

Poincaré’s energetic approach to linear elasticity

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SUMMARY. Modern theories of complex materials rely on the construction of specific potentials for inner actions; such a procedure may be linked with an approach by Poincaré. In this contribution we examine Poincaré’s approach to the ordinary theory of linear elasticity and find out how it is related to the standard molecular model by Navier, Cauchy and Poisson and to the refined molecular model by Voigt. In the end, we comment on the relationships among these approaches and the contemporary theories of complex material behaviour.

1 INTRODUCTION

In the XIXth century most of the studies on elasticity were developed in a linearised framework adopting a central-force scheme. The matter constituting physical bodies was thought composed of ultimate elements considered as body-points exchanging opposite forces through the line joining them. Such models, developed by Navier, Cauchy and Poisson, led to experimental contradictions as far as the number of elastic constants was concerned (‘rari-constant’ theories [1, 2]).

Other studies, initiated by Green’s research on the mechanical properties of the luminiferous ether, by-passed the question by resorting to a continuous model of matter, giving up an explanation *per causas* of elasticity. Green solely admitted that the internal actions derive from a potential; the results of such a model were confirmed by experiments but gave rise to a long debate among mechanicians as to the ‘real’ number of elastic constants and the ‘correct’ model for elastic phenomena.

Voigt [3, 4] presented a way to solve the problem (‘multi-constant’ theory [2, 5, 6]) on one hand by improving the molecular model: the ultimate components of matter, or ‘molecules’, are not body-points but small rigid bodies; on the other hand by considering an elastic potential of both the forces and the moments exchanged by the ‘molecules’. His results – obtained by adopting a molecular model but abandoning the central-force scheme – were confirmed by experiments.

Poincaré proposed a slightly different approach to the subject [7]. He did not abandon a molecular description of the matter and made use of an elastic potential that does not specify which kind of actions are exchanged by the ultimate components of bodies. Both the views of Voigt and Poincaré were well accepted by the scientific community [8].

The mechanistic/molecular and the energetic/continuum approaches to standard problems in physics, like that of linear elasticity for solids, are present also in modern problems. Indeed, when studying new materials, either the simple molecular or the energetic approach may seem inadequate: the ultimate components of these materials are far from being simply body-points, and postulating a reasonable form for the potential of inner actions may not be an easy task. A constitutive characterization of such materials is necessary to perform a thorough study of their behaviour.

In physics the inadequacy of the central-force scheme is often avoided by resorting to multi-body interaction potentials. Yet, papers in which the validity of the central-force scheme is assumed are also present. In many other circumstances the physicists resort to non-harmonic pair central-force potentials, leading to suitable constitutive characterizations; an overview is found in [9].

In this contribution we will present a modern exposition of Voigt's model [3, 4] first, then Poincaré's approach [7], still valid and predictive in the theories of new complex materials. Correspondences between the multi-body and Voigt approaches will also be indicated, observing that in both cases angular potentials appear, respectively depending on the angles between the lines connecting particles and on the particle orientations.

2 VOIGT'S MODEL FOR ELASTICITY

Around the beginning of the XXth century Voigt [3, 4] advanced the hypothesis that the critical points in the 'ancient' molecular theory of elasticity, that of Navier, Cauchy and Poisson, lie in the assumption of molecules exchanging only central opposite forces. Voigt, on the basis of studies on crystals, proposed a different point of view: matter is composed by ultimate elements (*Bausteine*, or 'bricks') which are aggregations of atoms that behave like rigid bodies, assembled in regular lattices in space. These bricks-molecules interact in pairs via a system of actions reducible to a force and a couple and in conservative processes the potential function of a pair of bricks h, k is

$$-d\Phi_{hk} = \mathbf{f}_{hk} \cdot \delta\mathbf{p}_h + \mathbf{m}_{hk} \cdot \delta\boldsymbol{\theta}_h + \mathbf{f}_{kh} \cdot \delta\mathbf{p}_k + \mathbf{m}_{kh} \cdot \delta\boldsymbol{\theta}_k \quad (1)$$

where $\mathbf{f}_{hk}, \mathbf{m}_{hk}$ are the force and the couple exerted by k on h , respectively, $\delta\mathbf{p}_h, \delta\boldsymbol{\theta}_h$ are the first-order displacement of the centre of gravity and the rotation of h , respectively; and similarly for the actions of h on k and the first-order rigid motion characteristics for k .

If the pair h, k undergoes a rigid motion, the equation of virtual work provides the balance equations for inner actions, once posed \times the cross product between vectors:

$$\begin{aligned} \mathbf{f}_{hk} + \mathbf{f}_{kh} &= \mathbf{0}, \\ \mathbf{m}_{hk} + \mathbf{m}_{kh} + (\mathbf{p}_k - \mathbf{p}_h) \times \mathbf{f}_{kh} &= \mathbf{0} \end{aligned} \quad (2)$$

and, by inserting (2) into (1) and posing $\mathbf{p}_{hk} = \mathbf{p}_h - \mathbf{p}_k$, one obtains the following equivalent reduced expressions for the potential:

$$\begin{aligned} -d\Phi_{hk} &= \mathbf{f}_{hk} \cdot (\delta\mathbf{p}_{hk} + \mathbf{p}_{hk} \times \delta\boldsymbol{\theta}_k) + \mathbf{m}_{hk} \cdot (\delta\boldsymbol{\theta}_h - \delta\boldsymbol{\theta}_k) = \\ &= \mathbf{f}_{kh} \cdot (\delta\mathbf{p}_{hk} + \mathbf{p}_{hk} \times \delta\boldsymbol{\theta}_h) + \mathbf{m}_{kh} \cdot (\delta\boldsymbol{\theta}_k - \delta\boldsymbol{\theta}_h) \end{aligned} \quad (3)$$

Voigt accepts the existence of a sphere of molecular action, following Navier, Cauchy and Poisson: the molecular interaction is appreciable only inside this sphere and vanishes outside. The radius of the molecular sphere of action is negligible with respect to ordinary dimensions, yet contains a huge amount of molecules. Voigt advances the strong hypothesis that within this sphere the bricks have the same first-order rotation. This inner constraint is implicitly assumed perfect, hence the power expended by constraint reactions shall vanish on any motion compatible with the constraint and (3) imply that the intermolecular force $\mathbf{f}_{hk} = -\mathbf{f}_{kh}$ is entirely active, while there exists a reactive part of the intermolecular couples $\mathbf{m}_{hk}, \mathbf{m}_{kh}$. Keeping into account this constraint the reduced form for the pair potential is

$$-d\Phi_{hk} = \mathbf{f}_{hk} \cdot (\delta\mathbf{p}_{hk} + \mathbf{p}_{hk} \times \delta\boldsymbol{\theta}_h) \quad (4)$$

Since the bricks inside the sphere of actions rotate of the same amount Voigt remarks that it is always possible to refer the relative positions of the pair h, k to a new basis. This is rigidly rotated with respect to the basis in the reference shape by the same amount of the bricks. The expressions for the relative motion of rigid bases provides, denoting with an asterisk the vectors with respect to the moving basis,

$$\delta\mathbf{p}_{hk}^* = \delta\mathbf{p}_{hk} + \mathbf{p}_{hk} \times \delta\boldsymbol{\theta}_h \quad (5)$$

Voigt proves, by introducing (5) into (4), that the final reduced form for the pair potential

$$-d\Phi_{hk} = \mathbf{f}_{hk} \cdot \delta\mathbf{p}_{hk}^*, \quad (6)$$

does not depend on rotation, which can be skipped via a change of basis.

Thus, the active part of intermolecular forces are

$$\mathbf{f}_{hk} = \frac{\partial(-d\Phi_{hk})}{\partial(\delta\mathbf{p}_{hk}^*)} \quad (7)$$

while there is no active part of the molecular couples \mathbf{m}_{hk} , \mathbf{m}_{kh} , which are mere constraint reactions and can be determined only via balance equations.

Voigt follows Poisson's approach in terms of forces in order to define the densities of contact force \mathbf{f}_n (*Druck*, or 'pressure'— nowadays stress) and couple \mathbf{m}_n (*flachenhafte Moment*, or stress-couple). His results can however be obtained and will be presented here by means of a purely energetic approach.

Voigt considers a surface element of area dA with outer unit normal \mathbf{n} which is the base of a straight cylinder with height ρ equal to the radius of the sphere of molecular action. We denote by the subscript i (e) the molecules inside (outside) the cylinder (that is, on opposite sides of \mathbf{n}), and we consider only those pairs i, e separated by a distance less than ρ . Indeed, the other pairs do not interact since the elements of the pair lie outside the sphere of molecular action.

The work expended by the actions that the molecules outside the cylinder exert on those inside is

$$\begin{aligned} \delta W_{ie} &= \sum_i \sum_e \mathbf{f}_{ie} \cdot (\delta\mathbf{p}_{ie} + \mathbf{p}_{ie} \times \delta\boldsymbol{\theta}_i) \\ &= \sum_i \sum_e (\delta\mathbf{p}_{ie} \cdot \mathbf{f}_{ie}) + \delta\boldsymbol{\theta}_i \cdot \sum_i \sum_e (\mathbf{p}_{ie} \times \mathbf{f}_{ie}) \end{aligned} \quad (8)$$

We define the stress \mathbf{f}_n and the couple-stress \mathbf{m}_n by means of the following equivalence of expended works:

$$\delta W_{ie} = (\mathbf{f}_n dA) \cdot (\delta\rho)\mathbf{n} + (\mathbf{m}_n dA) \cdot \delta\boldsymbol{\theta}_i, \quad (9)$$

where the first addend has the same form of the work spent by a pressure on the elementary variation of volume in thermodynamics and the second is obvious.

From (8), (9) standard arguments of calculus of variations provide, on one hand,

$$\mathbf{f}_n \cdot (\delta\rho)\mathbf{n} = \frac{1}{dA} \sum_i \sum_e \mathbf{f}_{ie} \cdot \delta\mathbf{p}_{ie}, \quad (10)$$

and stress is an average of intermolecular forces crossing the surface dA .

On the other hand, (8), (9) yield

$$\mathbf{m}_n = \frac{1}{dA} \sum_i \sum_e (\mathbf{p}_{ie} \times \mathbf{f}_{ie}) \quad (11)$$

Hence, the couple-stress is an average of the moments of intermolecular forces; from (10), (11) a constitutive relation for the force suffices to define both the stress and the couple-stress.

Voigt remarks that in the definition for the couple-stress (11) the lever arm is small and the sums are vanishingly small when compared with those in (10), hence if the stress is finite (which is implicitly assumed) the couple-stress vanishes.

Voigt can so recover the standard results on stress known since Navier, Cauchy and Poisson: external surface actions and inner contact actions are well described by the stress field and Voigt proves that, on the basis of (10), the latter is linear in the normal to the surface element on which stress acts.

Voigt operates a standard linearization procedure on the pair potential (6), which is a function only of the relative distances between the centres of gravity of the elementary bricks. Indeed, as we have already seen, the assumption of the constraint on the rotation of the bricks inside the sphere of molecular action makes the pair potential independent of the rotation.

By means of standard passages, the first-order approximation to the change in the relative distance between points is given by the gradient of the displacement, well defined by 9 independent coefficients. Since stress is linear in the unit normal to the considered surface element, it is also well defined by 9 components. Thus, the most general linear elastic constitutive relation contains 81 coefficients C_{hk}^{mn} . Voigt remarks, however, that these coefficients derive from an elastic potential (we nowadays call such materials hyperelastic) and are expressed, after lengthy calculations which are only mentioned by Voigt, by

$$C_{hk}^{mn} = \frac{1}{2}\zeta^0 \sum_i x_m^0 x_n^0 \left(\frac{\partial^2 \Phi}{\partial x_h \partial x_k} \right)^0 \quad (12)$$

where the superscript 0 indicates that the considered fields are evaluated in the reference shape, ζ is the number of bricks per unit volume (the body is supposed homogeneous) and the sum may be extended, for symmetry reasons, only to one half of the molecules inside the cylinder used for the definition of the stress.

It is obvious, then, that by Schwartz's theorem on mixed derivatives and the symmetry in the product $x_m^0 x_n^0$ in (12) reduce the actual number of elastic coefficients. Voigt further remarks that under his assumption on rotation: a) the gradient of the displacement does not depend on micro-rotation and hence reduces to the infinitesimal strain, which is symmetric and well defined by 6 coefficients; b) couple-stresses do not exist and the stress is defined by a linear operator \mathbf{S} which is also symmetric and well defined by 6 coefficients. The hyperelastic potential is thus provided by 21 coefficients because of the symmetries of the quadratic form built on the infinitesimal strain:

$$(\mathbf{S})_{lm} = (\mathbf{C})_{lm}^{pq} (\mathbf{E})_{pq}, \quad \mathbf{S} = \mathbf{S}^\top, \quad \mathbf{E} = \mathbf{E}^\top, \quad (\mathbf{C})_{lm}^{pq} = (\mathbf{C})_{pq}^{lm}. \quad (13)$$

Voigt proves that for homogeneous isotropic bodies the number of elastic constants is 2, as confirmed by experiments. As a corollary, he shows that under the ancient traditional hypothesis that intermolecular forces are central and opposite he can easily obtain the so-called relations of Cauchy and Poisson, which reduce the number of elastic coefficients to 1 for isotropic homogeneous linear elastic bodies, as it was remarked for instance also by Marcolongo in [8].

3 POINCARÉ'S MODEL FOR ELASTICITY

In his monograph on elasticity [7] Poincaré assumes a discrete model of matter made up of molecules of negligible dimension, or body-points, which exchange forces \mathbf{f} . Intermolecular forces are characterized by a force function (potential energy) U depending on the present placement of all the molecules, sum of the placement \mathbf{x}_i in the reference shape and of the displacement \mathbf{u}_i

$$U = \hat{U}(\mathbf{x}_i + \mathbf{u}_i), \quad \mathbf{f}_i = \frac{\partial \hat{U}}{\partial \mathbf{u}_i}. \quad (14)$$

The orientation of the body to which the molecules belong is immaterial, since it can be skipped via a rigid motion (remark that a similar reasoning was put forward by Voigt). Then U depends on the sole distance r_{ij} between pairs of molecules i, j , which can be collected in the N -dimensional vector \mathbf{r} , N being the number of the pairs of molecules composing the body:

$$U = U(\mathbf{r}), \quad (\mathbf{r}) = (r_{12}, r_{13}, r_{14}, \dots). \quad (15)$$

Poincaré points out that the potential energy being the sum of the potential of pairs of molecules,

$$U = \sum_{ij} U_{ij}(r_{ij}), \quad (16)$$

is but a particular case, when intermolecular forces are central and opposite and depend only on the relative position of the two molecules i, j , not on the relative position of other molecules. This particular case, remarks Poincaré, is that of the molecular model by Navier, Cauchy and Poisson.

In general, however, intermolecular forces depend on the whole amount of the considered molecules, even if they are necessarily opposite, as it is easily shown as follows. Consider any two molecules m_1, m_2 , the placements of which are $\mathbf{x}_1, \mathbf{x}_2$; the forces $\mathbf{f}_1, \mathbf{f}_2$ on the two molecules are provided, by the definition of potential energy (15), by

$$\begin{aligned} \mathbf{f}_1 &= \frac{\partial U}{\partial \mathbf{x}_1} = \frac{\partial U}{\partial \mathbf{r}} \frac{\partial \mathbf{r}}{\partial \mathbf{x}_1} = \sum_{ij} \frac{\partial U}{\partial r_{ij}} \frac{\partial [(\mathbf{x}_i - \mathbf{x}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j)]^{\frac{1}{2}}}{\partial \mathbf{x}_1} = \\ &= \frac{\partial U}{\partial r_{12}} \frac{\mathbf{x}_1 - \mathbf{x}_2}{r_{12}} + \frac{\partial U}{\partial r_{13}} \frac{\mathbf{x}_1 - \mathbf{x}_3}{r_{13}} + \dots \\ \mathbf{f}_2 &= \frac{\partial U}{\partial \mathbf{x}_2} = \frac{\partial U}{\partial \mathbf{r}} \frac{\partial \mathbf{r}}{\partial \mathbf{x}_2} = \sum_{ij} \frac{\partial U}{\partial r_{ij}} \frac{\partial [(\mathbf{x}_i - \mathbf{x}_j) \cdot (\mathbf{x}_i - \mathbf{x}_j)]^{\frac{1}{2}}}{\partial \mathbf{x}_2} = \\ &= -\frac{\partial U}{\partial r_{12}} \frac{\mathbf{x}_1 - \mathbf{x}_2}{r_{12}} + \frac{\partial U}{\partial r_{23}} \frac{\mathbf{x}_2 - \mathbf{x}_3}{r_{23}} + \dots \end{aligned} \quad (17)$$

It is apparent that $\mathbf{f}_1, \mathbf{f}_2$ are the sum of terms which can be interpreted as the forces exchanged between the pairs of molecules $m_1, m_2; m_1, m_3; m_2, m_3$; and so on. It is also apparent that the forces between m_1, m_2 (hence between any pair of molecules) are opposite and central.

Poincaré assumes that U admits a power series expansion in terms of \mathbf{r} in a neighbourhood of the natural shape, described by \mathbf{r}_0 and characterized by the absence of external forces¹:

$$U(\mathbf{r}) = U(\mathbf{r}_0) + \frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot \Delta \mathbf{r} + \frac{1}{2} \frac{\partial^2 U}{\partial \mathbf{r} \otimes \partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r} \otimes \Delta \mathbf{r}) + \dots \quad (18)$$

The increments $\Delta \mathbf{r}$ are expressed in terms of the displacements \mathbf{u}_i of the molecules and of their relative variation $\Delta \mathbf{u}_{ij} = \mathbf{u}_i - \mathbf{u}_j$:

$$\Delta r_{ij} = 2\mathbf{r}_{ij} \cdot \Delta \mathbf{u}_{ij} + \Delta \mathbf{u}_{ij} \cdot \Delta \mathbf{u}_{ij} = (\Delta r_{ij})_1 + (\Delta r_{ij})_2 \quad (19)$$

where $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$. Since the magnitudes of the $\Delta \mathbf{u}_{ij}$ are much smaller than the relative distances r_{ij} , the term $(\Delta r_{ij})_1$ is a first-order infinitesimal, while $(\Delta r_{ij})_2$ is of second order with respect to the magnitude of the $\Delta \mathbf{u}_{ij}$.

¹This condition, as Poincaré remarks, does not coincide with the usual definition, dating back to Lamé and accepted also nowadays, of natural state as stress-free. Indeed, a stress-free state implies the absence of external forces but the reverse is not true since intermolecular forces can be self-balanced, like in a redundant system subject to a thermal action.

Hence, by arresting the development (18) to the second order and using (19)

$$\begin{aligned}
U(\mathbf{r}) &= U(\mathbf{r}_0) \\
&+ \frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_1 \\
&+ \frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_2 + \frac{1}{2} \frac{\partial^2 U}{\partial \mathbf{r} \otimes \partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_1 \otimes (\Delta \mathbf{r})_1
\end{aligned} \tag{20}$$

where $(\Delta \mathbf{r})_1, (\Delta \mathbf{r})_2$ are vectors collecting the $(\Delta r_{ij})_1, (\Delta r_{ij})_2$, respectively.

Let us pose, with Poincaré,

$$\begin{aligned}
U_0 &= U(\mathbf{r}_0), \\
U_1 &= \frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_1, \\
U_2 &= \frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_2 + \frac{1}{2} \frac{\partial^2 U}{\partial \mathbf{r} \otimes \partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_1 \otimes (\Delta \mathbf{r})_1
\end{aligned} \tag{21}$$

where the terms are polynomials of order zero, one and two in the Δr_{ij} , respectively.

The second addend in U_2 is divided into two other addends, one keeping into account the distances between the same pair, characterized by $r_{ij}, \Delta r_{ij}$,

$$\bar{U}_2 = \frac{1}{2} \sum_{ij} \frac{\partial^2 U}{\partial r_{ij}^2} \Big|_{\mathbf{r}=\mathbf{r}_0} (\Delta r_{ij})_1^2, \tag{22}$$

where the sum is extended over all the pairs of molecules i, j . The other addend keeps into account the distances between different pairs of molecules:

$$\hat{U}_2 = \sum_{ij, hk} \frac{\partial^2 U}{\partial r_{ij} \partial r_{hk}} \Big|_{\mathbf{r}=\mathbf{r}_0} (\Delta r_{ij})_1 (\Delta r_{hk})_1. \tag{23}$$

and the sum is extended over all the different pairs of molecules $i, j; h, k$.

Poincaré operates what nowadays would be called homogenization: he divides the body into very small cubes with edge much larger than the radius of molecular action (the same concept of the classical theory by Navier, Cauchy and Poisson) and hence containing a vast amount of molecules. Then he shows that the potential energy of the whole body is expressed by the sum of the potential energies of each cube, once admitted that the potential energy of the layer of molecules next to the common surface of adjacent cubes is negligible (the number of molecules in that layer is much smaller than in the rest of the cube because of the dimension of the radius of molecular action). Thus, keeping into account only the distances r_{ij} between molecules inside the volume dV of the small cubes, Poincaré obtains that U_1 is obtained via the volume density W_1

$$W_1 = \frac{1}{dV} \left(\frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_1 \right) \tag{24}$$

while U_2 is obtained via the volume density W_2

$$W_2 = \frac{1}{dV} \left(\frac{\partial U}{\partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_2 + \frac{1}{2} \frac{\partial^2 U}{\partial \mathbf{r} \otimes \partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta \mathbf{r})_1 \otimes (\Delta \mathbf{r})_1 \right) \tag{25}$$

and the second addend of W_2 may be split in two, \bar{W}_2, \hat{W}_2 , by using (22), (23).

If the displacement \mathbf{u} is a regular vector field the expressions for $(\Delta\mathbf{r})_1, (\Delta\mathbf{r})_2$ are obtained by considering the displacements of the centres of the small cubes and their first-order derivatives, because of the smallness of the considered cubes.

Hence, recalling (19) and posing $\mathbf{H} = \text{grad } \mathbf{u}$, one has

$$(\Delta r_{ij})_1 = 2\mathbf{r}_{ij} \cdot \Delta\mathbf{u}_{ij} = 2\mathbf{r}_{ij} \cdot \left(\frac{\partial\mathbf{u}}{\partial\mathbf{x}} \mathbf{r}_{ij} \right) = 2(\mathbf{r}_{ij} \otimes \mathbf{r}_{ij}) \cdot \mathbf{E}, \quad \mathbf{E} = \text{sym } \mathbf{H} \quad (26)$$

for the first-order term and

$$(\Delta r_{ij})_2 = \Delta\mathbf{u}_{ij} \cdot \Delta\mathbf{u}_{ij} = \left(\frac{\partial\mathbf{u}}{\partial\mathbf{x}} \mathbf{r}_{ij} \right) \cdot \left(\frac{\partial\mathbf{u}}{\partial\mathbf{x}} \mathbf{r}_{ij} \right) = (\mathbf{r}_{ij} \otimes \mathbf{r}_{ij}) \cdot (\mathbf{H}^\top \mathbf{H}) \quad (27)$$

for the second-order term. It turns out that $(\Delta r_{ij})_1$ is a linear function of the six components of the symmetric tensor \mathbf{E} , the infinitesimal strain, while $(\Delta r_{ij})_2$ is a linear function of the six components of the symmetric tensor $\mathbf{H}^\top \mathbf{H}$, the quadratic strain. That is, the potential energy is expressed, as it is standard also nowadays, in terms of the strain measure.

It is now possible to compute the number of coefficients necessary to define the potential energy, or better the two density functions W_1, W_2 ; this will result in defining the elastic constitutive relations, because of the definition of potential function.

The density function W_1 , by (24), (26), is a linear function of the 6 components of the infinitesimal strain, hence its knowledge requires 6 independent coefficients. From a constitutive point of view, however, the complete characterization of W_1 lets us know the intermolecular force in the natural state (which, as already remarked, need not be stress-free), hence it can be skipped.

Indeed, in order to know the intermolecular forces in the present deformed shape it is necessary to characterize the density function W_2 , which, apart from the term $1/dV$, is the sum of two terms.

The first, by (25), (27), is linear in the 6 components of the quadratic strain $\mathbf{H}^\top \mathbf{H}$, hence requires 6 independent coefficients.

The second, by (22), (23), (25), (26), may be expressed as

$$\begin{aligned} \frac{1}{2} \frac{\partial^2 U}{\partial \mathbf{r} \otimes \partial \mathbf{r}} \Big|_{\mathbf{r}=\mathbf{r}_0} \cdot (\Delta\mathbf{r})_1 \otimes (\Delta\mathbf{r})_1 &= 2 \sum_{ij} \frac{\partial^2 U}{\partial r_{ij}^2} \Big|_{\mathbf{r}=\mathbf{r}_0} (\mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \otimes \mathbf{r}_{ij}) \cdot (\mathbf{E} \otimes \mathbf{E}) + \\ &+ 4 \sum_{ij, hk} \frac{\partial^2 U}{\partial r_{ij} \partial r_{hk}} \Big|_{\mathbf{r}=\mathbf{r}_0} (\mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \otimes \mathbf{r}_{hk} \otimes \mathbf{r}_{hk}) \cdot (\mathbf{E} \otimes \mathbf{E}), \end{aligned} \quad (28)$$

hence is quadratic in the infinitesimal strain and requires 21 independent coefficients.

Of these, 15 are necessary to identify the term of the energy density coming from \bar{U}_2 , see equation (22). Indeed, \bar{U}_2 is a quadratic form in the $(\Delta r_{ij})_1$, but 6 of the 21 coefficients multiplying it are dependent, those comig from posing $\mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \otimes \mathbf{r}_{hk} \otimes \mathbf{r}_{hk} = \mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \otimes \mathbf{r}_{ij}$ in (28). These dependent relations are called ‘relations of Cauchy and Poisson’ in the literature [8].

The remaining 6 independent coefficients are necessary to identify also the term of the energy density coming from \hat{U}_2 , see equation (23).

So, a complete characterization of an elastic material requires $21+6=27$ independent coefficients. This number can be reduced if:

1. the reference shape is free of external forces: indeed, Poincaré proves that the coefficients of the first term defining W_2 have the same form as those defining W_1 , hence in this case they vanish and one needs only 21 elastic coefficients;

2. the potential U is the sum of pair potentials, as provided by (16); then the last addend in (28) vanishes, because the partial derivatives in the coefficients are zero (each term depends only on the distance of the considered pair and not on others). Hence in this case the number of independent coefficients are reduced to 15 (as in the model by Navier, Cauchy and Poisson).

Poincaré also proves that for isotropic bodies the number of elastic constants reduces to two, as confirmed by experiments.

The following table can then be considered:

Potential	External forces	Coefficients
Coupled	Present	27
	Absent	21
Uncoupled	Present	21
	Absent	15

4 A MENTION TO MODERN ATOMISTIC THEORIES

Continuum models derived from discrete descriptions of materials at different length scales, spanning several orders of magnitude from the submicron scale to the millimeter or even larger scales, are at present among the most promising approaches in the mechanics of materials with microstructure.

The development of atomistic-continuous models based on energetic links between continuum and discrete solid mechanics can be seen as originated from molecular modelling of elastic materials developed in the 19th century, in particular by Voigt and Poincaré.

These models are based on the assumption that there is an implicit mapping from the large set of atomistic degrees of freedom to a single displacement vector field. A standard hypothesis to obtain such a correspondence is the so-called Cauchy-Born rule, which simplistically applies the same continuum linear transformation to the atom positions in such a way that each point in the solid is subjected to local homogeneous deformations [10]

$$\mathbf{x}_i = \mathbf{F}\mathbf{X}_i, \quad (29)$$

where \mathbf{X}_i and \mathbf{x}_i are the i -th atom positions in the reference and deformed configuration, respectively, while $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ is the continuum local deformation gradient. In this way a strain energy density $W(\mathbf{F})$ can be computed using an atomistic interaction potential, and the continuum stress as well as the constitutive tensors, i.e. the first Piola-Kirchhoff tensor \mathbf{P} and the Lagrangian tangent stiffness fourth order tensor, \mathbf{C} , can be derived as

$$\mathbf{P} = \frac{\partial W}{\partial \mathbf{F}}, \quad \mathbf{C} = \frac{\partial^2 W}{\partial \mathbf{F} \otimes \partial \mathbf{F}}. \quad (30)$$

Such an hypothesis (29) derives from an intuitive judgment and holds when interactions are quite of short range. It is easy to recognize that in a linearized framework Voigt's and Poincaré's coarse-graining processes imply the same hypothesis. Moreover, the same conceptual framework applies for the derivation of the stress measures and constitutive relations of non standard continua equivalent to systems of particles endowed with extension [13, 14].

In this framework, the potential energy of a system of particles has a continuum quadratic form strain-energy counterpart. In a more general case, the introduction of potentials of order higher than

two and/or the recourse to multi-body interaction terms are often necessary, for example when long-range interactions must be considered. In any case, an implicit mapping between the large set of atomistic degrees of freedom to one or, in the non-standard continua, few vector fields is assumed.

Let $\mathbf{x}_j, \mathbf{x}_h, \dots, \mathbf{x}_N$ be the current positions of the $j^{th}, h^{th}, \dots, N^{th}$ particle/atom interacting with the i^{th} -atom. The multi-body potential of a system of N -particles interacting with the i^{th} -particle is a function of the N distances $r_{i\alpha} = |\mathbf{x}_i - \mathbf{x}_\alpha|$, $\alpha = j, h, \dots, N$. A basic issue in the physics of solids is the construction of a good interaction model which provides an accurate estimation of the total energy and related quantities (e.g. the energy derivatives) of the material. The simplest way to do that is to expand the potential into series of two-body U^{2B} , three-body U^{3B} , ..., n -body U^{nB} terms

$$U(r_{ij}, r_{ih}, \dots, r_{iN}) \cong \sum_{i \neq j} U^{2B}(r_{ij}) + \sum_{i \neq j \neq h} U^{3B}(r_{ij}, r_{ih}) + \dots + \sum_{i \neq j \neq h \dots \neq n} U^{nB}(r_{ij}, r_{ih}, \dots, r_{in}), \quad (31)$$

establishing a criterion for the potential cut-off for a suitable number $n \leq N$ of interacting particles. If the multi-body potential is expanded in Taylor series it can be recognized that the second order term depends on the product $r_{ij}r_{ih}$, and then the series expansion up to the same order is a three-body or at least a two-body (for $j = h$) potential. The n -order term depends on $r_{ij}r_{ih} \dots r_{in}$, and then the series expansion up to the same order is at most an $n + 1$ -body potential.

The so-called central-force scheme implies the definition of a potential as the sum of two-body potentials depending only on the relative distance between the two particles. As mentioned above, in elasticity for instance, this scheme early showed to be inadequate since the symmetries of the constitutive tensors, including the six Cauchy-Poisson relations, provide a number of independent coefficients which is in contradiction with experiments (15 in the general anisotropic and 1 in the isotropic case). In Poincaré's model, the second order potential depends on the product $r_{ij}r_{ih}$, or equivalently on the angle between r_{ij} and r_{ih} : $\theta_{ijh} = (\mathbf{r}_{ij} \cdot \mathbf{r}_{ih})/|\mathbf{r}_{ij} \cdot \mathbf{r}_{ih}|$, and it is in general a three-body potential providing, as shown in the previous session, the necessary 21 elasticities for anisotropic bodies in the natural state. At the same time, the model by Voigt, having rigid bodies with constrained rotations, provides a two-body potential description enriched by the presence of non-central forces, which entails that the Cauchy-Poisson relations are not valid and the resulting independent elastic coefficients are 21 ([4], pp. 607–608).

From the beginning of the 20th century it was recognized that both these non-central force schemes were necessary to correctly describe the elastic behaviour of elastic isotropic media [8, 11]. In particular, the latter model was generally interpreted as reduced to the former since the variations of angles were accounted for.

As mentioned above, in current atomistic modelling there are many circumstances in which the inadequateness of the central-force scheme calls for the need of improved multi-body potential descriptions, often obtained resorting to atomistics. This could happen both when the structure of regular lattices must be properly taken into account in deriving energy-equivalent continuous models for crystals, and when the developed potentials must be able to capture complex phenomena, such as brittle fracture in covalent materials accounting for the structures of extended defects [12, 9].

Most of these improved atomistic/continuum models of materials, based on lattice microscopic (atomistic/molecular) information and on energy equivalence between models at different material scales, can then be seen as generalized Voigt and Poincaré approaches which allow to describe materials with various microstructures at different scales (nano-micro-meso) and various (non-linear and/or non-elastic) behaviours.

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