

GENESIS OF THE MULTISCALE APPROACH FOR MATERIALS WITH MICROSTRUCTURE

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Monday, 17 November 2008

Abstract

This paper presents an overview of the origin of multiscale approaches in mechanics. While the pioneer molecular models of linear elastic bodies by Navier, Cauchy and Poisson were contradicted by experiments, the phenomenological energetic approach by Green still seems suitable for simple materials only. Voigt's molecular model, here reinterpreted in the light of contemporary mechanics, reconciled the two approaches providing a conceptual guideline for developing constitutive models based on a direct link between continuum and discrete solid mechanics. Such a theoretical background proves to be especially suitable for new complex materials. An example referred to masonry-like materials is given.

Keywords: Molecular theory of elasticity, multiscale modelling, constitutive models, lattice mechanics.

1. Introduction: the multiscale approach between past and present

A basic issue of mechanics of materials, starting from modern nanoscience up to structural engineering, is the definition of constitutive models for materials with internal structure that can be detected at different (meso, micro/nano, atomistic, electronic) scales [1]. Based on their internal structure, these complex materials can be classified as composite, fibre-reinforced, granular, amorphous, defected or martensitic. Moreover, these materials are defined as complex because of their mechanical behaviour, which is essentially non-linear, due to damage, fracture, growth, piezoelectricity, etc.

In order to develop theoretical, mathematical and computational tools for the modelling of mechanical properties of such materials various approaches have been proposed within a truly multidisciplinary framework. In many cases, direct modelling at scales smaller than macroscopic, such as atomic-scale, molecular or dislocation dynamics simulations [2]-[4], can lead to numerically cumbersome problems. Micromechanic modelling, focused on retaining memory of the fine material organization without forsaking the advantages of the field description, appears to be more effective for this purpose [5]-[7]. In particular multiscale approaches, which aim to deduce properties and relations at a given

scale by bridging information at proper underlying levels, offer useful new insights into complex materials [8], [9] opening the way to various challenging applications in material science and engineering [10].

For many years, multiscale mechanics has provided several strategies (homogenization, coarse graining) to identify relationships among different material scales, in particular to derive macroscopic constitutive functions for continuous linear or non-linear materials [11]-[14]. These strategies allow replacing a fine-grained description with a lower-resolution coarse-grained model and have often been applied to describe the macroscopic behaviour of heterogeneous materials made of parts of significant shape, size and distribution at various microscopic levels (composites, masonry-like, bio-materials, materials with voids or defects, etc.). Moreover, the possibility of microstructure evolution has also been taken into account within the framework of finite inelasticity with ‘internal variables’ [15]. And also in order to extend the results within the framework of non-simple materials, various models particularly addressing non-local and higher-order materials have also been proposed [16]-[18]. Such formulations become significant in problems in which macroscopic length scales are comparable to material internal length scales and the field equations for the classical continuum become ill-posed. With this regard, various homogenization techniques, also addressed to numerical simulations, have also been developed within the framework of micromorphic materials [19]-[25] or other multifield materials [26]-[29].

In addition, many other multiscale strategies have been developed for studying the transition from the fine-grain to the coarse-grain description for materials with microstructure at length scales with several orders of magnitude smaller than the macroscopic scale, such as defects at the atomic scale, nano-composite materials or dislocated bodies. A comprehensive review of classical methods by which boundary-value problems can be solved exploiting atomic information can be found in the article by Ortiz and Phillips [30]. With this regard, various other approaches searching for direct links between discrete and continuum solid mechanics have been proposed and are currently still being researched [31]-[36].

Originally, analogous multiscale strategies were developed to predict the constitutive relationships for standard elastic continua starting from the discrete description of materials at a supposed atomic level. This work focuses particular attention on the genesis of the multiscale approach in the mechanics of materials that essentially coincides with the genesis of continuum mechanics. During the 19th century, the basic principle of classical physics and, in particular, of the energetic theory of elasticity - the principle of continuity of matter - had often been discussed, also on the basis of the discoveries of the time regarding the existence of atoms. Theories of material behaviour [36]-[41], like other mean field theories in physics [42]-[44], searched for justification and a rational basis by taking into account the discrete nature of matter. The molecular theory of elasticity, as developed by Navier, Cauchy and Poisson, represented one of the first steps in this direction. The aim of this theory was to predict the macroscopic constitutive behaviour on the basis of the definition of microscopic laws for atomic/molecular interactions, depending on the inter-molecular distance (central-force model). Macroscopic quantities (stress, elastic moduli, etc.) were then derived as averages of atomic material quantities. A further important step was achieved by Voigt [45]-[47] who proposed a molecular approach which took into account both interatomic forces and couples, also based on the description of the potential of particle interactions.

The molecular theory of elasticity was long supported by important scientists, including Saint-Venant [48], mostly because it seemed to be a theory which was physically motivated by its mechanical background, made of forces perceived as mechanical interactions between material particles. This theory was, however, later abandoned due to experimental discrepancies. Despite the significant work of Voigt, which bypassed the limitations of the central-force scheme providing results in agreement with experimental data, the molecular approach was no longer adopted and from then on the constitutive theories were based on macroscopic criteria following the mathematical theory of elastic potential by Green [49].

Green's theory was based on the single assumption that the internal work of any force system be an exact differential. This approach can be quite easily pursued until ideal materials with quadratic energy functionals can be found. On the other hand, in the mechanics of new complex materials, which are quite different mechanical objects to the ideal homogeneous medium of classical continuum mechanics, finding weak macroscopic principles for describing complex phenomena, such as damage, fracture, growth, etc., is not an easy task [50]. Therefore, a multiscale-molecular approach aimed at building an explicit version of a stored energy function starting from the Lagrangian description of particle interactions encounters renewed interest. This is both because the macroscopic behaviour is greatly influenced by the internal structure of the material and must be taken into account, and because the development of procedures governing transitions among material descriptions at different length scales often allows to derive theoretical constitutive models which are physically motivated.¹

The aim of this work is to study and reinterpret the basic issues of molecular elasticity and propose a current formulation of the classical approaches in order to point out the historical and epistemological basis of the present coarse-graining multiscale strategies. Upon summarizing the basic stages of the classical molecular models of the 19th century, in Section 2 we present the central-force model as developed by Cauchy [39] focusing on the definition of the stress and the derivation of the so-called *rari-constant* constitutive relations; in Section 3 we rewrite and interpret Voigt's molecular work [45]-[47] governed by potentials of forces and couples leading, after introducing suitable constraints, to a *multi-constant* constitutive model of Green's type. In Section 4, with the aid of an example referred to masonry-like materials, we point out how Voigt's molecular approach allows to bridge the gap between the mechanistic/corpuscular and energetic/continuous conceptions. Such an approach can be seen as a sample pioneer strategy to describe macroscopic phenomenology interpreted and rationalised using microscopic information, as occurs in current advanced material science.

2. The molecular theory of elasticity: the central-force model

2.1. Historical notes

The aim of the molecular theory of elasticity was to predict the macroscopic constitutive behaviour on the basis of the definition of microscopic laws for particle interactions, depending on the inter-molecular distance, going through the definition of macroscopic stress quantities as averages of atomic material quantities.

¹ See for example the discussion contained in the work by Ericksen ([51], pp. 189-192).

Originally the molecular models were introduced to justify the ‘causes’ of elasticity, which were presumed to lie on the natural attractive or repulsive properties of atoms depending on their mutual distance, as in the original idea of Newton specified later by Laplace and Boscovich.² This mechanistic approach allowed to preserve the concept of force as mechanical interaction between material particles and was extremely appreciated by the scientists of the period. The earlier formulations of the mathematical theory of elasticity by Navier [36], Cauchy [39] and Poisson [40] were based on such a corpuscular interpretation. Although the description of the material behaviour originates from the modelling of discrete systems of interacting particles, the aim of each formulation was the derivation of continuous models in which macroscopic quantities were derived in statistical terms. All these models were based on differential calculus in agreement with the Lagrangian tradition of analytical mechanics.

Analogous molecular approaches were developed in various fields of physics at the same time. The 19th century was characterized by the attempt at providing a mechanical interpretation for any physical phenomena. For instance light was described as propagated in space through an elastic medium called ether, as in elasticity. This is the case with Fresnel’s theory of light propagation [53], in which the ether was described as a system of material particles interacting through springs. A number of other phenomena were also explained in terms of interactions at the molecular level. Thermodynamics and electro-magnetism were the most important frameworks in which the multiscale-molecular approach was developed. The kinetic theory of gases, for example, from Boyle, Euler, D. Bernouilli and Avogadro to Clausius and Maxwell and more generally the statistical-mechanics, by Boltzmann and Gibbs, describe interatomic actions as depending on interatomic distances and derive both macroscopic average quantities (pressure, temperature, volume, strain energy, free energy, entropy) and laws from atomistic information. As is well known, further developments of such statistical approaches also led to quantum mechanics.

Apart from any physical basis, in these theories the molecules were considered as ultimate material particles without extension. As done by Voigt in elasticity (Section 3), in some cases experimental discrepancies were solved by properly enriching the molecular models, as occurred for instance by adding degrees of freedom to the molecular model of the ideal gas. This key idea that elementary material particles gained extension, becoming ‘structured molecules’ according to current terminology, was destined to be followed-up in the mechanics of materials.

In 1821 at the *Académie des Sciences* of Paris Navier presented the first systematic memoir on the molecular theory of elasticity. In this work, which was not published until 1827 [36], the balance equations in terms of displacements for elastic bodies were derived. Navier started from the mechanical description of a system of material points interacting through forces connecting the points by pair and depending on the distance between these points. In this memoir he proposed an approach followed by many 19th century scientists, and was therefore a forerunner of modern homogenization techniques. Some years later, Cauchy read a memoir at the *Académie des Sciences* in which all the basic concepts of continuum mechanics, the definition of stress and the constitutive relations, were derived on the basis of a molecular central-force approach [39]. Here below the basic assumptions of the Cauchy model are described and reinterpreted.

² For a general overview concerning the history of the theory of elasticity, and especially of the outcome of the molecular theory of elasticity with particular reference to the Italian framework see the book by Capecchi *et al.* [52].

In Cauchy's model a body is composed of identical molecules, possibly without extension. Let us consider a reference molecule b , located in the initial configuration at \mathbf{b} , and a surrounding molecule a , located at \mathbf{a} along the direction $\mathbf{n} = (\mathbf{a} - \mathbf{b}) / \|\mathbf{a} - \mathbf{b}\|$ at a distance $r = \|\mathbf{a} - \mathbf{b}\|$. Cauchy's basic assumptions are the following.

1 - Molecules a , b move from their initial position to their final one \mathbf{a}' , \mathbf{b}' by undertaking a displacement which is considered a regular vector field $\mathbf{u}(\mathbf{x})$ on the whole Euclidean space:

$$\begin{aligned}\mathbf{a}' &= \mathbf{a} + \mathbf{u}_a \\ \mathbf{a}' - \mathbf{b}' &= \mathbf{a} - \mathbf{b} + \mathbf{u}_a - \mathbf{u}_b = \mathbf{a} - \mathbf{b} + \mathbf{u}_{ab}\end{aligned}\quad (1)$$

where $\mathbf{u}_a = \mathbf{u}(\mathbf{a})$, $\mathbf{u}_b = \mathbf{u}(\mathbf{b})$ and $\mathbf{u}_{ab} = \mathbf{u}_a - \mathbf{u}_b$. The regular vector field $\mathbf{u}(\mathbf{x})$, though defined everywhere, assumes physical meaning only for $\mathbf{x} = \mathbf{a}$ and $\mathbf{x} = \mathbf{b}$; that is only where molecules are present.³

2 - The pair of molecules a , b interact through a force \mathbf{f}_{ab} which is a vector function of their current distance, $r' = \|\mathbf{a}' - \mathbf{b}'\|$, through a given function $f(r')$, equal for all the molecules, proportional to the masses m_a and m_b of a and b :

$$\mathbf{f}_{ab} = m_a m_b f(r') \mathbf{n}', \quad (2)$$

where $\mathbf{n}' = (\mathbf{a}' - \mathbf{b}') / \|\mathbf{a}' - \mathbf{b}'\|$.

3 - Function $f(r')$ is considered as continuous to any order for all values of r' . However it assumes physical meaning only for discrete values of the distance r' between molecules a and b .

4 - Function $f(r')$ is negligible at considerable distances r' . This means that only very small values of r' must be considered, and the expansion of quantities depending on r' can be stopped at the first order. In particular, the expression of the displacement variation \mathbf{u}_{ab} is approximated by

$$\mathbf{u}_{ab} = \nabla \mathbf{u}(\mathbf{a} - \mathbf{b}), \quad (3)$$

where

$$\nabla \mathbf{u} = \frac{\partial \mathbf{u}}{\partial \mathbf{x}}. \quad (4)$$

The region outside which the intermolecular forces are negligible is called *sphère d'activité sensible* [56].⁴

³ The introduction of such a regular field can be ascribed to the so-called Cauchy-Born hypothesis in Physics. The validity of such an hypothesis has been discussed in various papers (e.g. [54], [55]).

⁴ Poisson called this region *sphère d'action moléculaire* [40], [41].

5 - The displacement field \mathbf{u} and its variation \mathbf{u}_{ab} are very small. This has two important consequences:

a - The strain ε , given the variation in distance between a and b , can be assumed to be linear in displacements:

$$\varepsilon = \frac{1}{\|\mathbf{a}-\mathbf{b}\|} \mathbf{u}_{ab} \cdot \mathbf{n} \cong \frac{1}{\|\mathbf{a}-\mathbf{b}\|^2} \nabla \mathbf{u} (\mathbf{a}-\mathbf{b}) \cdot (\mathbf{a}-\mathbf{b}) = \mathbf{E} \cdot \mathbf{n} \otimes \mathbf{n} \quad (5)$$

where $\mathbf{E} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$.

b - Function $f(r')$ can be linearized with respect to r' . Cauchy, however, prefers to linearize $f(r')/r'$ and obtains:⁵

$$\frac{f(r')}{r'} = A + B\varepsilon, \quad (6)$$

where A and B are coefficients depending on the value of f and its derivative evaluated at the reference point \mathbf{b} .

2.2. Measure of stress

To define the stress measure Cauchy considers an infinitesimal surface of area dA_m , with outward unit normal \mathbf{m} , and a cylinder, with base dA_m and height l greater than the radius of molecular activity, built in the negative half-space defined by \mathbf{m} (Figure 1). The stress vector \mathbf{t}_m acting over the base of the cylinder is given by the forces exerted on all the molecules b of the cylinder by all the molecules a contained in the positive half-space, divided by dA_m . That is, from Equation (2), by the summation over the molecules a, b

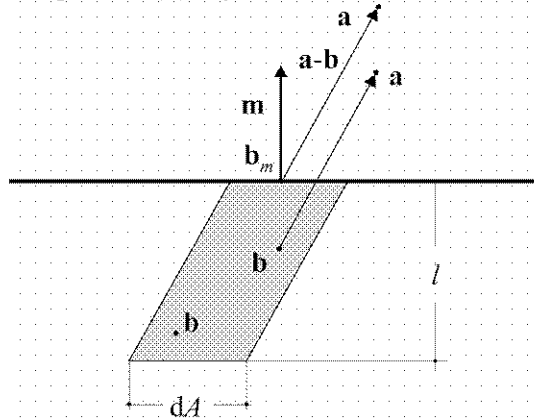


Figure 1. The cylinder of molecular interactions according to Cauchy

$$\mathbf{t}_m = \frac{1}{dA_m} \sum_{ab} m_a m_b f(r') \mathbf{n}' = \frac{1}{dA_m} \sum_{ab} m_a m_b \frac{f(r')}{r'} (\mathbf{a}' - \mathbf{b}') . \quad (7)$$

The summation can be easily performed if the further assumption is made.

⁵ Cauchy ([39], p. 230).

6 - Molecules b are distributed uniformly and it can be assumed that their relative distance is much smaller than the diameter of the section of the cylinder, which is supposed to be greater than the radius of molecular activity.

Under this assumption, the summation of the force of all the molecules with a given value of $\|\mathbf{a}' - \mathbf{b}'\|$ is simply obtained by multiplying Equation (7) for the number ν of molecules contained in the cylinder of height $l = (\mathbf{a}' - \mathbf{b}') \cdot \mathbf{m}$ and area dA_m

$$\nu = \gamma \frac{l dA_m}{m_b}, \quad (8)$$

with γ representing the mass density. Then, with the use of Equations (7) and (8), the stress vector on the surface of normal \mathbf{m} is given by:

$$\mathbf{t}_m = \gamma \sum_a m_a \frac{f(r')}{r'} ((\mathbf{a}' - \mathbf{b}'_m) \cdot \mathbf{m})(\mathbf{a}' - \mathbf{b}'_m), \quad (9)$$

where the summation is now extended to all the molecules a lying in the positive half-space defined by \mathbf{m} acting on the molecule b_m (Figure 1).

Equation (9) can be written as:

$$\mathbf{t}_m = \frac{\gamma}{2} \sum_a m_a \frac{f(r')}{r'} (\mathbf{a}' - \mathbf{b}'_m) \otimes (\mathbf{a}' - \mathbf{b}'_m) \mathbf{m} = \mathbf{Tm}, \quad (10)$$

where for the sake of symmetry the summation has been extended to all the molecules surrounding b_m ,⁶ which entails the introduction of the factor 1/2.

The symmetric tensor \mathbf{T} :

$$\mathbf{T} = \frac{\gamma}{2} \sum_a m_a \frac{f(r')}{r'} (\mathbf{a}' - \mathbf{b}') \otimes (\mathbf{a}' - \mathbf{b}'), \quad (11)$$

is the Cauchy stress tensor.

2.3. Constitutive relations

The constitutive relations can be obtained by introducing the displacement and strain in Equation (11). This can be done on the basis of relation (6) for $f(r')$, and expressions (1) for the final configuration \mathbf{a}' and \mathbf{b}' of the molecules:

$$\mathbf{T} = \frac{\gamma}{2} \sum_a m_a (A + \varepsilon B) (\mathbf{a} - \mathbf{b} + \mathbf{u}_{ab}) \otimes (\mathbf{a} - \mathbf{b} + \mathbf{u}_{ab}). \quad (12)$$

By expanding the tensor product, neglecting higher order terms, and taking into account Equation (5) one obtains:

⁶ For the sake of simplicity from now on the index 'm' on \mathbf{b} will be omitted.

$$\begin{aligned}\mathbf{T} &= \frac{\gamma}{2} \sum_a m_a (A + \varepsilon B) [(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) + (\mathbf{a} - \mathbf{b}) \otimes \mathbf{u}_{ab} + \mathbf{u}_{ab} \otimes (\mathbf{a} - \mathbf{b})] \\ &= \frac{\gamma}{2} \sum_a m_a [(A + \varepsilon B)(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) + A(\mathbf{a} - \mathbf{b}) \otimes \mathbf{u}_{ab} + A\mathbf{u}_{ab} \otimes (\mathbf{a} - \mathbf{b})] ,\end{aligned}\quad (13)$$

Which, by considering relation (3), yields:

$$\mathbf{T} = \frac{\gamma}{2} \sum_a m_a [(A + \varepsilon B)(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) + A(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b})\mathbf{E} + A\mathbf{E}(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b})] . \quad (14)$$

By assuming that in the initial configuration, when $\varepsilon = 0$ and $\mathbf{E} = \mathbf{0}$, the stress is zero the following relation holds

$$\sum_a m_a A [(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b})] = \mathbf{0} , \quad (15)$$

which, by considering \mathbf{E} independent over the summation, furnishes

$$\mathbf{T} = \frac{\gamma}{2} \sum_a m_a \varepsilon B (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) , \quad (16)$$

and as $\mathbf{a} - \mathbf{b} = r \mathbf{n}$

$$\mathbf{T} = \frac{\gamma}{2} \sum_a m_a r^2 B \mathbf{E} \cdot (\mathbf{n} \otimes \mathbf{n}) \mathbf{n} \otimes \mathbf{n} = \frac{\gamma}{2} \sum_a m_a r^2 B \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \mathbf{E} = \mathbf{A} \mathbf{E} . \quad (17)$$

Considering an orthonormal basis of unit vectors $\{\mathbf{e}_i\}$ ($i=1,3$), the fourth order elastic tensor \mathbf{A} has components:

$$(\mathbf{A})_{ijkl} = \frac{\gamma}{2} \sum_a m_a r^2 (\mathbf{n})_i (\mathbf{n})_j (\mathbf{n})_h (\mathbf{n})_k . \quad (18)$$

with $i, j, h, k=1, 3$.

This equation shows that each coefficient of the elastic tensor \mathbf{A} is function of r and \mathbf{n} (that is of the director cosines $(\mathbf{n})_i$ ($i=1,2,3$)). Since the dependence on r is the same for all the coefficients, each coefficient can be considered as a function of $(\mathbf{n})_i$ ($i=1,3$) only. In the general anisotropic case the number of independent coefficients is equal to the number N of combinations with repetition of the 3 objects $(\mathbf{n})_i$ ($i=1,2,3$), of class 4:

$$N = \binom{4+3-1}{4} = \frac{6!}{4!2!} = 15 .$$

Cauchy then introduces further assumptions based on material symmetry.

a – The body has three orthogonal planes of symmetry (*orthotropy*).

In such a case the coefficients with odd exponents for the director cosines vanish, because the summation (18) vanishes for these coefficients. This reduces to *six* the number of independent coefficients.

b - The body has three orthogonal planes of symmetry and the arrangement of molecules is the same in the three directions (*identical orthotropy*). This means that the

coefficients depending on $(\mathbf{n})_i$ are the same as those depending on $(\mathbf{n})_j$, for any i and j . This reduces to *three* the number of coefficients.

c - The body has the same arrangement of molecules in all directions (*isotropy*).

By means of lengthy mathematical passages Cauchy shows that in this case only *one* independent coefficient remains. In all the symmetry considerations Cauchy assumes that matter is continuous because there is no arrangement of molecules that can satisfy the symmetry properties, isotropy in particular.

3. Voigt's contribution to the molecular theory of elasticity

3.1. Historical notes

Many scientists of the 19th century participated in the debate about the molecular theory of elasticity developed by Navier, Cauchy and Poisson. This theory was supported for a long time by important scientists of the period, including Saint-Venant,⁷ mostly because of its mechanical background in which forces were perceived as mechanical interactions between material particles. Soon after its publication, however, this theory led to experimental discrepancies regarding the number of elastic coefficients.

As described in Section 2, Cauchy, as well as Navier and Poisson, obtained the constitutive relationships of linear elastic anisotropic materials depending on *fifteen* constants which were reducible to only *one* constant in the case of isotropy.⁸ Around mid-century some experimental researches showed the inaccuracy of the latter prediction by measuring Poisson's coefficients for metallic materials [57].

Some years after, George Green [49] presented a model of material, which was not corpuscular but continuous, in which he followed a phenomenological approach: he bypassed the explanation of the 'causes' of elasticity and the description of the actual (unknown) nature of matter by referring to a unique general principle which allowed to exploit the whole potentiality of differential calculus. Green's theory of potential based on the sole assumption that the internal work of any force system is an exact differential, gave results confirmed by experiments - that is *twenty-one* elasticities for anisotropic materials which were reducible to *two* in the case of isotropy - and it is well known that this was definitively adopted in elasticity [58].

Due essentially to the previously mentioned experimental discrepancies, the molecular theory of elasticity was eventually abandoned. The possibility to clarify the basic defects of this theory was initially found outside the canonical studies on mechanics. In 1866 Auguste Bravais [59] published a work on crystallography which prompted Woldemar Voigt to improve the molecular model in order to bypass the difficulties related to the identification of the material constants [57]. Voigt also published various works on crystallography and elasticity [45]-[47] which reconciled the results of both the mechanistic/corpuscular and the energetic/continuous theories of matter. Although his work was noticed by his contemporaries, as for instance demonstrated by the attention focused on his approach in didactic handbooks of his day,⁹ this important contribution was mostly ignored by the scientific literature for about a century.

⁷ Navier ([48], p. 541 and ff.).

⁸ Even if Cauchy, using another continuum model, also obtained equations of motion in which *two* constants appeared ([38], p. 184).

⁹ See for example the handbook by the Italian elasticist Roberto Marcolongo ([60], pp. 176-194), in which Voigt's theory of elasticity was widely illustrated, together with Poincaré's approach [61].

Voigt considered the classical molecular theory by Navier, Cauchy and Poisson (*théorie des actions à distance*) old-fashioned and judged it to be inadmissible, not only because of the results, which differed from those of experiments on the mechanical characteristics of materials, but also because the hypothesis of central actions depending on mutual distance was incompatible with the growth mechanism of crystals.

[...] le mécanisme de l'accroissement des cristaux aurait dû d'ailleurs convaincre de l'inadmissibilité de cette conception, car la formation régulier d'un cristal dans une dissolution ou dans une masse fondue n'est compréhensible que si un *moment directeur* agit sur la particule qui va s'associer au cristal en lui donnant une orientation parallèle à celles qui font déjà partie de l'édifice ([46], p. 289).

He recognized that Green's theory of potential (*théorie des actions immédiates*) gave results which were in agreement with experiments but he considered this theory to be satisfactory only if the purpose was the deduction of the elementary laws of elasticity, without knowing the causes of such a phenomenon. Instead, Voigt thought that causes must have mechanical origin; he tried to derive a general theory of matter and was interested in finding the reasons for which the molecular hypothesis led to incorrect results. He found the reason in the hypothesis of mutual forces directed along the line connecting the centres of the particles.

Mais, d'après le principe de la conservation de l'énergie, des action mutuelles dirigées suivant la ligne des centres et ne dépendant que de la distance sont incompatibles avec de semblables moments. Car l'existence des moments exige un potentiel del l'action mutuelle dépendant de l'orientation, et celui-ci conduit à des forces qui varient avec l'orientation de la molécule et, en général, ne coïncident pas avec la ligne des centres ([46], p. 289).

He clearly demonstrated that the molecular theory failed simply because it assumed a central-force scheme depending only on mutual distance and not on the orientation of particles too.¹⁰

Voigt's molecular model is based on oriented material particles with extension, that is molecules or, according to current terminology, structured particles with uniform distribution and orientation. These molecules interact in pair through forces and couples.¹¹ Let a and b be two interacting elementary masses perceived as rigid particles (molecules) centred at \mathbf{a} and \mathbf{b} respectively. The pair of vectors \mathbf{f}^a and \mathbf{f}^b and of skew-symmetric tensors \mathbf{C}^a and \mathbf{C}^b represent respectively the force and the couple that a exerts on b and vice versa. The forces act through two points \mathbf{p}^a and \mathbf{p}^b belonging to a and b respectively. The vectors \mathbf{u}_p^a and \mathbf{u}_p^b represent the infinitesimal displacement of the two points respectively, while the skew-symmetric tensors \mathbf{W}^a and \mathbf{W}^b respectively represent the infinitesimal

¹⁰ It should be noted that both Born and Poincaré had already verified that Cauchy's relations (Eq. 17) were not valid if the intermolecular forces were not central [61], [62].

¹¹ The concept of force systems reducible to a force and a couple in mechanics was clarified by L. Poinsoit [63] who, by studying the equilibrium of rigid bodies, investigated how a system of forces could be resolved into a single force and a couple. Successively, Lord Kelvin [64] defined a continuum body as a material made of points interacting through forces and moments. The treatise of the Cosserat brothers on the deformable bodies with translational and rotational degrees of freedom appeared in 1909 [65].

rotations of the two molecules a and b . In order to study the equilibrium Voigt introduces the interacting potential, defined as a function which takes into account the work of both forces and couples¹²

$$-d\Phi_{ab} = (\mathbf{f}^a \cdot d\mathbf{r}_p^a + \mathbf{f}^b \cdot d\mathbf{r}_p^b) + \frac{1}{2}(\mathbf{C}^a \cdot d\mathbf{W}^a + \mathbf{C}^b \cdot d\mathbf{W}^b), \quad (19)$$

By requiring $d\Phi_{ab} = 0$ for any rigid infinitesimal displacement, the balance equations between the pair of molecules are obtained:

$$\begin{aligned} \mathbf{f}^a + \mathbf{f}^b &= \mathbf{0} \\ \mathbf{C}^a + \mathbf{C}^b + [(\mathbf{p}^a - \mathbf{p}^b) \otimes \mathbf{f}^a - \mathbf{f}^a \otimes (\mathbf{p}^a - \mathbf{p}^b)] &= \mathbf{0}. \end{aligned} \quad (20)$$

At this point Voigt introduces a strong constitutive prescription: molecules have the same orientation within the *sphère d'action moléculaire*¹³

$$\mathbf{W}^a = \mathbf{W}^b = \mathbf{W} \quad \forall a \text{ and } b. \quad (21)$$

As a consequence, taking into account the balance equations (20) and putting $\mathbf{f}_{ab} = \mathbf{f}^a = -\mathbf{f}^b$, the potential formula becomes¹⁴

$$-d\Phi_{ab} = \mathbf{f}_{ab} \cdot d[\mathbf{u}_p^a - \mathbf{u}_p^b - \mathbf{W}(\mathbf{p}^a - \mathbf{p}^b)] , \quad (22)$$

Considering the displacement vectors, \mathbf{u}^a and \mathbf{u}^b , of the centres \mathbf{a} and \mathbf{b} of a and b one has

$$\mathbf{u}_p^a = \mathbf{u}^a + \mathbf{W}(\mathbf{p}^a - \mathbf{a}) \quad \text{and} \quad \mathbf{u}_p^b = \mathbf{u}^b + \mathbf{W}(\mathbf{p}^b - \mathbf{b}). \quad (23)$$

Then defining

$$\mathbf{u}_{ab} = \mathbf{u}_p^a - \mathbf{u}_p^b - \mathbf{W}(\mathbf{p}^a - \mathbf{p}^b) = \mathbf{u}^a - \mathbf{u}^b - \mathbf{W}(\mathbf{a} - \mathbf{b}). \quad (24)$$

one has

$$-d\Phi_{ab} = \mathbf{f}_{ab} \cdot d\mathbf{u}_{ab}, \quad (25)$$

and the interaction force can be derived as

$$\mathbf{f}_{ab} = -\frac{\partial \Phi_{ab}}{\partial \mathbf{u}_{ab}}. \quad (26)$$

¹² In the present paper Voigt's notations and treatment have been adapted to facilitate the current reader. In particular, Voigt introduces the potential function as the work of interacting forces and couples in the variation of displacements and rotations, and then as the first variation of the energy ([47], p. 598). Here we have directly introduced infinitesimal kinematical quantities.

¹³ Voigt ([46], p. 293; [47], p. 599). We use the representation of infinitesimal rotations and moments through skew-symmetric tensors instead of axial vectors. It is worth noting that there exists a one-to-one relation between the two notations: $\Theta \mathbf{v} = \Theta \times \mathbf{v}$, $\forall \mathbf{v} \in \mathcal{V}$, where Θ is a skew-symmetric tensor, Θ is its axial vector and \mathcal{V} is a vector space.

¹⁴ Voigt ([47], p. 600).

Moreover, due to symmetry considerations,¹⁵ he assumes

$$\mathbf{C}^a = \mathbf{C}^b = \mathbf{C}_{ab} . \quad (27)$$

where, because of the balance equation (20)₂,

$$\mathbf{C}_{ab} = -\frac{1}{2}[(\mathbf{p}^a - \mathbf{p}^b) \otimes \mathbf{f}^a - \mathbf{f}^a \otimes (\mathbf{p}^a - \mathbf{p}^b)] . \quad (28)$$

3.2. Measure of stress

In order to evaluate the stress due to internal forces Voigt follows the Cauchy and Poisson approach, resorting to the definition of a representative volume element (RVE)

[...] un élément de volume, grand par le rapport à la sphère d'action moléculaire et contenant, par conséquent, un nombre extrêmement grand de molécules. Les molécules environnant l'élément de volume n'agissent alors que sur les molécules intérieures immédiatement voisines de la surface de séparation et se combinent pour donner les composants de la pression. ([46], p. 290)

Voigt then considers a cylinder elevated on a surface element of area A_m defined by the outward unit vector \mathbf{m} . The plane containing this surface divides the body into two portions. Let a be a molecule in the half body which does not contain the cylinder and b the molecule within the cylinder in the opposite half body, Voigt then defines the stress vector \mathbf{t}_m (*la pression des forces*) over the surface element as the summation extended to each molecule a and each molecule b of the interactions \mathbf{f}_{ab} per unit surface

$$\mathbf{t}_m = \frac{1}{A_m} \sum_{ab} \mathbf{f}_{ab} . \quad (29)$$

Moreover, as molecules also interact through couples, the couple-stress tensor \mathbf{C}_m (*la pression des moments*) is analogously defined as the summation extended to each molecule a and each molecule of the interactions \mathbf{C}_{ab} per unit surface

$$\mathbf{C}_m = \frac{1}{A_m} \sum_{ab} \mathbf{C}_{ab} . \quad (30)$$

According to Voigt,¹⁶ the distance between molecules within the sphere of actions is small in comparison with the diameter of A_m , then as this diameter is infinitesimal, $\|\mathbf{p}^a - \mathbf{p}^b\|$ is infinitesimal of higher order and, considering Equation (28), $\mathbf{C}_{ab} = \mathbf{0}$.

The continuous model derived by Voigt is a continuum with constrained rotations in which the couple stresses, perceived as moments of forces of negligible arm are null. This continuum can be considered as a particular case of the continuum studied by the Cosserat brothers some years later [65].

¹⁵ These symmetry considerations that Voigt mentions ([46], p. 293; [47], p. 599) implicitly involve linear constitutive relations between interaction couples and rotations.

¹⁶ Voigt ([46], p. 294).

By providing a mechanical criterion to build up a potential function from which to obtain derived intermolecular forces, Voigt reconciles the mechanistic and the energetic approaches. Moreover, the advantage of introducing couples, albeit as moments of forces vanishing in the localisation process, lies in the definition of a lattice model with forces which are not directed along the line $\mathbf{a}-\mathbf{b}$ connecting the centres of molecules. This circumstance allows to derive an elastic model with the number of elastic constants required by experiments.

3.3. Constitutive relations

To derive the stress-strain relations for the continuum intermolecular forces, which are null in the reference state, Voigt assumes linear functions of the relative displacement between molecules

$$\mathbf{f}_{ab} = \mathbf{f}(\mathbf{u}_{ab}) \cong \mathbf{f}(\mathbf{u}_{ab})|_0 + \nabla \mathbf{f}(\mathbf{u}_{ab})|_0 \cdot \mathbf{u}_{ab} + \dots = \mathbf{K}_{ab} \mathbf{u}_{ab} \quad , \quad (31)$$

where \mathbf{K}_{ab} is a symmetric second order tensor. Moreover, by assuming homogeneous deformations,¹⁷

$$\mathbf{u}_a - \mathbf{u}_b = \nabla \mathbf{u} (\mathbf{a} - \mathbf{b}) \quad , \quad (32)$$

which are null in the reference state, and putting $\mathbf{W} = \frac{1}{2}(\nabla \mathbf{u} - \nabla \mathbf{u}^T)$ and $\mathbf{E} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ he obtains

$$\mathbf{u}_{ab} = (\nabla \mathbf{u} - \mathbf{W}) (\mathbf{a} - \mathbf{b}) = \mathbf{E} (\mathbf{a} - \mathbf{b}) \quad . \quad (33)$$

Equation (31) then becomes

$$\mathbf{f}_{ab} = \mathbf{K}_{ab} \mathbf{E} (\mathbf{a} - \mathbf{b}) \quad . \quad (34)$$

In such a way the potential function is quadratic in $\mathbf{a} - \mathbf{b}$

$$\begin{aligned} -d\Phi_{ab} &= \mathbf{f}_{ab} \cdot d\mathbf{E} (\mathbf{a} - \mathbf{b}) = \mathbf{K}_{ab} \mathbf{E} (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) \cdot d\mathbf{E} \\ &= \frac{1}{2} \{ [\mathbf{K}_{ab} \mathbf{E} (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b})] + [(\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) \mathbf{E} \mathbf{K}_{ab}] \cdot d\mathbf{E} \} \end{aligned} \quad (35)$$

The mean potential energy over the RVE of volume V is¹⁸

¹⁷ This is the linearized representation of the Cauchy-Born rule (see footnote 2). This assumption leads to the so called Voigt's hypothesis used in classical simplified homogenization methods (see for example [17]).

¹⁸ Unlike current formulations, in which the size of the RVE must be properly defined, in Voigt's model no assumptions are made about the size of the intermolecular sphere of actions because his aim was the definition of the field equations of a continuum model, rather than the computation of the effective material constants. The volume V of the module is then introduced in order to be able to evaluate the average value of the potential and the derived stress.

$$d\Phi = \frac{1}{V} \sum_{ab} d\Phi_{ab}. \quad (36)$$

Then the stress-strain relationships for the continuum are derived as

$$\mathbf{T} = -\frac{\partial\Phi}{\partial\mathbf{E}} = \frac{1}{2V} \sum_{ab} \{[\mathbf{K}_{ab}\mathbf{E}(\mathbf{a}-\mathbf{b}) \otimes (\mathbf{a}-\mathbf{b})] - [(\mathbf{a}-\mathbf{b}) \otimes (\mathbf{a}-\mathbf{b})\mathbf{E}\mathbf{K}_{ab}]\} = \hat{\mathbf{A}} \mathbf{E} \quad (37)$$

Based on Equations (26) and (33), Equation (37) corresponds to the so-called *virial* of the forces for the stress of a particle system under a generic deformation state.

Considering an orthonormal basis of unit vectors $\{\mathbf{e}_i\}$ ($i=1,3$), the fourth order elastic tensor $\hat{\mathbf{A}}$ has components

$$(\hat{\mathbf{A}})_{ijkl} = \frac{1}{2V} \sum_{ab} \{(\mathbf{K}_{ab})_{ih}(\mathbf{a}-\mathbf{b})_j(\mathbf{a}-\mathbf{b})_k + (\mathbf{K}_{ab})_{kj}(\mathbf{a}-\mathbf{b})_i(\mathbf{a}-\mathbf{b})_h\} \quad (38)$$

with $i, j, h, k=1,3$.

Considering the major symmetry of $\hat{\mathbf{A}}$ due to hyperelasticity and the symmetries of \mathbf{E} and \mathbf{T} , the number of independent parameters turns out to be *twenty-one*. Voigt also examines other cases of material symmetry, and in the case of *isotropy* the independent constants reduce to *two*.

In Voigt's model, the removal of the central forces scheme led to constitutive equations depending, according to Green's theory and experimental results, on the expected number of constants. As the scientists of the time had already recognized ([60], p.105), the molecular model by Navier and Cauchy failed only because of the central force scheme.

4. Molecular-multiscale approach: the present

4.1. Background

In the 19th century most studies on molecular theories of elasticity were developed, in a linearised framework, adopting central-force schemes that led to experimental contradictions concerning the number of elastic constants ("rari-constant" theories). Voigt (Section 3.) presented a way to solve the problem considering an elastic potential of both forces and moments. It can also be noticed that, probably starting from an original idea by Poincaré [61], in the current physical literature many examples can be found in which the inadequacy of the central force scheme is discussed and avoided by resorting to multi-body interaction potentials [62], [30], [36]. The Voigt approach can be reduced to the Poincaré's and other multi-body approaches because in both cases angular potentials appear, respectively depending on the angles between the lines connecting particles and on the particle orientations, and the number of elastic constants corresponds to the number required by experiments ("multi-constant" theories).¹⁹

¹⁹ In many other circumstances physicists resort to non-harmonic pair central-force potentials that lead to the right number of constants. This matter, however, exceeds the limits of this work and is being treated in a forthcoming manuscript.

Putting aside the strong debate about the material constants, the idea that many physical phenomena could have been described by resorting to a mechanical corpuscular (Newtonian) model was central in that century.

Molecular theories in mechanics, as well as in thermodynamics and in the theory of light propagation, were essentially based on the concept of the discrete nature of matter. Despite the experimental support derived from the first discoveries of the existence of atoms,²⁰ the introduction of the concept of discreteness in Physics, and of the corresponding ‘simple mathematics’ (matrix algebra), was difficult and was opposed for a long time. The main difficulties consisted in removing the Laplacian principle of ‘continuum indispensability’ and the related differential mathematics [66]. On the other hand, in agreement with the predominant tradition of Lagrange’s analytical mechanics, even the goal of the elasticians of the period was the construction of continuous models using the apparatus of differential mathematics, although they resorted to the discrete description of matter to give mechanical meaning to the fields of interest (stress, strain, etc.). Therefore, in a scientific framework dominated by classical analytical mechanics, it does not seem strange that in the presence of experimental discrepancies, the molecular approach was no longer adopted and that, thenceforward, continuum constitutive theories were based on macroscopic criteria following Green’s hypothesis or other phenomenological approaches. The significant work of Voigt was then abandoned, although his enriched molecular model led to results in agreement with Green’s approach and with the experimental data.

By contrast, at present the determination of structure-property relationships for complex materials often requires the bridging of many length scales and multiscale approaches, based on discrete modelling at microscopic levels, encounter renewed interest in the mechanics of materials with microstructure. In fact, they also provide many suggestions for deriving physically motivated constitutive relations (e.g. [51], [36]).

The key ideas arising from Voigt’s work can be summarized as follows: *i)* no ‘a priori’ general principles governing macroscopic phenomena must be assumed; *ii)* at the microscopic level the material can be described as an assemblage of interacting elements which desist from being material point-particles, as in Cauchy’s model, to become structured molecules; in a wider meaning these molecules can represent internal material phases with size ranging from fibres in composites to dislocations in metals etc.; *iii)* inter-molecular actions can be forces directed other than along the line connecting centres *iv)* inter-molecular actions can be of different natures, both linear and non-linear, depending not only on the mutual particle distances; *v)* the large set of degrees of freedom of molecular models can be connected to one or more field variables through affine or not affine mappings, respectively accounting for shorter or longer range interactions, and these mappings allow one to build in various inter-atomic potentials generating different hyperelastic solid models.

The means of accounting for these suggestions has progressed along many lines within the statistical-mechanics framework, ranging from classical hyperelastic models derived from atomistic pair or multi-body potentials [62], [51] and generalized continua, not always hyperelastic, derived from lattices [67]-[70], to complex atomistic-continuum models [71]-[73] up to statistical higher-order hyperelastic lattice models accounting for non-linear

²⁰ J. Dalton, On the absorption of gases by water and other liquids, *Memoirs of the Literary and Philosophical Society of Manchester*, Second Series, **1**, 1805, 271-87 (Read Oct. 21, 1803); W. Prout, On the relation between the specific gravities of bodies in their gaseous state and the weights of their atoms, *Annals of Philosophy*, **6**, 1815, 321-330; R. Brown, A brief account of microscopical observations made in the months of June, July and August, 1827, on the particles contained in the pollen of plants; and on the general existence of active molecules in organic and inorganic bodies, *Philosophical Magazine*, **4**, 1828, 161-173; J. J. Thomson, Cathode rays, *Philosophical Magazine*, **44**, 1897.

and non-local effects [74]-[76], [36].²¹ Finally, even homogenization theories based on energetic methods [77] and, in particular, mathematical multiscale models [78]-[80] developed in the non-linear elasticity frame, also using Gamma-convergence techniques, could be ascribed to the domain of molecular/atomistic theories.

Many other examples which refer to the described conceptual framework can be found in literature. Various difficulties often arise in the case of materials with microstructure several orders of magnitude smaller than macroscopic scale and with generally random microstructure. Besides the determination of the size of the so-called statistical volume element [81]-[82], most difficulties are related to the definition of the empirical parameters for the molecular models. However, recent developments of experimental techniques, high resolution electron microscopes for instance, as well as studies at microscopic levels to define internal phase interactions [83] allow one to define with growing precision the material response at microscopic level taking into account their internal structure and symmetries (dislocations, grain boundaries, nanoindentations, etc.).

Otherwise, referring to materials with periodic internal structure, it is possible to find a mesoscopic level at which the material response can be more easily detected than at a nano/micro level. A paradigmatic example of the application of Voigt's molecular approach to derive the linear elastic constitutive relation of a micropolar continuum of the Cosserat type is described in the section below. The proposed procedure has also been extended to the non-linear framework and the derived multifield continuum has been shown to suitably represent the behaviour of block-masonry materials [23], [24].

4.2. A model for masonry-like materials based on Voigt's approach

The reference material is a material made of brick/blocks embedded in a mortar matrix. At the molecular level such a material is described by a lattice system made of interacting rigid particles. The continuous model of the generalized homogeneous material (macromodel) is built up based on the linearized kinematics of the lattice model (micromodel).

Let a and b be two rigid particles of the system with centres \mathbf{a} and \mathbf{b} . The particles interact through two points \mathbf{p}^a and \mathbf{p}^b , placed respectively at a and b , occupying the same position \mathbf{p} in the reference shape. The vectors \mathbf{u}^a and \mathbf{u}^b represent the infinitesimal displacement of the centres of particles and the skew-symmetric tensors \mathbf{W}^a and \mathbf{W}^b represent the infinitesimal rotations of the particles. Denoting by \mathbf{u}_p^a and \mathbf{u}_p^b the displacement vectors of \mathbf{p}^a and \mathbf{p}^b , respectively, the linearized strain measures of the lattice system are defined as the relative displacement between the two points and the relative rotation between a and b

$$\mathbf{u}_{ab} = \mathbf{u}_p^a - \mathbf{u}_p^b = \mathbf{u}^a - \mathbf{u}^b + \mathbf{W}^a(\mathbf{p}^a - \mathbf{a}) - \mathbf{W}^b(\mathbf{p}^b - \mathbf{b})$$

²¹ In this framework the classical papers by J. H. Irving and J. G. Kirkwood (The statistical mechanical theory of transport processes IV: The Equations of Hydrodynamics, *Journal of Chemical Physics*, **18**, 1950, 817-829) and by W. Noll (Die Herleitung der Grundgleichungen der Thermomechanik and der Continua aus der Statistischen Mechanik, *Journal of Rational Mechanics and Analysis*, **4**, 1955, 627-646) played a central role. Nevertheless, it must be noticed that, even if the reference to classical statistical-mechanics is due, attention in this paper is focused on models concerning only pure mechanical processes, where the thermal properties of continua are not relevant.

$$\mathbf{W}_{ab} = \mathbf{W}^a - \mathbf{W}^b. \quad (39)$$

Denoting with \mathbf{f}^a and \mathbf{f}^b the vectors of forces acting through \mathbf{p}^a and \mathbf{p}^b , and with \mathbf{C}^a and \mathbf{C}^b the skew-symmetric tensors of couples that a exerts on b and vice versa, the balance equations between the pair of particles can be written as

$$\begin{aligned} \mathbf{f}^a + \mathbf{f}^b &= \mathbf{0} \\ \mathbf{C}^a + \mathbf{C}^b &= \mathbf{0}. \end{aligned} \quad (40)$$

Considering brick textures for which a representative volume element can be defined, here referred to as the module, and taking into account equations (40) the mean strain energy of the module of volume V reads

$$\bar{\Phi} = \frac{1}{2V} \sum_{ab} \left\{ \mathbf{f}_{ab} \cdot \mathbf{u}_{ab} + \frac{1}{2} \mathbf{C}_{ab} \cdot \mathbf{W}^{ab} \right\} \quad (41)$$

where $\mathbf{f}_{ab} = \mathbf{f}^a = -\mathbf{f}^b$ and $\mathbf{C}_{ab} = \mathbf{C}^a = -\mathbf{C}^b$.

Let $\mathbf{u}(\mathbf{x})$ be a displacement vector field and $\mathbf{W}(\mathbf{x})$ a rotation skew-symmetric tensor field. Under the hypothesis of homogeneous deformations in the module of centre \mathbf{x}

$$\begin{aligned} \mathbf{u}^a &= \mathbf{u}(\mathbf{x}) + \nabla \mathbf{u}(\mathbf{a} - \mathbf{x}) \\ \mathbf{W}^a &= \mathbf{W}(\mathbf{x}) + \nabla \mathbf{W}(\mathbf{a} - \mathbf{x}), \end{aligned} \quad (42)$$

the strain measures (39) can be expressed in terms of the regular fields $\nabla \mathbf{u}(\mathbf{x}) - \mathbf{W}(\mathbf{x}), \nabla \mathbf{W}(\mathbf{x})$

$$\begin{aligned} \mathbf{u}_{ab}(\nabla \mathbf{u} - \mathbf{W}, \nabla \mathbf{W}) &= (\nabla \mathbf{u} - \mathbf{W})(\mathbf{a} - \mathbf{b}) + \mathbf{W}(\mathbf{a} - \mathbf{x})(\mathbf{p} - \mathbf{a}) - \nabla \mathbf{W}(\mathbf{b} - \mathbf{x})(\mathbf{p} - \mathbf{b}) \\ \mathbf{W}_{ab}(\nabla \mathbf{u} - \mathbf{W}, \nabla \mathbf{W}) &= \nabla \mathbf{W}(\mathbf{a} - \mathbf{b}) \end{aligned} \quad (43)$$

as well as the mean strain energy function over the module

$$\begin{aligned} \bar{\Phi}(\nabla \mathbf{u} - \mathbf{W}, \nabla \mathbf{W}) &= (\nabla \mathbf{u} - \mathbf{W}) \cdot \frac{1}{2V} \sum_{ab} \mathbf{f}_{ab} \otimes (\mathbf{a} - \mathbf{b}) \\ &+ \nabla \mathbf{W} \cdot \frac{1}{2V} \sum_{ab} \left\{ \mathbf{f}_{ab} \otimes [(\mathbf{p} - \mathbf{a}) \otimes (\mathbf{a} - \mathbf{x}) - (\mathbf{p} - \mathbf{b}) \otimes (\mathbf{b} - \mathbf{x})] + \frac{1}{2} \mathbf{C}_{ab} \otimes (\mathbf{a} - \mathbf{b}) \right\} \end{aligned} \quad (44)$$

Assuming the following linear elastic response functions for the contact actions in the module

$$\begin{aligned} \mathbf{f}_{ab} &= \mathbf{K}_{ab} \mathbf{u}_{ab} \\ \mathbf{C}_{ab} &= \mathbf{K}_{ab} \mathbf{W}_{ab}, \end{aligned} \quad (45)$$

where \mathbf{K}_{ab} and \mathbf{K}_{ab} are symmetric constitutive tensors of the second and fourth order respectively, and using Equations (43) again, the mean strain energy function over the module can be written as²²

$$\bar{\Phi}(\nabla\mathbf{u}-\mathbf{W},\nabla\mathbf{W}) = \frac{1}{2}\{(\nabla\mathbf{u}-\mathbf{W})\cdot\mathbf{A}(\nabla\mathbf{u}-\mathbf{W})+2(\nabla\mathbf{u}-\mathbf{W})\cdot\mathbf{B}\nabla\mathbf{W}+\nabla\mathbf{W}\cdot\mathbf{C}\nabla\mathbf{W}\} \quad (46)$$

The tensors \mathbf{A} , \mathbf{B} , and \mathbf{C} , of the fourth, fifth and sixth order respectively have components depending on the elastic constants of the matrix and on the shape, the size, the orientation and the arrangement of the elements of the lattice system.

Let us now suppose we replace the module with a neighbourhood of a continuum centred at \mathbf{x} . Considering a closed ball N_δ of radius δ ($\delta>0$), centre \mathbf{x} and volume $V(N_\delta)$, through the localization theorem, we assume the mean strain energy of the module (44) to coincide with the stored energy function per unit volume of the continuum

$$\lim_{\delta\rightarrow 0} \frac{1}{V(N_\delta)} \int_{N_\delta} \Phi dV = \Phi(\mathbf{x}) := \bar{\Phi}(\nabla\mathbf{u}-\mathbf{W},\nabla\mathbf{W}) \quad (47)$$

Then, in analogy with Voigt's approach, the constitutive relations of the equivalent continuum can be derived as²³

$$\begin{aligned} \mathbf{S} &= \frac{\partial\bar{\Phi}(\nabla\mathbf{u}-\mathbf{W},\nabla\mathbf{W})}{\partial(\nabla\mathbf{u}-\mathbf{W})} = \mathbf{A}(\nabla\mathbf{u}-\mathbf{W}) + \mathbf{B}\nabla\mathbf{W} \\ \mathbf{S} &= \frac{\partial\bar{\Phi}(\nabla\mathbf{u}-\mathbf{W},\nabla\mathbf{W})}{\partial(\nabla\mathbf{W})} = \mathbf{B}^T(\nabla\mathbf{u}-\mathbf{W}) + \mathbf{C}\nabla\mathbf{W} \end{aligned} \quad (48)$$

Equations (48) correspond to the stress-strain relations of a Cosserat continuum in which \mathbf{u} is the standard displacement field and \mathbf{W} is the microrotation field. The tensor fields \mathbf{S} and \mathbf{S} are the second-order stress-tensor and the third-order tensor of the microcouples, respectively.

Considering an orthonormal basis of unit vectors $\{\mathbf{e}_i\}$ ($i=1,3$), the components of the elastic tensors \mathbf{A} , \mathbf{B} , and \mathbf{C} are given by the following relations

²² It can be shown that if the central symmetry for the module holds the tensor \mathbf{B} is null and the strain energy function is a quadratic form [84]. Such a material symmetry characterizes periodic lattices.

²³ \mathbf{B}^T is the transpose of the fifth order tensor \mathbf{B} such that, for each second order tensor \mathbf{T} and each third order tensor \mathbf{T} , it has $\mathbf{B}\mathbf{T}\cdot\mathbf{T} = \mathbf{B}^T\mathbf{T}\cdot\mathbf{T}$.

$$\begin{aligned}
(\mathbf{A})_{ijhk} &= \frac{\partial^2 \bar{\Phi}(\nabla \mathbf{u} - \mathbf{W}, \nabla \mathbf{W})}{\partial (\nabla \mathbf{u} - \mathbf{W})_{ij} \partial (\nabla \mathbf{u} - \mathbf{W})_{hk}} = \frac{1}{V} \sum_{ab} \{ (\mathbf{K}_{ab})_{ih} (\mathbf{a} - \mathbf{b})_k (\mathbf{a} - \mathbf{b})_j \} \\
(\mathbf{B})_{ijhkl} &= \frac{\partial^2 \bar{\Phi}(\nabla \mathbf{u} - \mathbf{W}, \nabla \mathbf{W})}{\partial (\nabla \mathbf{u} - \mathbf{W})_{ij} \partial (\nabla \mathbf{W})_{hkl}} = \frac{1}{V} \sum_{ab} \{ (\mathbf{K}_{ab})_{ih} [(\mathbf{a} - \mathbf{x})_i (\mathbf{p} - \mathbf{a})_k - (\mathbf{b} - \mathbf{x})_i (\mathbf{p} - \mathbf{b})_k] (\mathbf{a} - \mathbf{b})_j \} \\
(\mathbf{C})_{hklmng} &= \frac{\partial^2 \bar{\Phi}(\nabla \mathbf{u} - \mathbf{W}, \nabla \mathbf{W})}{\partial (\nabla \mathbf{W})_{hkl} \partial (\nabla \mathbf{W})_{mng}} = \frac{1}{V} \sum_{ab} \{ (\mathbf{K}_{ab})_{hm} [(\mathbf{a} - \mathbf{x})_q (\mathbf{p} - \mathbf{a})_n - (\mathbf{b} - \mathbf{x})_q (\mathbf{p} - \mathbf{b})_n] \\
&\quad [(\mathbf{p} - \mathbf{a})_k (\mathbf{a} - \mathbf{x})_i - (\mathbf{p} - \mathbf{b})_k (\mathbf{b} - \mathbf{x})_i] + \frac{1}{2} (\mathbf{K}_{ab})_{hkmn} (\mathbf{a} - \mathbf{b})_q (\mathbf{a} - \mathbf{b})_i \}
\end{aligned} \tag{49}$$

where $i, j, h, k, l, m, n, q = 1, 3$. In particular, the tensor \mathbf{A} does not contain any internal length parameter while the tensors \mathbf{B} and \mathbf{C} have components depending also on the size of the elements. This circumstance allows us to take size effects into account properly [23].

If Voigt's internal constraints are then posed, that is, the rotation of the particles in the module is assumed constant and equal to the local rigid rotation

$$\begin{aligned}
\mathbf{W} &= \frac{1}{2} (\nabla \mathbf{u} - \nabla \mathbf{u}^T) \\
\nabla \mathbf{W} &= \mathbf{0} ,
\end{aligned} \tag{50}$$

by putting $\mathbf{E} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$, the strain energy density of the equivalent continuum, Equation (44), becomes

$$\begin{aligned}
\bar{\Phi}(\mathbf{E}) &= \frac{1}{2V} \sum_{ab} [\mathbf{f}_{ab} \otimes (\mathbf{a} - \mathbf{b})] \cdot \mathbf{E} \\
&= \frac{1}{4V} \sum_{ab} [\mathbf{K}_{ab} \mathbf{E} (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) + (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) \mathbf{E} \mathbf{K}_{ab}] \cdot \mathbf{E}
\end{aligned} \tag{51}$$

The constitutive relations can then be derived as in the Voigt model (Equation (37)) for the standard symmetric stress tensor \mathbf{T}

$$\mathbf{T} = \frac{\partial \bar{\Phi}(\mathbf{E})}{\partial \mathbf{E}} = \frac{1}{2V} \sum_{ab} [\mathbf{K}_{ab} \mathbf{E} (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) + (\mathbf{a} - \mathbf{b}) \otimes (\mathbf{a} - \mathbf{b}) \mathbf{E} \mathbf{K}_{ab}] = \hat{\mathbf{A}} \mathbf{E} . \tag{52}$$

The components of the fourth order elastic tensor $\hat{\mathbf{A}}$ are the same as in Equations (38)

$$(\hat{\mathbf{A}})_{ijhk} = \frac{\partial^2 \bar{\Phi}(\mathbf{E})}{\partial \mathbf{E}_{ij} \partial \mathbf{E}_{hk}} = \frac{1}{2V} \sum_{ab} \{ (\mathbf{K}_{ab})_{ih} (\mathbf{a} - \mathbf{b})_j (\mathbf{a} - \mathbf{b})_k + (\mathbf{K}_{ab})_{kj} (\mathbf{a} - \mathbf{b})_i (\mathbf{a} - \mathbf{b})_h \} \tag{53}$$

with $i, j, h, k, h = 1, 3$.

This example shows how the approach of the classical molecular theory of elasticity based on the assumptions of affine mappings for all the degrees of freedom of the lattice system (Equations (43)) and of energy equivalence (Equation (47)) naturally leads to a multifield continuum model [85]-[87] characterized by the presence of more field

descriptors than the classical continuum; in the present case it is a continuum with local rigid microstructure.

The derived continuum is linear elastic but the response functions for the interactions in the module can be defined in order to take also into account non-linear behaviours [23]-[24]. In addition, the kinematics of the lattice micromodel can be enriched by non-affine mappings between lattice and macroscopic field descriptors deriving higher order continua accounting for long range interactions [76] or by other additional degrees of freedom. In the latter case the integral procedure of equivalence presented above led to the identification of multifield continua specifically derived to describe microcracked and fibre-composite materials [26]-[29].

Finally, an advantage of the energy equivalence procedure is that this ensures the preservation of the material symmetry class in the transition from the discrete to the continuum description [84]. From a more general point of view, this approach could allow one to properly account for symmetry-induced instabilities describing important features related to re-arrangements of the material microstructure, such as a symmetry-breaking phase transition [51], [88], a defect-induced damage [89] or other material instabilities [90]. Molecular modelling combined with statistical-mechanics-based approaches, proves to be very suitable for providing the constitutive support that higher-order theories and the theories of multifield continua needed for engineering applications.

5. Final Remarks

In this paper we present an overview of the origin of multiscale approaches in mechanics. The pioneer molecular models of linear elastic bodies by Navier, Cauchy and Poisson rested on the hypothesis that in ordinary materials the basic components of matter, called molecules, interact via central forces depending on the variation in distance between their centres of gravity. The constitutive equations obtained by means of these models saw linear elasticity described by 15 material constants, reducible to only one constant for isotropic bodies. Such a result, contradicted by experiments, was bypassed by Green's phenomenological approach. The idea of explaining the 'causes' of elasticity was then definitively abandoned. Towards the end of the 19th century, the work of Voigt based on a mechanical description solved the paradox: Voigt used a different model for the molecule, actually seeing matter as a structured continuum (to put it in contemporary language), yet not abandoning the power of the useful energetic description.

Cauchy's and Voigt's molecular models are here rewritten and reinterpreted in the light of contemporary micromechanics. We show how the latter approach reconciles the mechanistic/corpuscular with the energetic/continuous conceptions, providing a conceptual guideline for developing constitutive models based on a direct link between continuum and discrete solid mechanics. Such a theoretical background proves to be especially suitable for new complex materials. This allows to describe enriched kinematics and introduce multi-field mechanical models as well as conjugating the advantages of the continuous derivation of multi-field balance and compatibility equations with the discrete derivation of (possibly) complex, non-trivial constitutive relations. It seems that, from this viewpoint, the study of Voigt's original approach by means of a contemporary synthetic language provides a useful tool to formulate new complex and refined models.

Acknowledgements

The authors thank Prof. Martin Ostoja-Starzewski for the suggestions concerning the material presented here and the encouragement in writing this paper. This research has been partially supported by the ‘Ministero dell’Università e della Ricerca Scientifica’ under a grant MIUR 2006.

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