{\partial F_M^i} + \frac{\partial W^{\text{cap}}}{\partial F_M^i} - \frac{\partial}{\partial X^A} \left(\frac{\partial W^{\text{cap}}}{\partial F_{M,A}^i} \right) \quad (31)$$

as the quantity that appears in the Lagrangian balance equation

$$-\frac{\partial}{\partial t} (\rho_0 v_i) + \frac{\partial \mathbb{P}_i^A}{\partial X^A} - \frac{\partial U^{\text{ext}}}{\partial \chi^i} = 0$$

This tensor is an *effective tensor* (in the following effective tensor are written using blackboard fonts) since it is composed of tensors of different order

$$\mathbb{P}_i^M := \mathbf{P}_i^M + \frac{\partial}{\partial X^A} (\mathbf{H}_i^{MA})$$

where \mathbf{P}_i^M is the classical Piola stress, and \mathbf{H}_i^{MA} is third-order *Hyper Piola* stress defined as

$$\mathbf{H}_i^{MN} := \frac{\partial W}{\partial F_{M,N}^i}$$

It is worth noting that for capillary fluids, the classical Piola stress can be decomposed as

$$\mathbf{P}_i^M := (\mathbf{P}^{\text{eul}})_i^M + (\mathbf{P}^{\text{cal}})_i^M$$

Hence, another *effective* tensor can be defined

$$(\mathbb{P}^{\text{cal}})_i^M := (\mathbf{P}^{\text{cal}})_i^M + \frac{\partial}{\partial X^A} (\mathbf{H}_i^{MA})$$

resulting in the following additive decomposition of the following *bulk Piola* stress

$$\mathbb{P}_i^M := (\mathbf{P}^{\text{eul}})_i^M + (\mathbb{P}^{\text{cal}})_i^M$$

4.8.4 Piola stress for capillary fluids

Now we will effectively compute the effective *bulk Piola tensor*. To that aim, we start by calculating the addend by using (28) and (56)

$$\begin{aligned} \frac{\partial \beta}{\partial F_{M,N}^i} &= -2g^{ab} \rho_{\rho,a} (F^{-1})_i^M (F^{-1})_b^N \\ -\frac{\partial}{\partial X^A} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial F_{M,A}^i} \right) &= -\frac{\partial}{\partial X^A} \left(J \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial F_{M,A}^i} \right) = \frac{\partial}{\partial X^A} \left(\rho_0 2g^{ab} \rho_{\rho,a} \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} (F^{-1})_i^M (F^{-1})_b^A \right) \\ &= \frac{\partial}{\partial X^A} \left(\rho_0 2g^{ab} \rho_{\rho,a} \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} (F^{-1})_i^M \right) (F^{-1})_b^A + \rho_0 2g^{ab} \rho_{\rho,a} \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} (F^{-1})_i^M \frac{\partial}{\partial X^A} \left((F^{-1})_b^A \right) \\ &= \frac{\partial}{\partial x^b} \left(\rho_0 2g^{ab} \rho_{\rho,a} \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} (F^{-1})_i^M \right) + \rho_0 2g^{ab} \rho_{\rho,a} \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} (F^{-1})_i^M (F^{-1})_{b,A}^A \end{aligned}$$

Now we use the (42)

$$(F^{-1})_{i,A}^A = \frac{\rho_{,A}}{\rho} (F^{-1})_i^A = \frac{\rho_{,i}}{\rho}$$

to get

$$-\frac{\partial}{\partial X^A} \left(\frac{\partial W^{\text{cap}}}{\partial F_{M,A}^i} \right) = \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \rho_0 g^{ab} \rho_{\rho,a} \right) (F^{-1})_i^M + 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \rho_0 g^{ab} \rho_{\rho,a} (F^{-1})_{i,b}^M + 2\beta \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} J (F^{-1})_i^M \quad (32)$$

Using (30) and (32) in (31) we obtain

$$\mathbb{P}_i^M = \left(-(p(\rho) + \mathcal{P}^{\text{cap}}) + \rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{ab} \rho_{\rho,a} \right) \right) J (F^{-1})_i^M - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{ab} \rho_{\rho,a} \rho_{,i} J (F^{-1})_b^M$$

where we have used

$$\frac{\partial W^{\text{eul}}}{\partial F_M^i} = -Jp(\rho) (F^{-1})_i^M$$

4.8.5 Cauchy stress for capillary fluids

As for the effective bulk Piola stress, we define the effective bulk Cauchy stress as the quantity that appears in the Eulerian balance equation

$$-\rho \left(\frac{\partial v_i(\vec{\mathcal{E}})}{\partial t} + \frac{\partial v_i(\vec{\mathcal{E}})}{\partial x^a} (v^a)^i(\vec{\mathcal{E}}) \right) - \frac{\partial}{\partial x^b} (\mathbb{T}_i^b) - \rho \left(\frac{\partial (U^{\text{exp}}/\rho_0)}{\partial \chi^i} \right) (\vec{\mathcal{E}}) = 0$$

This *effective tensor* can be decomposed as

$$\mathbb{T}_i^j := \mathbb{T}_i^j + \frac{\partial}{\partial x^A} (\mathbb{S}_i^{jA})$$

where \mathbb{T}_i^j is the second-order capillary Cauchy stress, and \mathbb{S}_i^{jk} is the third-order *capillary Hyper Cauchy* stress. As previously done, the second-order Cauchy stress can be decomposed as

$$\mathbb{T}_i^j := (\mathbb{T}^{\text{eul}})_i^j + (\mathbb{T}^{\text{cap}})_i^j$$

Hence, another *effective* tensor can be defined

$$(\mathbb{T}^{\text{cap}})_i^j := (\mathbb{T}^{\text{cap}})_i^j + \frac{\partial}{\partial x^a} (\mathbb{S}_i^{ja})$$

resulting in the following additive decomposition of the following *bulk Cauchy* stress

$$\mathbb{T}_i^j := (\mathbb{T}^{\text{eul}})_i^j + (\mathbb{T}^{\text{cap}})_i^j$$

Let now get back to the explicit determination of \mathbb{T}_i^j . By recalling (see Appendix A) the Piola transformation of tensors from the Lagrangian to the Eulerian description

$$\mathbb{T}_i^j = J^{-1} \left(\mathbb{P}_i^A F_A^j \right) (\overline{\mathcal{E}})$$

the *bulk Cauchy* stress tensor for capillary fluids is obtained

$$\mathbb{T}_i^j = \left(- (p(\rho) + \mathcal{P}^{\text{cap}}) + \rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{ab} \rho_{,a} \right) \right) \delta_i^j - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{aj} \rho_{,a} \rho_{,i}$$

In the case of Cahn-Hilliard fluids with a constant λ we have

$$2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} = \lambda, \quad \check{W}^{\text{cap}} = -\mathcal{P}^{\text{cap}} = \frac{\lambda}{2} g^{ab} \rho_{,a} \rho_{,b}$$

so that

$$\mathbb{T}_i^j = \left(-p(\rho) + \frac{\lambda}{2} g^{ab} \rho_{,a} \rho_{,b} + \rho \frac{\partial}{\partial x^b} (\lambda g^{ab} \rho_{,a}) \right) \delta_i^j - \lambda g^{aj} \rho_{,a} \rho_{,i}$$

which is exactly the result found in the literature (see Seppacher [140] or Casal and Gouin [25, 26]). Let us now develop the Eulerian divergence of the effective capillary Cauchy tensor

$$\begin{aligned} \frac{\partial}{\partial x^c} (\mathbb{T}_i^c) &= \frac{\partial}{\partial x^c} \left(\left(-p(\rho) + \frac{\lambda}{2} g^{ab} \rho_{,a} \rho_{,b} + \rho \frac{\partial}{\partial x^b} (\lambda g^{ab} \rho_{,a}) \right) \delta_i^c - \lambda g^{ac} \rho_{,a} \rho_{,i} \right) \\ &= -\frac{\partial}{\partial x^i} p(\rho) + \lambda g^{ab} \rho_{,a} \rho_{,b,i} + \frac{\partial}{\partial x^i} (\rho \lambda g^{ab} \rho_{,ab}) - \lambda g^{ac} \rho_{,ac} \rho_{,i} - \lambda g^{ac} \rho_{,a} \rho_{,ic} \\ &= -\frac{\partial}{\partial x^i} p(\rho) + \lambda \rho \frac{\partial}{\partial x^i} (g^{ab} \rho_{,ab}) \end{aligned}$$

In conclusion the Eulerian balance equation for Cahn-Hilliard fluids is:

$$-\rho \left(\frac{\partial v_i(\overline{\mathcal{E}})}{\partial t} + \frac{\partial v_i(\overline{\mathcal{E}})}{\partial x^a} (v^a) \overline{\mathcal{E}} \right) - \frac{\partial}{\partial x^i} p(\rho) + \lambda \rho \frac{\partial}{\partial x^i} (g^{ab} \rho_{,ab}) - \rho \left(\frac{\partial (U^{\text{exp}}/\rho_0)}{\partial \chi^i} \right) (\overline{\mathcal{E}}) = 0$$

To complete the description of the model, the associated boundary conditions have to be supplied.

4.8.6 Boundary terms

In the particular case of capillary fluids the *Hyper Piola* tensor has the following explicit expression

$$\mathbb{H}_i^{MN} = \frac{\partial W^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial F_{M,N}^i} = -\lambda \rho_0 g^{ab} (F^{-1})_b^M (F^{-1})_i^N$$

Its Eulerian equivalent is the following *Hyper Cauchy* tensor

$$\mathbb{S}_i^{jk} = -J^{-1} H_i^{AB} F_B^j F_A^k = -J^{-1} \rho_0 g^{ab} \rho_{,a} \lambda (F^{-1})_i^B (F^{-1})_b^A F_B^j F_A^k = -\lambda \rho g^{ak} \rho_{,a} \delta_i^j$$

Double force The expression of contact double force will first be proceed. In the absence of surface external double force, the boundary conditions read

$$\frac{\partial W^{\text{cap}}}{\partial \nabla F} \cdot (N \otimes N) = 0$$

or, in components

$$\frac{\partial W^{\text{cap}}}{\partial F_{A,B}^i} N_A N_B = -\lambda \rho_0 \rho_{,a} g^{ab} (F^{-1})_b^A (F^{-1})_i^B N_A N_B = 0$$

Using the Piola transformation for normals (43), the former expression is rewritten

$$-\lambda \rho_0 \rho_{,a} g^{ab} (F^{-1})_b^M (F^{-1})_i^N J^{-1} F_M^c n_c J^{-1} F_N^e n_e = 0$$

Hence, for line forces (23) we obtain

$$-J^{-1} \lambda \rho \rho_{,a} g^{ab} n_b \nu_i = 0$$

Force In absence of external force, the new boundary conditions read

$$\mathbb{P}_i^A N_A + \frac{\partial}{\partial X^E} (P_C^D (H_i^{BC} N_B)) P_D^E = 0$$

or, using the Piola transformation, in Eulerian form

$$\mathbb{T}_i^a n_a + \frac{\partial}{\partial x^e} (P_c^d (S_i^{bc} n_b)) P_d^e = 0$$

The first term will first be considered. This term can be expanded as

$$\begin{aligned} \mathbb{T}_i^a n_a &= \left[\left(-p(\rho) + \frac{\lambda}{2} g^{bc} \rho_{,b} \rho_{,c} + \rho \frac{\partial}{\partial x^c} (\lambda g^{bc} \rho_{,b}) \right) \delta_i^a - \lambda g^{ba} \rho_{,b} \rho_{,i} \right] n_a \\ &= \left(-p(\rho) + \frac{\lambda}{2} g^{bc} \rho_{,b} \rho_{,c} + \rho \frac{\partial}{\partial x^c} (\lambda g^{bc} \rho_{,b}) \right) n_i - \lambda g^{ab} \rho_{,b} \rho_{,i} n_a \\ &= \left(-p(\rho) + \frac{\lambda}{2} g^{bc} \rho_{,b} \rho_{,c} + \rho \frac{\partial}{\partial x^c} (\lambda g^{bc} \rho_{,b}) \right) n_i - \lambda n^b \rho_{,b} \rho_{,i} \\ &= \left(-p(\rho) + \frac{\lambda}{2} g^{bc} \rho_{,b} \rho_{,c} + \rho \frac{\partial}{\partial x^c} (\lambda g^{bc} \rho_{,b}) - \lambda n^i \rho_{,i} n^b \rho_{,b} \right) n_i \end{aligned}$$

It remains now to consider the last part of the boundary conditions, i.e.

$$\frac{\partial}{\partial x^d} (P_b^c (S_i^{ab} n_a)) P_c^d$$

This computation is a bit more tricky. In order to easily proceed their expression, the following identities need to be established:

$$\begin{aligned} Q \cdot (v \otimes n) &= (v \cdot n) Q \\ P \cdot (v \otimes n) &= (v \cdot n) P \end{aligned} \tag{33}$$

Their demonstration is straightforward:

$$\begin{aligned} Q_a^i v^a n_j &= n^i n_a v^a n_j = n_a v^a n^i n_j = Q_j^i v^a n_a \\ P_a^i v^a n_j &= (\delta_a^i - Q_a^i) v^a n_j = (\delta_j^i \delta_a^j v^a n_j) + Q_j^i v^a n_a \\ &= \delta_j^i v^a n_a + Q_j^i v^a n_a = (\delta_j^i + Q_j^i) v^a n_a \\ &= P_j^i v^a n_a \end{aligned}$$

Now, using the definition of the hyperstress for capillary fluids

$$S_i^{aj} n_a = -\lambda \rho \rho^j n_i$$

In the following, the factor $-\lambda\rho$ will be dropped down and only added at the end. Using the identity (33) we have the first transformation relation

$$P_a^i (\rho^a n_j) = \rho^a n_a P_j^i$$

Therefore

$$\nabla_k^S (P_a^i (\rho^a n_j)) = \nabla_k^S (\rho^a n_a P_j^i) = \nabla_k^S (\rho^a n_a) P_j^i + \rho^a n_a \nabla_k^S (P_j^i)$$

where $\nabla_k^S := P_k^a \frac{\partial}{\partial x_a}$ denotes the surface gradient. Let us now compute the surface gradient of the projection operator P ,

$$\begin{aligned} \nabla_k^S (P_j^i) &= \nabla_k^S \delta_j^i - \nabla_k^S (n^i n_j) = -(\nabla_k^S (n^i) n_j + n^i \nabla_k^S (n_j)) \\ &= L_k^i n_j + n^i L_{kj} \end{aligned}$$

where $L_{ij} := -P_i^a n_{aj}$ is the Weingarten curvature tensor. Therefore, at the end

$$\nabla_k^S (P_a^i (\rho^a n_j)) = \nabla_k^S (\rho^a n_a) P_j^i + \rho^a n_a (L_k^i n_j + n^i L_{kj})$$

To obtain the surface divergence it remains to multiply the previous result by δ_k^i

$$\nabla_i^S (P_a^i (\rho^a n_j)) = \nabla_i^S (\rho^a n_a) P_j^i + \rho^a n_a (L_i^i n_j + n^i L_{ij})$$

This expression can be simplified, we have

$$\begin{aligned} \nabla_i^S P_j^i &= P_i^a \frac{\partial}{\partial x_a} P_j^i = P_i^a P_j^i \frac{\partial}{\partial x_a} = \nabla_j^S \\ n^i L_{ij} &= n^i P_i^a n_{aj} = 0 \end{aligned}$$

and

$$2H := L_i^i$$

where H is the surface mean curvature. Therefore, at the end of the journey

$$\nabla_i^S (P_a^i (\rho^a n_j)) = \nabla_j^S (\rho^a n_a) + 2\rho^a n_a H n_j$$

Once the two parts added, we obtain

$$\left(-p(\rho) + \frac{\lambda}{2} g^{ab} \rho_{,a} \rho_{,b} + \rho \frac{\partial}{\partial x^b} (\lambda g^{ab} \rho_{,a}) - \lambda n^i \rho_{,i} n^a \rho_{,a} + 2\rho^a n_a H \right) n_i + \nabla_i^S (\rho^a n_a) = 0$$

or

$$-p^* n_i + \nabla_i^S (\rho^a n_a) = 0$$

in which

$$p^* = \left(p(\rho) - \frac{\lambda}{2} g^{ab} \rho_{,a} \rho_{,b} - \rho \frac{\partial}{\partial x^b} (\lambda g^{ab} \rho_{,a}) + \lambda n^i \rho_{,i} n^a \rho_{,a} + 2\rho^a n_a H \right)$$

This is exactly the result found in [140, 141, 25, 26].

4.8.7 Bernoulli Law for capillary fluids

The results in the previous sections imply that for capillary fluids the following Eulerian Balance of force holds (see also [24, 25])

$$-\rho \left(\frac{\partial v_i^{\overline{(\mathcal{E})}}}{\partial t} + \frac{\partial v_i^{\overline{(\mathcal{E})}}}{\partial x^a} (v^a)^{\overline{(\mathcal{E})}} \right) - \frac{\partial}{\partial x^i} (p(\rho)) + \frac{\partial}{\partial x^b} (\mathbb{T}^{\text{cap}})^b_i - \rho \left(\frac{\partial U / \rho_0}{\partial \chi^i} \right)^{\overline{(\mathcal{E})}} = 0.$$

where we have introduced the constitutive equations

$$(\mathbb{T}^{\text{cap}})^b_i = \left(-\mathcal{P}^{\text{cap}}(\rho, \beta) + \rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{ab} \rho_{,a} \right) \right) \delta_i^j - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{aj} \rho_{,a} \rho_{,i}$$

$$-\mathcal{P}^{\text{cap}} := \check{W}^{\text{cap}} - \rho \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \quad ; \quad p(\rho) := \rho^2 \frac{\partial(\check{W}/\rho_0)}{\partial \rho} .$$

If the last relationship is invertible one can express the density as a function $\hat{\rho}$ of the pressure and introduce the function

$$Q(p) = \int \frac{1}{\hat{\rho}(p)} dp$$

which has the remarkable property

$$\frac{\partial Q(p)}{\partial x^i} = \frac{1}{\hat{\rho}(p)} \frac{\partial p}{\partial x^i} .$$

As a consequence, once divided by ρ the equations become

$$-\frac{\partial v_i(\vec{\mathcal{E}})}{\partial t} - \frac{\partial v_i(\vec{\mathcal{E}})}{\partial x^a} (v^a) \vec{\mathcal{E}} - \frac{\partial}{\partial x^i} (Q(p)) + \frac{1}{\rho} \frac{\partial}{\partial x^b} (\mathbb{T}^{\text{cap}})^b_i - \left(\frac{\partial U/\rho_0}{\partial \chi^i} \right) \vec{\mathcal{E}} = 0 \quad (34)$$

The calculation of $\frac{\partial}{\partial x^a} (\mathbb{T}^{\text{cap}})^a_i$ We have to compute the following term

$$\begin{aligned} \frac{\partial}{\partial x^a} (\mathbb{T}^{\text{cap}})^a_i &= \frac{\partial}{\partial x^a} \left(\left(-\mathcal{P}^{\text{cap}}(\rho, \beta) + \rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \right) \delta_i^a - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{da} \rho_{,d} \rho_{,i} \right) \\ &= \underbrace{\frac{\partial}{\partial x^i} \left(\check{W}^{\text{cap}} - \rho \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} + \rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \right)}_A - \underbrace{2 \frac{\partial}{\partial x^a} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{da} \rho_{,d} \rho_{,i} \right)}_B \end{aligned}$$

Let process first the term labeled A

$$\begin{aligned} A &= \frac{\partial}{\partial x^i} \check{W}^{\text{cap}} - \frac{\partial}{\partial x^i} \left(\rho \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \right) + \frac{\partial}{\partial x^i} \left(\rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \right) \\ &= \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \frac{\partial \rho}{\partial x^i} + \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial x^i} - \rho_{,i} \frac{\partial \check{W}^{\text{cap}}}{\partial \rho} - \rho \frac{\partial}{\partial x^i} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \right) + \frac{\partial}{\partial x^i} \left(\rho \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \right) \\ &= \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial x^i} - \rho \frac{\partial}{\partial x^i} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \right) + \rho_{,i} \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) + \left(\rho \frac{\partial}{\partial x^i} \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \right) \end{aligned}$$

the term B is easy to determine

$$B = -2\rho_{,i} \frac{\partial}{\partial x^a} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{ad} \rho_{,d} \right) - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{da} \rho_{,d} \rho_{,ia}$$

Therefore we have

$$\frac{\partial}{\partial x^a} (\mathbb{T}^{\text{cap}})^a_i = -\rho \frac{\partial}{\partial x^i} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \right) + \left(\rho \frac{\partial}{\partial x^i} \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \right) + \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} \frac{\partial \beta}{\partial x^i} - 2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{da} \rho_{,d} \rho_{,ia}$$

and recalling that

$$\frac{\partial \beta}{\partial x^i} = \frac{\partial}{\partial x^i} (g^{ab} \rho_{,a} \rho_{,b}) = 2g^{ab} \rho_{,a} \rho_{,bi}$$

the sought result is finally obtained

$$\begin{aligned} \frac{\partial}{\partial x^a} (\mathbb{T}^{\text{cap}})^a_i &= -\rho \frac{\partial}{\partial x^i} \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \right) + \rho \frac{\partial}{\partial x^i} \frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) \\ &= \rho \frac{\partial}{\partial x^i} \left(\frac{\partial}{\partial x^b} \left(2 \frac{\partial \check{W}^{\text{cap}}}{\partial \beta} g^{bc} \rho_{,c} \right) - \left(\frac{\partial \check{W}^{\text{cap}}}{\partial \rho} \right) \right) \\ &= \rho \frac{\partial}{\partial x^i} (\mathcal{P}^{\text{eff}}(\rho; \rho_{,a}; g^{ab} \rho_{,ab})) \end{aligned}$$

4.8.8 Bernoulli constant of motion along flow curves

In order to be able to conclude our argument we need a last tensorial equality (see e.g. Lebedev et al. [86])

$$\frac{\partial v_i}{\partial x^a} v^a = \frac{\partial v^a}{\partial x^i} v_a + \left(\frac{\partial v_i}{\partial x^a} v^a - \frac{\partial v^a}{\partial x^i} v_a \right) = \frac{\partial}{\partial x^i} \left(\frac{1}{2} v^a v_a \right) + W_i^a v_a \quad (35)$$

where the tensor W_i^j defined by

$$W_i^j := \frac{\partial v_i}{\partial x^j} - \frac{\partial v^j}{\partial x^i}$$

clearly verifies the equality

$$W_b^a v_a v^b = \left(\frac{\partial v_b}{\partial x^a} v^b v^a - \frac{\partial v^a}{\partial x^b} v^b v_a \right) = \frac{1}{2} \left(\frac{\partial (v_b v^b)}{\partial x^a} v^a - \frac{\partial (v^a v_a)}{\partial x^b} v^b \right) = 0$$

Let consider the equations (34)

$$-\frac{\partial v_i^{\overline{(\mathcal{E})}}}{\partial t} - \frac{\partial v_i^{\overline{(\mathcal{E})}}}{\partial x^a} (v^a)^{\overline{(\mathcal{E})}} - \frac{\partial}{\partial x^i} (Q(p)) + \frac{1}{\rho} \frac{\partial}{\partial x^b} (\mathbb{S}_i^b) - \left(\frac{\partial U / \rho_0}{\partial \chi^i} \right)^{\overline{(\mathcal{E})}} = 0$$

if the applied bulk external forces are such that there exists a scalar Eulerian function V for which the following equality holds

$$\left(\frac{\partial U / \rho_0}{\partial \chi^i} \right)^{\overline{(\mathcal{E})}} = \frac{\partial V}{\partial x^i}$$

and by making use of (35) (the notation $(\cdot)^{\overline{(\mathcal{E})}}$ has been dropped down), we obtain

$$-\frac{\partial v_i}{\partial t} - \frac{\partial}{\partial x^i} \left(\frac{1}{2} v^c v_c \right) + W_i^d v_d - \frac{\partial}{\partial x^i} (Q(p)) + \frac{\partial}{\partial x^i} \left(\frac{\partial}{\partial x^b} \left(2 \frac{\partial \dot{W}^{\text{cap}}}{\partial \beta} g^{ab} \rho_{,a} \right) - \left(\frac{\partial \dot{W}^{\text{cap}}}{\partial \rho} \right) \right) - \frac{\partial V}{\partial x^i} = 0.$$

By calculating the inner product with v we get

$$\frac{\partial}{\partial t} \left(\frac{1}{2} v \cdot v \right) + \nabla \left(\frac{1}{2} v \cdot v + Q(p(\rho)) - \mathcal{P}^{\text{eff}} (\rho; \rho_{,a}; g^{ab} \rho_{,ab}) + V \right) \cdot v = 0$$

And if the field v be stationary, i.e. if

$$\frac{\partial v}{\partial t} = 0$$

the last equation becomes

$$\nabla \left(\frac{1}{2} v \cdot v + Q(p(\rho)) - \mathcal{P}^{\text{eff}} (\rho; \rho_{,a}; g^{ab} \rho_{,ab}) + V \right) \cdot v = 0$$

i.e. along flow curves there exists a constant K_0 such that

$$\frac{1}{2} v \cdot v + Q(p(\rho)) - \mathcal{P}^{\text{eff}} (\rho; \rho_{,a}; g^{ab} \rho_{,ab}) + V = K_0.$$

5 Conclusions: towards continuum analytical mechanics ?

The role of the principle of least action (or of its weaker version the principle of virtual works) in applied mathematics, and in particular in mathematical physics, has been controversial since its very first formulations. The attitude towards this postulation is often a total refuse. Indeed, both the supporters of *variational* postulations and the supporters of *balance of everything* behave often as if the controversy does not exist. They simply pretend that the other postulation process is not used at all or anymore. Of course the supporters of *balance of everything* are aware of the importance of a variational principle, especially when a numerical code has to be designed or an existence and uniqueness theorem need to be proven. They treat the variational principle as a theorem to be proven in their postulation scheme. Very strange and somehow clumsy expressions are used like: *theorem of the principle of virtual works* which is rather an oxymoron. Their attitude (see the section variational principles in Truesdell

and Toupin [165]) is that a variational formulation cannot be generally obtained. Their existence are considered as mathematical curiosities that make easier the work of the mathematicians. For them the search of variational principles is a secondary task devoted to the applied mathematicians.

On the contrary the supporters of *variational* postulations behave as if their point of view were the only possible: they do not even care to announce that they use it as, in their opinion, everybody has to do so. To these supporters are directed the words of Piola which we already cited:

“Somebody could here object that this [i.e. the variational foundations of Analytical mechanics] is a very old knowledge, which does not deserve to be newly promulgate by me: however [it seems that my efforts are needed] as my beautiful theories [after being published] are then criticized.”

Actually the elitist attitude of many supporters of *variational* postulations is the true cause of the frequent *rediscoveries* of the same variational principles in different times and the loss of the information about their first historical appearance. Variational principles have to be regarded as the most powerful heuristic tool in applied mathematics. The wise attitude of Hamilton and Rayleigh consisted in refraining from the effort of describing dissipative phenomena directly and explicitly by means of the least action principle, but including them in the picture only in a second step, by means of the introduction of a suitable dissipation functional. Of course this *heuristic* attitude does not imply that a purely variational formulation of given model cannot be obtained, at worst by embedding the original space of configurations in a wider one. When this further step can be performed then the value of the improved mathematical model will increase.

In this context we found interesting the works Carcaterra and Sestieri [17], Carcaterra et al. [18], Culla et al. [33], Carcaterra [19], Carcaterra and Akai [21], which were initially motivated by the need of developing innovative technological solutions. In these papers it is proven that a conservative system can show, if one restricts his attention to a subset of its degrees of freedom, an apparent dissipative behavior. Actually in suitably designed conservative systems the energy may flow from some primary degrees of freedom into a precise set of other (secondary or hidden) ones, and remain there trapped for a very long (from the point of view of practical application: infinite) time. Therefore, in some cases, a non-conservative description of a primary system, including an *ad-hoc* dissipation functional, is a realistic and effective modeling simplification, even if the *true* and complete system is actually Hamiltonian and conservative. The greatest advantage in variational based models is that, if the action functional is well-behaving, they always produce intrinsically well-posed mathematical problems. Somebody claimed that this is a purely mathematical requirement: actually this is not the case. *It is a "physical" prescription that a model could give a "unique" prevision of the modalities of occurrence of a physical phenomenon!*

There is also a *practical* advantage in the variational formulation of models as they are easily transformed into numerical codes. Of course after having considered Lagrangian systems (the evolution of which are governed by a least action functional) the study of non-Lagrangian ones (for which such a functional may not exist) may appear very difficult. It is often stated that dissipation cannot be described by means of a least action principle. This is not exactly true, as it is possible to find some action functionals for a large class of dissipative systems (see e.g. Maugin [97], Vujanovic and Jones [168] or Moiseiwitsch [111]). However it is true that not every conceived system can be regarded as a Lagrangian one. This point is mathematically delicate and will be only evoked here (see e.g. Santilli [131] for more details). In general, a non-Lagrangian system can be regarded as Lagrangian in two different ways: i) because it is an *approximation* of a Lagrangian system (see the case of Cattaneo equation for heat propagation in e.g. Vujanovic and Jones [168]), and this approximation leads to *cancel* the lacking part of the *true* action functional ii) because the considered system is simply a subsystem of a larger one which is truly Lagrangian. (see e.g. Carcaterra and Sestieri [17], Carcaterra et al. [18] Carcaterra [19], Carcaterra and Akai [21] [21]). The assumption that variational principles can be used only for non-dissipative systems is contradicted by, e.g., Bourdin et al. [10], Maugin and Trimarco [96] or Rinaldi and Lai [127] where variational principles modeling dissipative phenomena occurring in damage and fracture are formulated. In our opinion models for surface phenomena in presence of thermodynamical phenomena and diffusion or phase transitions in solids developed e.g. in McBride et al [101, 102], Steeb and Diebels [158] and Steinmann et al. [160] or for growth phenomena in living tissues as those presented in [93] (with suitable modifications!) should be formulated in a variational form.

One should not believe that the aforementioned considerations are limited to the description of mechanical phenomena only: actually the formulation of *variational principles* proved to be a powerful tool in many different research fields. In the following list (which cannot be exhaustive) we simply want to indicate the enormous variety of phenomena which were considered, up to now, from the variational point of view, by citing only those few works among the many available in the literature which we know better

- for biological evolutionary phenomena (see e.g. Edwards [54], Klimek et al. [77] and references therein);
- for the mathematical study of mutation and selection phenomena in species evolution (see e.g. Baake and Georgii [4]);

- for some phenomena of solid/solid phase transitions in plates and shells (see e.g. to Eremeyev Pietraszkiewicz et al. [124], Eremeev et al. [56], Eremeyev and Pietraszkiewicz [57]);
- for mechanical vibration control (see e.g. Carcaterra and Akai [21]);
- for electromagnetic phenomena (see e.g. Daher and Maugin [36] and references therein);
- for vibration control using distributed arrays of piezoelectric actuators (see e.g. dell’Isola Vidoli [47, 48]);
- for interfacial phenomena (see e.g. Eremeyev and Pietraszkiewicz [57], [34]Rangamani et al. [126] Steigmann and Ogden [155, 154], Daher and Maugin [37] and references therein);
- for the theory of membranes and rods (see e.g. Steigmann [153], Steigmann and Faulkner [157]);
- for mechanical phenomena involving different length scales (see e.g. Steigmann [156], dell’Isola et al. [50] and references therein);
- for phase transition phenomena in fluids (see Seppecher [65, 138, 139, 140, 141] or Casal and Gouin [25, 26]);
- for damage and fracture phenomena (see e.g. Francfort and Marigo [64], Yang and Misra [108, 109], Contrafatto and Cuomo [30, 31, 32], [35]);
- for some phenomena related to fluid flow in deformable porous media (see e.g. to dell’Isola et al. [49], dell’Isola et al. [50], Sciarra et al. [133, 134, 135], Quiligotti et al. [125]);
- for some piezoelectromechanical or magnetoelastic coupling phenomena (see e.g. to Barham et al. [5], Steigmann [152], Maurini et al. [99], Maugin and Attou [95], Maurini, et al. [100], dell’Isola and Vidoli [47, 48]).

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A Piola transformations and the formula of material derivative

A.1 Geometric framework

Let χ be a C^2 -diffeomorphism between the domains D_α and D_β . The following notations will be considered

$$F := \nabla \chi, \quad J := \det F, \quad F^{-T} := (F^{-1})^T$$

These fields are all defined in D_α . Conversely, the fields

$$F^{-1}, \quad J^{-1} := \det F^{-1}, \quad F^T$$

are obviously defined in D_β . These relations are summed up in the following diagram:

$$\begin{array}{ccc}
 T_X D_\alpha & \begin{array}{c} \xrightarrow{F} \\ \xleftarrow{F^T} \end{array} & T_x D_\beta \\
 \uparrow & & \uparrow \\
 D_\alpha & \xrightarrow{\chi} & D_\beta \\
 \downarrow & & \downarrow \\
 T_X^* D_\alpha & \begin{array}{c} \xrightarrow{F^{-T}} \\ \xleftarrow{F^{-1}} \end{array} & T_x^* D_\beta
 \end{array}$$

in which $T_p D$ and $T_p^* D$ denote, respectively, the tangent and cotangent plane to D at p . For every tensor field T_α defined in D_α , and for every tensor field T_β defined in D_β we use the notations

$$T_\alpha^{\overrightarrow{(\beta)}} := T_\alpha \circ \chi^{-1}, \quad T_\beta^{\overrightarrow{(\alpha)}} := T_\beta \circ \chi$$

We will say that $T_\alpha^{\overrightarrow{(\beta)}}$ is the field T_α displaced in D_β and conversely. These relations are exemplified in the following diagram in the specific case of two vectors fields:

$$\begin{array}{ccc}
 T_X D_\alpha & \begin{array}{c} \xrightarrow{F} \\ \xleftarrow{F^T} \end{array} & T_x D_\beta \\
 \uparrow T_\alpha & \begin{array}{c} \nearrow T_\beta^{\overrightarrow{(\alpha)}} \\ \nwarrow T_\alpha^{\overrightarrow{(\beta)}} \end{array} & \uparrow T_\beta \\
 D_\alpha & \begin{array}{c} \xrightarrow{\chi} \\ \xleftarrow{\chi^{-1}} \end{array} & D_\beta
 \end{array}$$

A.2 Transposition of linear mappings

The transposed F^T of the linear mapping F from the vector space $T_X D_\alpha$ to the vector space $T_x D_\beta$ is defined as the unique linear mapping from $T_x^* D_\beta$ to $T_X^* D_\alpha$ such that for every couple $(V, l) \in T_X D_\alpha \times T_x^* D_\beta$

$$\langle l, FV \rangle_{(T_x^* D_\beta, T_x D_\beta)} = \langle F^T l, V \rangle_{(T_X^* D_\alpha, T_X D_\alpha)}$$

where the bracket denotes the duality product. If both D_α and D_β are equipped with an inner product on their tangent space at each point⁹, tangent and cotangent space can be identified. Let us denote by g_α and g_β these fields of metric defined, respectively, on D_α and D_β . Through g_β a vector w can be associated to any covector l , more precisely:

$$\forall l \in T_x^* D_\beta, \exists w \in T_x D_\beta, \quad l = g_\beta w$$

Therefore the equality between the duality bracket can be rewritten

$$\langle g_\beta w, FV \rangle_{(T_x^* D_\beta, T_x D_\beta)} = \langle F^T g_\beta w, V \rangle_{(T_X^* D_\alpha, T_X D_\alpha)}$$

This construction can be summarized by the following diagram

$$\begin{array}{ccccc}
 & & T_X^* D_\alpha & \xleftarrow{F^T} & T_x^* D_\beta & & \\
 & \swarrow & \uparrow & & \uparrow & \searrow & \\
 \mathbb{R} & & & & & & \mathbb{R} \\
 & \swarrow & \uparrow g_\alpha & & \uparrow g_\beta & \searrow & \\
 & & T_X D_\alpha & \xrightarrow{F} & T_x D_\beta & &
 \end{array}$$

⁹In others terms, if both D_α and D_β are Riemannian manifolds.

Once introduced bases in $T_X D_\alpha$ and $T_x D_\beta$, we can represent vectors, tensors and inner products in terms of their components. The following relation is written in the domain D_β , hence quantities defined on D_α have to be transported:

$$g_{ab} w^b (F_A^a V^A)^{\vec{\beta}} = V^A (F^T)_A^a g_{ab} w^b (V^A)^{\vec{\beta}} \quad \forall V^A, \forall w^b$$

which implies

$$g_{ab} \left((F_A^a)^{\vec{\beta}} - (F^T)_A^a \right) V^A w^b = 0 \quad \forall V^A, \forall w^b$$

Therefore we have

$$(F_M^i)^{\vec{\beta}} = (F^T)_M^i \quad (36)$$

and, conversely,

$$(F^{-1})_i^M \overrightarrow{(\alpha)} = (F^{-T})_i^M \quad (37)$$

These relations will be important in the next subsection to properly define Piola transformation.

Let us now consider the following inner product (with a slight abuse of notation)

$$\langle FV, FW \rangle_{T_x D_\beta}$$

where F is the same linear mapping as before. By considering the transposed mapping one gets

$$\langle FV, FW \rangle_{T_x D_\beta} = \langle F^T FV, W \rangle_{T_X D_\alpha}$$

which in terms of components becomes

$$(g_{ab})^{\vec{\alpha}} F_A^a V^A F_B^b W^B = g_{CB} (F^T F)_B^C V^A W^B$$

therefore

$$(F^T F)_{MN} = (g_{ab})^{\vec{\alpha}} F_M^a F_N^b = (F_{Ma})^{\vec{\alpha}} F_N^a$$

or more simply, dropping down the change of domain:

$$(F^T F)_{MN} = F_{Ma} F_N^a \quad ; \quad (F^T F)^{MN} = F_a^M F^{aN}$$

A.3 Piola transformation for virtual works and stress tensors

We call virtual displacement stemming from χ a vector field $\delta\chi$ defined in D_α and such that, for every X in D_α , the vector $\delta\chi(X)$ belongs to the tangent space at the point $\chi(X)$. We will denote \mathcal{D} the space of such virtual displacements.

$$\mathcal{D} = \{ \delta\chi : D_\alpha \rightarrow TD_\beta, X \mapsto \delta\chi(X) \}$$

A virtual work functional must obviously be identified as a linear and continuous functional defined on \mathcal{D} (for a detailed discussion of this point see dell'Isola et al. [53] and references therein), i.e to an element of \mathcal{D}^* the dual space of \mathcal{D}

$$\mathcal{D}^* = \{ \mathcal{W} : \mathcal{D} \rightarrow \mathbb{R}, \delta\chi \mapsto W \}$$

Because of a representation theorem due to Schwartz [132] we can state that for any virtual work functional \mathcal{W} defined in D_α there exist N regular fields \mathbb{P}_γ (where $\gamma = 1, \dots, N$) such that

$$\mathcal{W}(\delta\chi) = \sum_{\gamma=1}^N \int_{D_\alpha} \mathbb{P}_\gamma \nabla_\alpha^\gamma (\delta\chi) dV_\alpha.$$

where

$$\nabla_\alpha^\gamma = D_\alpha \rightarrow \otimes^\gamma T^* D_\alpha \otimes TD_\beta \quad ; \quad \mathbb{P}_\gamma = D_\alpha \rightarrow \otimes^\gamma TD_\alpha \otimes T^* D_\beta$$

Modifying slightly the nomenclature introduced by Truesdell and Toupin [165] we can call \mathbb{P}_γ the γ -th order Piola stress tensor. Now, following Piola [119], we can transport the field $\delta\chi$ on D_β and define the corresponding Cauchy stress tensors \mathbb{T}_γ by means of the equality

$$\int_{D_\alpha} \mathbb{P}_{\gamma}^{\nabla_\alpha}(\delta\chi) dV_\alpha := \int_{D_\beta} \mathbb{T}_{\gamma}^{\nabla_\beta}(\delta\chi^{\overrightarrow{(\beta)}}) dV_\beta \quad \forall \delta\chi \in \mathcal{D}$$

in which

$$\nabla_\beta = D_\beta \rightarrow \otimes^\gamma T^* D_\beta \otimes T D_\beta \quad ; \quad \mathbb{T}_\gamma = D_\alpha \rightarrow \otimes^\gamma T D_\beta \otimes T^* D_\beta$$

To prove that such a tensor exists, and to get its representation, let us write component-wise the previous equation

$$\int_{D_\alpha} \mathbb{P}_i^{A_1 \dots A_\gamma} (\delta\chi)_{,A_1 \dots A_\gamma}^i dV_\alpha = \int_{D_\beta} \mathbb{T}_i^{j_1 \dots j_\gamma} (\delta\chi^{\overrightarrow{(\beta)}})_{,j_1 \dots j_\gamma}^i dV_\beta \quad \forall \delta\chi \in \mathcal{D}$$

Then using the chain rule the derivatives

$$(\delta\chi^{\overrightarrow{(\beta)}})_{,j_1 \dots j_\gamma}^i = \left((\delta\chi)_{,A_1 \dots A_\gamma}^i \right)^{\overrightarrow{(\beta)}} (F^{-1})_{j_1}^{A_1} \dots (F^{-1})_{j_\gamma}^{A_\gamma}$$

and a change of variable in the second integral, we obtain

$$\int_{D_\alpha} \mathbb{P}_i^{A_1 \dots A_\gamma} (\delta\chi)_{,A_1 \dots A_\gamma}^i dV_\alpha = \int_{D_\alpha} J \left(\mathbb{T}_i^{j_1 \dots j_\gamma} (F^{-1})_{j_1}^{A_1} \dots (F^{-1})_{j_\gamma}^{A_\gamma} \right)^{\overrightarrow{(\alpha)}} (\delta\chi)_{,A_1 \dots A_\gamma}^i dV_\alpha \quad \forall \delta\chi \in \mathcal{D}$$

which is equivalent to the following Piola formula of transformation of stress tensors

$$\mathbb{P}_i^{A_1 \dots A_\gamma} = J \left(\mathbb{T}_i^{j_1 \dots j_\gamma} (F^{-1})_{j_1}^{A_1} \dots (F^{-1})_{j_\gamma}^{A_\gamma} \right)^{\overrightarrow{(\alpha)}}$$

or, using the transformation (37) :

$$\mathbb{P}_\gamma = J \left(\mathbb{T}_\gamma \right)^{\overrightarrow{(\alpha)}} \underbrace{F^{-T} \dots F^{-T}}_\gamma$$

With simple algebra we also get

$$J^{-1} \left(\mathbb{P}_i^{A_1 \dots A_\gamma} F_{A_1}^{i_1} \dots F_{A_\gamma}^{i_\gamma} \right)^{\overrightarrow{(\beta)}} = \mathbb{T}_{\gamma i}^{i_1 \dots i_\gamma}$$

or, using the transformation (36) :

$$\mathbb{T}_\gamma = J^{-1} \left(\mathbb{P}_\gamma \right)^{\overrightarrow{(\beta)}} \underbrace{F^T \dots F^T}_\gamma$$

A.4 Piola transformation for divergence

For any tensor field T_α the following equality holds (for a proof see e.g. dell'Isola et al. [52] or Hughes and Marsden [94]).

$$\nabla_\alpha \cdot T_\alpha = J \left(\nabla_\beta \cdot \left(J^{-1} T_\alpha^{\overrightarrow{(\beta)}} F^T \right) \right)^{\overrightarrow{(\alpha)}} \quad (38)$$

which obviously implies the other one

$$(\nabla_\alpha \cdot T_\alpha)^{\overrightarrow{(\beta)}} = J^{\overrightarrow{(\beta)}} \nabla_\beta \cdot \left(J^{-1} T_\alpha^{\overrightarrow{(\beta)}} F^T \right)$$

In components this relation reads (where X^L and x^j denote the components of the position vector in D_α and D_β respectively)

$$\left(\frac{\partial T_\alpha^A}{\partial X^A}\right)^{\overrightarrow{(\beta)}} = J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^a} \left(J^{-1} (T_\alpha^A F_A^a)^{\overrightarrow{(\beta)}} \right) \quad (39)$$

Similarly we have that the following relationship, in some sense inverse of the relation (38)

$$\nabla_\beta \cdot T_\beta = J^{-1} \left(\nabla_\alpha \cdot \left(J T_\beta^{\overrightarrow{(\alpha)}} F^{-T} \right) \right)^{\overrightarrow{(\beta)}} \quad (40)$$

A.5 The Piola-Ricci-Bianchi condition

The equation (40) was first found, without the help of tensor calculus, by Piola [119]. In the case where T_β reduces to the identity, the former equation takes the following form

$$\nabla \cdot (J F^{-T}) = 0 \quad (41)$$

which in components can be written

$$\frac{\partial}{\partial X^A} \left(J (F^{-1})_i^A \right) = 0$$

The equation (41) is a particular case of Bianchi condition for Ricci curvature tensor, when interpreting Lagrangian coordinates as a chart for the Eulerian configuration of the body. From Piola-Ricci-Bianchi condition

$$\frac{\partial}{\partial X^A} \left(J (F^{-1})_i^A \right) = 0$$

one gets

$$\begin{aligned} J_{,A} (F^{-1})_i^A + J (F^{-1})_{i,A}^A &= 0 \\ (F^{-1})_{i,A}^A &= -J^{-1} \left(\frac{\rho_0}{\rho} \right)_{,A} (F^{-1})_i^A = -\rho_0 J^{-1} \left(-\frac{1}{\rho^2} \right) \rho_{,A} (F^{-1})_i^A = \left(\frac{1}{\rho} \right) \rho_{,A} (F^{-1})_i^A \end{aligned}$$

In conclusion

$$(F^{-1})_{i,A}^A = \frac{\rho_{,A}}{\rho} (F^{-1})_i^A = \frac{\rho_{,i}}{\rho} \quad (42)$$

A.6 Piola transformation for double divergence

To obtain the Eulerian form for balance equation for capillary fluids we need to apply the divergence twice to calculate the transformation of double Lagrangian divergence. We proceed as follows: the equality (39) implies that (remark: we assume that the tensor T_α^{AB} is symmetric)

$$\left(\frac{\partial T_\alpha^{AB}}{\partial X^B}\right)^{\overrightarrow{(\beta)}} = J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^b} \left(J^{-1} (T_\alpha^{AB} F_B^b)^{\overrightarrow{(\beta)}} \right)$$

then

$$\begin{aligned} \left(\frac{\partial}{\partial X^A} \left(\frac{\partial T_\alpha^{AB}}{\partial X^B} \right) \right)^{\overrightarrow{(\beta)}} &= J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^a} \left(J^{-1} \left(\left(\frac{\partial T_\alpha^{AB}}{\partial X^B} \right)^{\overrightarrow{(\beta)}} (F_A^a)^{\overrightarrow{(\beta)}} \right) \right) \\ &= J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^a} \left(J^{-1} \left(J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^b} \left(J^{-1} (T_\alpha^{AB} F_B^b)^{\overrightarrow{(\beta)}} \right) (F_A^a)^{\overrightarrow{(\beta)}} \right) \right) \\ &= J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^a} \left(\frac{\partial}{\partial x^b} \left(J^{-1} (T_\alpha^{AB} F_B^b)^{\overrightarrow{(\beta)}} \right) (F_A^a)^{\overrightarrow{(\beta)}} \right) \end{aligned}$$

In conclusion we have:

$$\left(\frac{\partial}{\partial X^A} \left(\frac{\partial T_\alpha^{AB}}{\partial X^B} \right) \right)^{\overrightarrow{(\beta)}} = J^{\overrightarrow{(\beta)}} \frac{\partial}{\partial x^a} \left(\frac{\partial}{\partial x^b} \left(J^{-1} (T_\alpha^{AB} F_B^b)^{\overrightarrow{(\beta)}} \right) (F_A^a)^{\overrightarrow{(\beta)}} \right)$$

A.7 Piola transformation for normals

For normals we have the following formula (see e.g. dell'Isola et al. [50])

$$N_{\alpha}^{\overrightarrow{(\beta)}} = \frac{(J^{-1}F^T) N_{\beta}}{\|(J^{-1}F^T) N_{\beta}\|} \quad (43)$$

while, for the passage from α to β domain, the following transformation formula for areas holds

$$\left(\|(J^{-1}F^T) N_{\beta}\|^{-1}\right)^{\overrightarrow{(\alpha)}} = \|(JF^{-T}) N_{\alpha}\| = \frac{dA_{\beta}}{dA_{\alpha}}. \quad (44)$$

A.8 Material derivative

For what concerns the formula of material derivative we start by remarking that

$$\left(T_{\alpha}^{\overrightarrow{(\beta)}}\right)^{\overrightarrow{(\alpha)}} = T_{\alpha}$$

therefore

$$\begin{aligned} \left(\frac{\partial T_{\alpha}}{\partial t}\Big|_X\right) &= \left(\frac{\partial \left(T_{\alpha}^{\overrightarrow{(\beta)}}\right)^{\overrightarrow{(\alpha)}}}{\partial t}\Big|_X\right) = \left(\frac{\partial \left(T_{\alpha}^{\overrightarrow{(\beta)}} \circ \chi\right)}{\partial t}\Big|_X\right) = \left(\frac{\partial \left(T_{\alpha}^{\overrightarrow{(\beta)}}(\chi(X, t), t)\right)}{\partial t}\Big|_X\right) \\ &= \left(\frac{\partial \left(T_{\alpha}^{\overrightarrow{(\beta)}}(x, t)\right)}{\partial t}\Big|_x \circ \chi\right) + \left(\nabla_x T_{\alpha}^{\overrightarrow{(\beta)}}(x, t)\Big|_x \circ \chi\right) \cdot \frac{\partial \chi}{\partial t}\Big|_X \end{aligned}$$

as a consequence

$$\left(\frac{\partial T_{\alpha}}{\partial t}\Big|_X\right)^{\overrightarrow{(\beta)}} = \left(\frac{\partial \left(T_{\alpha}^{\overrightarrow{(\beta)}}(x, t)\right)}{\partial t}\Big|_x\right) + \left(\nabla_x T_{\alpha}^{\overrightarrow{(\beta)}}(x, t)\Big|_x\right) \cdot \frac{\partial \chi}{\partial t}\Big|_X^{\overrightarrow{(\beta)}}$$

B Basic kinematic formulas

In this section some useful kinematic formulas are proven (for a complete presentation of this subject see e.g. [86]). They are the basis of the procedure on which Hamilton-Piola postulation is founded. However, because of their central role, they cannot be avoided in any case: their use can be only postponed to subsequent steps, when different postulations are attempted and indeed kinematic formulas of this type are presented in any textbook of continuum mechanics. From now on, the α domain will coincide with the Lagrangian set of coordinates while β domain will coincide with the Eulerian domain and the notation $(\cdot)^{\overrightarrow{(\beta)}}$ and $(\cdot)^{\overrightarrow{(\mathcal{E})}}$ will be consistently used. They will be omitted occasionally for making readability easier.

B.1 Formulas on Eulerian mass density and its gradients

Mass density and its gradients play a pivotal role in strain energy of fluids. Here we gather some useful formulas relating them with C , F and ∇F (remark that we will omit the needed $(\cdot)^{\overrightarrow{(\beta)}}$, $(\cdot)^{\overrightarrow{(\mathcal{E})}}$ for making readability easier).

B.1.1 The derivative of the determinant a matrix with respect its entries

We start by recalling the well-known formula

$$\frac{\partial \det(A)}{\partial A_M^i} = \det A (A^{-T})_i^M$$

which can be recovered by using the Laplace rule for calculating the determinant

$$\delta_M^N \det A = A_M^a (A^*)_a^N$$

where $(A^*)_i^N$ is the cofactor of the element A_N^i . Remarking that the cofactors of all elements of the M -th row are independent of the entry A_M^i and the inversion theorem, for matrices one gets

$$\frac{\partial \det(A)}{\partial A_M^i} = (A^*)_i^M = \det A (A^{-T})_i^M$$

B.1.2 Partial derivatives of ρ , J and F^{-1} with respect to F

Once one recalls that

$$\rho_0 \det F = \rho$$

and having defined the cofactor of F as

$$(F^*)_i^A F_A^j = \det F \delta_i^j$$

it is easy to deduce

$$\begin{aligned} \frac{\partial J}{\partial F_M^i} &= J (F^{-T})_M^i = \frac{\rho_0}{\rho} (F^{-T})_M^i \\ \frac{\partial \rho}{\partial F_M^i} &= -\rho (F^{-1})_i^M \end{aligned} \quad (45)$$

$$\frac{\partial (F^{-1})_j^N}{\partial F_M^i} = -(F^{-1})_i^N (F^{-1})_j^M \quad (46)$$

B.1.3 Partial derivative of mass density with respect to C

In order to prove the following equality

$$\frac{\partial \rho}{\partial C_{MN}} = -\frac{\rho}{2} (F^{-1})^{Ma} (F^{-1})_a^N \quad (47)$$

We proceed in the following way:

$$\frac{\partial \rho}{\partial C_{MN}} = \rho_0 \frac{\partial (\det C)^{-\frac{1}{2}}}{\partial C_{MN}} = \rho_0 \frac{\partial (\det C)^{-\frac{1}{2}}}{\partial \det C} \frac{\partial \det C}{\partial C_{MN}} = -\frac{\rho_0}{2} (\det C)^{-\frac{3}{2}} \frac{\partial \det C}{\partial C_{MN}}$$

In conclusion we have

$$\frac{\partial \rho}{\partial C_{MN}} = -\frac{\rho_0}{2} (\det C)^{-\frac{1}{2}} (C^{-1})^{MN} = -\frac{\rho}{2} (F^{-1})^{Ma} (F^{-1})_a^{LN}$$

B.1.4 Lagrangian and Eulerian gradients of F^{-1}

Starting from

$$(F^{-1})_a^M F_N^a = \delta_N^M$$

after differentiation we obtain:

$$(F^{-1})_a^M F_{N,O}^a + F_N^a (F^{-1})_{a,O}^M = 0$$

which produces the following chain of equalities

$$\begin{aligned} F_N^a (F^{-1})_{a,O}^M &= -(F^{-1})_a^M F_{N,O}^a \\ (F^{-1})_{i,O}^M &= -(F^{-1})_i^A (F^{-1})_a^M F_{A,O}^a \end{aligned} \quad (48)$$

The last equality can be then multiplied times F^{-1} to get the Eulerian gradient

$$(F^{-1})_{i,j}^M = -(F^{-1})_j^A (F^{-1})_i^B (F^{-1})_a^M F_{B,A}^a$$

It can be useful to remark that:

$$-\left(\rho (F^{-1})_i^M\right)_{,j} = -\rho_{,j} (F^{-1})_i^M - \rho (F^{-1})_{i,j}^M = -\rho_{,j} (F^{-1})_i^M + \rho (F^{-1})_j^A (F^{-1})_i^B (F^{-1})_a^M F_{B,A}^a \quad (49)$$

B.1.5 Expression of Eulerian gradient of density in terms of F and its gradients

We start from the defining relationship:

$$\rho = \frac{\rho_0}{\det(F)} = \rho_0 \det(F^{-1}) \quad (50)$$

As it is possible to assume that ρ_0 is constant, we calculate the gradient of the density as follows

$$\rho_{,i} = \rho_0 \det(F^{-1})_{,i} = \rho_0 \frac{\partial \det(F^{-1})}{\partial (F^{-1})_a^A} \frac{\partial (F^{-1})_a^A}{\partial x^i} = \rho_0 \det(F^{-1}) F_A^a (F^{-1})_{a,i}^A$$

and finally

$$\rho_{,i}^{\overrightarrow{(B)}} = \rho F_A^b (F^{-1})_{b,B}^A (F^{-1})_i^B$$

To summarize, from all previous expressions we obtain the following useful formulas :

$$\begin{aligned} \frac{\rho_{,i}}{\rho} &= - (F^{-1})_a^A (F^{-1})_i^B F_{A,B}^a = - (F^{-1})_a^A F_{A,i}^a \\ \rho_{,i} &= \rho F_A^a (F^{-1})_i^B (F^{-1})_{a,B}^A = \rho F_A^a (F^{-1})_{a,i}^A \\ F_A^a (F^{-1})_{a,M}^A &= \frac{\rho_{,i}}{\rho} F_M^i \\ (F^{-1})_{j,A}^M (F^{-1})_i^A &= (F^{-1})_j^M \frac{\rho_{,i}}{\rho} \end{aligned} \quad (51)$$

B.1.6 Calculation of partial derivative of Eulerian gradient of mass density with respect to F

We need to estimate the following partial derivative:

$$\frac{\partial \rho_{,i}}{\partial F_M^j} = \frac{\partial}{\partial F_M^j} \left(-\rho (F^{-1})_a^A (F^{-1})_i^B \right) F_{A,B}^a$$

As we have that

$$\begin{aligned} &\left(\frac{\partial \rho}{\partial F_M^i} (F^{-1})_j^N (F^{-1})_k^O + \rho (F^{-1})_k^O \frac{\partial (F^{-1})_j^N}{\partial F_M^i} + \rho (F^{-1})_j^N \frac{\partial (F^{-1})_k^O}{\partial F_M^i} \right) = \\ &-\rho (F^{-1})_i^M (F^{-1})_j^N (F^{-1})_k^O - \rho (F^{-1})_i^N (F^{-1})_j^M (F^{-1})_k^O - \rho (F^{-1})_j^N (F^{-1})_i^O (F^{-1})_k^M \end{aligned}$$

where we used the equalities (45), (46). We can then conclude

$$\frac{\partial \rho_{,i}}{\partial F_M^j} = \rho \left((F^{-1})_j^M (F^{-1})_i^A (F^{-1})_a^B F_{B,A}^a + (F^{-1})_j^C (F^{-1})_i^M (F^{-1})_b^D F_{D,C}^b + (F^{-1})_i^E (F^{-1})_j^F (F^{-1})_c^G F_{F,E}^c \right)$$

by using (51) we get

$$\frac{\partial \rho_{,i}}{\partial F_M^j} = -\rho_{,i} (F^{-1})_j^M - \rho_{,j} (F^{-1})_i^M + \rho (F^{-1})_i^A (F^{-1})_{l_j}^B (F^{-1})_a^M F_{B,A}^a$$

Finally by replacing (49) we can conclude:

$$\frac{\partial \rho_{,i}}{\partial F_M^j} = -\rho_{,j} (F^{-1})_i^M - \left(\rho (F^{-1})_j^M \right)_{,i} \quad (52)$$

B.1.7 The derivatives of $(\beta)^{\overrightarrow{\mathcal{B}}}$ with respect F and ∇F

We start from a direct expression for $(\beta)^{\overrightarrow{\mathcal{B}}}$

$$(\beta)^{\overrightarrow{\mathcal{B}}} = (\nabla\rho \cdot \nabla\rho)^{\overrightarrow{\mathcal{B}}} = (g^{ab}\rho_{,a}\rho_{,b})^{\overrightarrow{\mathcal{B}}}$$

which implies the following two

$$\frac{\partial}{\partial F} (\beta)^{\overrightarrow{\mathcal{B}}} = 2(\nabla\rho)^{\overrightarrow{\mathcal{B}}} \cdot \frac{\partial(\nabla\rho)^{\overrightarrow{\mathcal{B}}}}{\partial F} \quad (53)$$

$$\frac{\partial}{\partial \nabla F} (\beta)^{\overrightarrow{\mathcal{B}}} = 2(\nabla\rho)^{\overrightarrow{\mathcal{B}}} \cdot \frac{\partial(\nabla\rho)^{\overrightarrow{\mathcal{B}}}}{\partial \nabla F} \quad (54)$$

Then using (55) and (52) we get easily:

$$\begin{aligned} \frac{\partial\beta}{\partial F_M^i} &= 2g^{ab}\rho_{,a} \frac{\partial(\rho_{,b})^{\overrightarrow{\mathcal{B}}}}{\partial F_M^i} \\ \frac{\partial(\beta)^{\overrightarrow{\mathcal{B}}}}{\partial F_M^i} &= -2g^{ab} \left(\rho_{,a}\rho_{,i} (F^{-1})^M_b + \rho_{,a} \left(\rho (F^{-1})^M_i \right)_{,b} \right)^{\overrightarrow{\mathcal{B}}} \end{aligned} \quad (55)$$

Similarly, using (54) and (51) we obtain

$$\frac{\partial(\beta)^{\overrightarrow{\mathcal{B}}}}{\partial F_{M,N}^i} = 2g^{ab}(\rho_{,a})^{\overrightarrow{\mathcal{B}}} \frac{\partial(\rho_{,b})^{\overrightarrow{\mathcal{B}}}}{\partial F_{M,N}^i} = -2g^{ab} \left(\rho\rho_{,a} (F^{-1})^M_i (F^{-1})^N_b \right)^{\overrightarrow{\mathcal{B}}} \quad (56)$$

B.2 Derivatives of $C, C^{-1}, \nabla C$ and ∇C^{-1} with respect to F and ∇F

B.2.1 Computation of $\frac{\partial C_{MN}}{\partial F_P^i}$

$$\begin{aligned} \frac{\partial C_{MN}}{\partial F_P^i} &= g_{ab} \frac{\partial}{\partial F_P^i} (F_M^a F_N^b) = g_{ab} \left(\frac{\partial F_M^b}{\partial F_P^i} F_N^a + F_M^b \frac{\partial F_N^a}{\partial F_P^i} \right) \\ &= g_{ab} (\delta_i^b \delta_M^P F_N^a + F_M^b \delta_i^a \delta_N^P) = (\delta_M^P F_{iN} + F_{iM} \delta_N^P) \end{aligned}$$

B.2.2 Computation of $\frac{\partial C_{MN,O}}{\partial F_P^i}$

$$\begin{aligned} \frac{\partial C_{MN,O}}{\partial F_P^i} &= \frac{\partial}{\partial F_P^i} \left(\frac{\partial F_M^a}{\partial X^O} F_{Na} + \frac{\partial F_N^b}{\partial X^O} F_{Lb} \right) \\ &= \frac{\partial}{\partial F_P^i} \left(\frac{\partial F_M^a}{\partial X^O} \right) F_{Na} + \frac{\partial F_M^b}{\partial X^O} \frac{\partial F_{Nb}}{\partial F_P^i} + \frac{\partial}{\partial F_P^i} \left(\frac{\partial F_N^c}{\partial X^O} \right) F_{Mc} + \frac{\partial F_N^d}{\partial X^O} \frac{\partial F_{Md}}{\partial F_P^i} \\ &= g_{ab} F_{M,O}^a \frac{\partial F_N^b}{\partial F_P^i} + g_{cd} F_{N,O}^c \frac{\partial F_M^d}{\partial F_P^i} = g_{ab} F_{M,O}^a \delta_i^b \delta_P^N + g_{cd} F_{N,O}^c \delta_i^d \delta_P^M \\ &= F_{iM,O} \delta_P^N + F_{iN,O} \delta_P^M \end{aligned}$$

B.2.3 Computation of $\frac{\partial C_{MN}^{-1}}{\partial F_P^i}$

$$\frac{\partial (C^{-1})_{MN}}{\partial F_P^i} = \frac{\partial \left((F^{-1})_{aM} (F^{-1})^a_N \right)}{\partial F_P^i} = \frac{\partial \left((F^{-1})_{aM} \right)}{\partial F_P^i} (F^{-1})^a_N + (F^{-1})_{bM} \frac{\partial \left((F^{-1})^b_N \right)}{\partial F_P^i}$$

Using equation (46) we obtain

$$\frac{\partial (C^{-1})_{MN}}{\partial F_P^i} = - (F^{-1})_{Mi} (F^{-1})^P_a (F^{-1})^a_N - (F^{-1})_{Ni} (F^{-1})^{bP} (F^{-1})_{bM}$$

B.2.4 Computation of $\frac{\partial C_{MN,O}^{-1}}{\partial F_P^i}$

$$\begin{aligned}\frac{\partial C_{MN,O}^{-1}}{\partial F_P^i} &= \left((F^{-1})_{Ma,O} \frac{\partial (F^{-1})_N^a}{\partial F_P^i} + \frac{\partial (F^{-1})_{Mb}}{\partial F_P^i} (F^{-1})_{N,O}^b \right) \\ &= - \left((F^{-1})_{Ni} (F^{-1})^{aP} (F^{-1})_{Ma,O} + (F^{-1})_{Mi} (F^{-1})^{aP} (F^{-1})_{aN,O} \right) \\ &= - (F^{-1})^{aP} \left((F^{-1})_{Ni} (F^{-1})_{Ma,O} + (F^{-1})_{Mi} (F^{-1})_{aN,O} \right)\end{aligned}$$

B.2.5 Computation of $\frac{\partial C_{MN,O}}{\partial F_{P,Q}^i}$

The computation is straightforward

$$\frac{\partial C_{MN,O}}{\partial F_{P,Q}^i} = \frac{\partial}{\partial F_{P,Q}^i} (F_{M,O}^a F_{Na} + F_{N,O}^b F_{Mb}) = \left(\delta_i^a \delta_M^P \delta_O^Q F_{Na} + \delta_i^b \delta_N^P \delta_O^Q F_{Mb} \right) = \left(\delta_M^P \delta_O^Q F_{Ni} + \delta_N^P \delta_O^Q F_{Mi} \right)$$

B.2.6 Computation of $\frac{\partial C_{MN,O}^{-1}}{\partial F_{P,Q}^i}$

We compute the partial derivative as the following product:

$$\frac{\partial C_{MN,O}^{-1}}{\partial F_{P,Q}^i} = \frac{\partial C_{MN,O}^{-1}}{\partial (F^{-1})_{A,B}^a} \frac{\partial (F^{-1})_{A,B}^a}{\partial F_{P,Q}^i}$$

The first term is directly proceed:

$$\begin{aligned}\frac{\partial C_{MN,O}^{-1}}{\partial (F^{-1})_{P,Q}^i} &= \frac{\partial}{\partial (F^{-1})_{P,Q}^i} \left(g_{ab} (F^{-1})_N^a (F^{-1})_{M,O}^b + (F^{-1})_{Mc} (F^{-1})_{N,O}^c \right) \\ &= g_{ab} \delta_i^b \delta_M^P \delta_Q^O (F^{-1})_N^a + \delta_i^c \delta_N^P \delta_Q^O (F^{-1})_{Mc} (F^{-1})_{N,L}^c \\ &= \delta_Q^O \left[\delta_M^P (F^{-1})_{iN} + \delta_N^P (F^{-1})_{Mi} \right]\end{aligned}$$

Deriving equation (48) with respect to $F_{P,Q}^i$ we obtain

$$\frac{\partial (F^{-1})_{i,N}^M}{\partial F_{P,Q}^j} = - (F^{-1})_j^M (F^{-1})_i^P \delta_N^Q$$

Combining the results and considering that

$$(F^{-1})_{M,N}^i = g^{ia} g_{MA} (F^{-1})_{a,N}^A$$

we finally have

$$\begin{aligned}\frac{\partial C_{MN,O}^{-1}}{\partial F_{P,Q}^i} &= -\delta_A^O \left[\delta_M^B (F^{-1})_{aN} + \delta_N^B (F^{-1})_{Ma} \right] (F^{-1})_{Bi} (F^{-1})^{aP} \delta_Q^A \\ &= -\delta_Q^O \left[(F^{-1})_{Mi} (F^{-1})^{aP} (F^{-1})_{aN} + (F^{-1})_{Ni} (F^{-1})^{bP} (F^{-1})_{Mb} \right]\end{aligned}$$

C Gauss divergence theorem for embedded Riemannian manifolds

We choose a global orthonormal basis $(e_i, i = 1, 2, 3)$ for the vector field of displacements in E^3 , the tridimensional Euclidean space. All tensor fields will be represented by their components with respect to this basis. In this section we consider an embedded Riemannian manifold \mathcal{M} in E^3 . This manifold can be therefore a regular curve or surface, but will be restricted to a surface in the present discussion. As \mathcal{M} can be equipped with a Gaussian coordinate systems, it is possible to introduce in the neighborhood of any point of \mathcal{M} (For more details see dell'Isola et al. [53]):

- P , the field of projection operator on tangent space;
- Q the field of projection operator on tangent space.

These projectors verify the following obvious identities:

$$\begin{aligned}\delta_i^j &= P_i^j + Q_i^j, & P_i^a P_a^j &= P_i^j, \\ Q_i^a Q_a^j &= Q_i^j, & P_i^a Q_a^j &= 0.\end{aligned}$$

In order to simplify the forthcoming calculations, instead of using curvilinear coordinates, we rather use a global Cartesian coordinate system, completed by P and Q in the neighborhood of \mathcal{M} . This technical choice is exactly the same one which allowed Germain to generalize, for second gradient materials, the results found by Green, Rivlin, Toupin and Mindlin.

The unit external normal to \mathcal{M} on its border, which is denoted ν , belongs to the tangent space to \mathcal{M} .

Using these notations the divergence theorem reads (see e.g. Spivak [161]) For any vector field W defined in the vicinity of M

$$\int_M (P_b^a W^b)_{,c} P_a^c dS = \int_{\partial M} W^a P_a^b \nu_b dL \quad (57)$$

This theorem together with relation

$$Q_{j,b}^a P_a^b = -Q_j^a P_{a,b}^b$$

implies that, for any vector field W defined in a neighborhood of \mathcal{M} .

$$\begin{aligned}\int_M (W^a)_{,b} P_a^b dS &= \int_M \left[(P_b^a W^b)_{,c} P_a^c + (Q_e^d W^e)_{,f} P_d^f \right] dS \\ &= \int_M W^a Q_{a,c}^b P_b^c dS + \int_{\partial M} W^d P_d^e \nu_e dL = - \int_M W^a Q_a^b P_{b,c}^c dS + \int_{\partial M} W^d P_d^f \nu_f dL\end{aligned}$$

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