Nineteenth century molecular models with a glance at modern discrete−continuum theories

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The origins of multiscale modelling, lying in the classical molecular models of Nineteenth century originally formulated to provide explanations per causas of elasticity, are investigated with the aim of drawing suggestions for the modelling of new complex materials. Conceptual guidelines for deriving scale dependent continuum formulations, here continuum models with additional degrees of freedom (multifield continua), are defined starting from non-classical corpuscular descriptions and the historical and epistemological settings of the current modelling proposals are highlighted.

1 Introduction. The mechanistic framework

This contribution focuses on the genesis of nonlocal theories for continuous models originated from refined discontinuous descriptions of materials. The molecular theory of elasticity, as developed by Navier, Cauchy and Poisson [2–4] in the 19^{th}century, represents the first attempt to derive the field equations of an elastic body basing on the definition of microscopic laws for systems of point–like particles ('molecules') close together, which cohere due to the presence of attractive forces. The molecules are perceived as ultimate particles without extension inside which no forces are accounted for. They interact in pairs through forces, depending on their mutual distance, directed along the line connecting their centres ('central–force' scheme). A kinematic corresponding map between the discrete degrees of freedom and the continuum fields guarantees the transition from the fine to the gross description. Macroscopic stress measures are then derived as averages of molecular material quantities over a convenient volume element, called 'molecular sphere of action', outside which intermolecular forces are negligible.

The mechanistic perspective of the molecular models of elasticity was much appreciated by the scientists of the period, among these Saint Venant [5], mostly because it preserved the Newtonian interpretation of internal forces as mechanical interactions between material particles. This belief was well framed within the recognized intent of reducing all natural phenomena to forces of attraction/repulsion. In his treatise on Opticks, and in particular at the 'Query 31', Newton indicated that: "the small particles of matter may cohere by the strongest attractions and, compose bigger particles of weaker virtues, and many of these may cohere and compose bigger particles, whose virtue is still weaker; and so on for diverse successions, until the progression end in the biggest particles which by adhering, compose Elastic bodies''. It is worth noting that at small distances the interactions are of unspecified nature ("perhaps chemical'') and of unknown cause. During the Eighteenth century, the Newtonian idea of matter coherence, not explicitly related to the presence of a medium between particles nor to the search for the causes of phenomena, was casted into a strictly mechanistic setting in which interact forces depending on the intermolecular distance. Various scientists as van Mussenbroeck interpreted the *coherentia corporum* as the effect of the attracting intermolecular action (*vis interna attrahens*) and Boscovich specified that this force depended on the mutual distance (see: [6]). This implied the forced introduction of a thin substance, thought as a fluid embedding the particles everywhere, which justified, in a sense, the molecular attraction. Thus recalling the "occult quality'' which Newton himself explicitly rejected, releasing his theory from the risks of Natural Philosophy of his detractors (Huygens and Leibniz among them).

Despite the limitations of the mechanistic point of view, which would have been recognized in the following years with the development of the concept of field theories of energy in thermodynamics and electromagnetism, the corpuscolar theories had a wide and important development in science, looking for instance at the kinetic theory of gases, statistical mechanics and later, when the discrete representation was extended to energy, quantum mechanics. Everything supported by the new discoveries about the existence of atoms. However, a discussion concerning the use of the concept of discrete in physics is beyond the scope of this short note which focuses on the idea, currently widely exploited in matter physics, of using refined discrete descriptions to built–up nonlocal field theories for complex materials.

2 Refined molecular models towards scale dependent continuum theories

The 'central–force' description led to experimental discrepancies concerning the number of elastic constants that were less that than those needed to represent the behaviour of materials belonging to various symmetry classes. Successively, Voigt and Poincaré introduced mixed energetic/mechanistic approaches providing refined descriptions of the classical molecular

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model that circumvented the problem of the underestimation of the number of the material constants related to the central–force scheme [7–9]. In particular, Voigt introduced a potential of force and moment interactions exerted between pairs of rigid bodies, while Poincaré proposed a multibody potential description. Both Voigt and Poincaré removed the local character of the Cauchy description by modifying the central–force scheme, thus obtaining continua which could be classifiable as 'implicitly' or 'weakly' non-local (e.g. [11]), since the presence of internal lengths and dispersion properties can be there recognized. Even if they finally led back to classical continuuous formulations by introducing internal constraints: Voigt imposing the same uniform rotation to the particles and Poincaré considering only pair–interaction terms. However, even if both Voigt and Poincaré, removing the local character of the central–force scheme, offered a good solution to the controversy about the elastic constants, the mechanistic–molecular approach was abandoned in favour of the energetic–continuum approach by Green, and their works have been neglected for long time [12–15].

Now these ideas found a renewed interest with particular reference to the problem of constitutive modelling of composite materials. The mechanical behaviour of materials characterized at finer scales by the presence of heterogeneities of significant size and texture, strongly depends on their internal structure, that is intrinsically heterogeneous and discrete because interfaces (grain boundaries, thin layers, etc.) dominate the gross behaviour. By lacking in material internal scale parameters, moreover, the classical continuum does not always seem appropriate to describe the macroscopic behaviour of such materials taking into account the size, the orientation and the disposition of the heterogeneities. This calls for the need of nonlocal continuum descriptions which can still be obtained through homogenization approaches aimed at deducing properties and relations by bridging information at proper underlying discrete micro–levels via energy equivalence criteria. As current researches in solid state physics, as well as in mechanics of materials, show, energy–equivalent continua obtained by defining direct links with lattice systems are still among the most promising approaches in material science.

Moving from discrete material descriptions, following the suggestions of Voigt and Poincaré, the original lattice models can be refined by extending the concept of molecule, in order to describe different internal phases (rigid inclusions, voids, etc.), and by taking into account of not only central intermolecular actions, or alternatively by introducing interaction potentials endowed of multibody terms. In this way, discrete–to–scale dependent nonlocal continua can be naturally derived using proper correspondence maps between discrete and continuum kinematic descriptors. Examples of such approaches are found in the works [12, 15, 16], where multifield continua with additional degrees of freedom [10] are derived from a lattice system made of rigid particles and distributed voids/defects (pores, microcracks, etc.) and then adopted for the description of ceramic matrix (polycrystals with interfaces) and fibre-reinforced composites.

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