

Title: Atomistic scale-dependent interpretation of continuum concepts and fields

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Abstract:

Any material system/body/identifiable set of molecules is modelled as a set of interacting point masses which undergo motions prescribed by Newtonian dynamics. Mass and momentum densities ρ and \mathbf{p} are defined, at any given scale ϵ , as locally-weighted molecular sums. Time differentiation of ρ yields the continuity equation with velocity $\mathbf{v} := \mathbf{p}/\rho$. The equation governing the motion of each molecule involves its interaction with all other molecules of the body of interest, together with the resultant force thereon due to external agency, such as gravitation or applied electromagnetic field. Multiplying this equation by a weighting dependent upon the distance of the molecule from any given geometrical point \mathbf{x} , and summing over all molecules, yield a local balance of linear momentum at \mathbf{x} corresponding to scale ϵ , of form $-\text{div } \mathcal{D} + \mathbf{f} + \mathbf{b} = \rho \mathbf{a}$ ($-\mathcal{D}_{ij,j} + f_i + b_i = \rho a_i$). Here \mathbf{f} is an interaction force density, \mathbf{b} the external force density ($\mathbf{b} = \rho \mathbf{g}$ if the only external agency is gravitational), \mathbf{a} is the acceleration, and \mathcal{D} is essentially thermal stress — the trace \mathcal{D}_{ii} of \mathcal{D} is twice the heat energy density. (In a moderately-rarefied gas $\mathbf{f} = \mathbf{0}$ and $-\mathcal{D}$ is the pressure tensor.) It is shown that \mathbf{f} can be expressed in terms of the divergence of a tensor field \mathbf{T}^- in a number of ways; for each such \mathbf{T}^- there is a corresponding Cauchy stress tensor $\mathbf{T} := \mathbf{T}^- - \mathcal{D}$. The geometrical/physical interpretation of \mathbf{T} associated with each way is outlined. Derivations of balances of generalised (tensor-valued) moment of momentum and energy are sketched. Remarks are made on the interpretation and scale-dependence of the notions of ‘material point’ and ‘boundary’ of a body. The rôle of additional averaging in time is discussed with relevance (i) to identification of field values with measurements, and (ii) to modelling systems whose molecular content changes with time. Implications and suggestions for modelling surface and edge effects are presented.