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An atomistically-meaningful pseudocontinuum representation for the finite monatomic chain with harmonic nearest-neighbor interactions

M. Charlotte

Université de Toulouse, ISAE-SupAero, Institut Clément ADER (CNRS, UMR 5312), 10 Ave Edouard Belin - BP 54032 - 31 055 TOULOUSE Cedex 4, France

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ABSTRACT

An atomistically-meaningful pseudocontinuum representation for the nontrivial lattice dynamics of a finite monatomic chain with linear elastic interactions between nearest neighbor atoms is analytically deduced by mean of a dynamic mechanical analysis extending the memory-dependent pseudocontinuum viewpoint suggested in [M. Charlotte and L. Truskinovsky, *Lattice dynamics from a continuum viewpoint*, J. Mech. Phys. Solids, 60, pages 1508–1544 (2012)]. For a correct description of the lattice dynamics at its interstice length scale, the pseudocontinuum model integrates both the bulk and boundary inertial (heat-vibration) effects of the atomistic medium through specific modifications of the classical elastodynamic Newton's law model: these modifications involve a generalization of the D'Alembert's principle of inertial forces and Neumann-Robin's boundary conditions, without increasing the number of initial and boundary conditions of the generic mechanical evolution problem, unlike all other generalized continuum models proposed in the literature up to this date. Owing to the spatially local and one-dimensional nature of the discrete and pseudocontinuum models, relationships are thus more clearly pinpointed between the elastodynamic normal stress field of that exact generalized continuum representation and the cohesive (or internal) and inertial forces operating at the lattice sites within the bulk of a finite-size monatomic chain and at its boundary.

1. Introduction

It has been already understood for long that, in order to reconcile the particle viewpoint with the continuum one, the solids with discrete/granular microstructures must be described with nonclassical continuum theories involving multiple length and time scales, and that in linear elasticity those ones are in part or essentially embedded into the phonon dispersion relations. Dispersive properties can be obtained in a continuum framework indeed with various enhancing ingredients such as spatial nonlocality (Blanc et al., 2002; Charlotte and Truskinovsky, 2008; Eringen, 1972; Eringen and Eringen, 1976; Eringen and Kim, 1977; Fafalis et al., 2012; Jirásek, 2004; Kroner, 1968; Krumshansl and Wallis, 1965; Kunin, 1982; Mindlin, 1964, 1965; Pichugin et al., 2008; Rogula, 1982; Silling, 2000; Suiker and de Borst, 2005; Sunyk and Steinmann, 2003; Toupin, 1962), temporal nonlocality (Askes et al., 2008; Bishop, 1952; Charlotte and Truskinovsky, 2012; Jirásek, 2004; Love, 2009; Metrikine and Askes, 2002a,b; Mindlin, 1964; Mindlin and Herrmann, 1950; Mindlin and McNiven, 1960; Mühlhaus and Oka, 1996; Pichugin et al., 2008; Rayleigh, 1945) or/and multi-fields/modes (Charlotte and Truskinovsky, 2008; Cosserat and Cosserat, 1909; Eringen, 1966; Eringen and Eringen, 1976; Eringen and Liebowitz, 1968; Il'iushina, 1969; Kunin, 1982; Mindlin and Herrmann, 1950; Mindlin and McNiven, 1960; Vasiliev et al., 2010) while using different kinematic and mechanic arguments. However, some of these enhanced continuum models lack of a physical reality or a mathematical consistency as they do not take into account correctly the dispersive, attenuating, and inertial effects related to the discrete distributions of masses (Charlotte and Truskinovsky, 2012; Milton and Willis, 2007; Willis, 1981; Willis and Suquet, 1997). One can meet for instance some difficulties to ensure the stability of these continuum models with respect to short wavelengths (Charlotte and Truskinovsky, 2008, 2012; Jirásek, 2004; Kunin, 1982; Pichugin et al., 2008; Rogula, 1982; Suiker and de Borst, 2005), or else to predict the filtering of high-frequency phonons that are linked to the natural capabilities of the aforementioned microstructured media to dissipate certain singularities in the material particle motions.

Besides, and apart from the fact that it is not always clear how to consider initial and boundary/interfacial conditions for the prior enhanced continuum models (except by variational formulation when possible), another important difficulty for all these continuum-atomistic connections is to correctly relate quantities

E-mail address: miguel.charlotte@isae.fr

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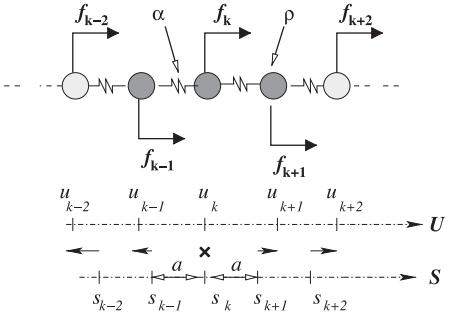

Fig. 1. The generic monatomic chain and its pseudocontinuum reference domain $\mathcal{S}$.

such as strain and stress tensors between two levels, but also these same quantities to forces and displacements used in the molecular model (Zimmerman et al., 2002, 2004, 2010). This may require in particular a correct atomistic interpretation of the local Cauchy's or Piola-Kirchhoff's stress tensors. That last nontrivial point has been a subject of great debate and controversy (see for instance Zhou, 2003). This important issue has been explored from many different perspectives for nearly two hundred years and has led to various definitions that do not appear to be consistent with each other; moreover those ones have not often fully appreciated the difference between pointwise stress measures and temporal and/or spatially-averaged quantities, as reported by Admal and Tadmor (2010, 2016); Murdoch (1982, 2003, 2007); Murdoch and Bedeaux (1993, 1994); Zimmerman et al. (2002, 2004, 2010). Currently, there are at least three definitions for the stress tensor which are commonly used in atomistic simulations: the virial stress (Clausius, 1870; Maxwell, 1870, 1874), the Tsai's traction (Tsai, 1979) and the Hardy's stress (Hardy, 1982). Other coarse grained continuum models use other averaged Cauchy's stress definitions associated with the names of Irving and Kirkwood (1950), Lehoucq and Lilienfeld-Toal (2010); Noll (1955, 2009) (which may be related to the one inferred for the peridynamics (Lehoucq and Silling, 2008; Silling, 2000)), or Murdoch and Bedeaux (Admal and Tadmor, 2010, 2016; Murdoch, 1982, 2003, 2007; Murdoch and Bedeaux, 1993, 1994), to mention just a few them; those ones are in a general multi-dimensional Eulerian's description of granular materials with arbitrary pair potentials of interactions or central cohesive forces between particles.

At the margins of these different viewpoints, this work attempts to identify what kind of local atomistic stress concept can be associated with an accurate *temporally nonlocal pseudocontinuum*[1] (**TN PC**) representation of a finite chain of particles with nearest neighbor harmonic interactions (**NNI**) like the one depicted on Fig. 1, that is submitted to soft loading devices and where the *surface dynamic pressure* generated by the particle vibration at the chain boundary needs to be accounted for as well. The elastodynamics of this Born-Von Kármán's finite, one-dimensional, monoatomic lattice corresponds to the simplest *medium of simple structure*, according to Kunin's classification (Kunin, 1982), since the only kinematic variable is a displacement (vector) that determines the state of the medium completely. However, from the continuum viewpoint, the fine dynamic behavior of such a simple lattice is in fact very complex already even in its linear regime due to the intrinsic occurrence of multiple scales of length and times of evolution (Brillouin and Parodi, 1956; Charlotte and Truskinovsky, 2008, 2012; Kunin, 1982; Maradudin et al., 1971) (as hereinafter the two time-scales ω_*^{-1} and T^* and two length-scales a and L) and to the importance of the micro-structural inertial forces.

The aforementioned TN PC viewpoint that is on target here is the one introduced previously in Charlotte and Truskinovsky (2012) for an infinite lattice domain: it assumes that the non-trivial dynamics of the considered lattice model can be interpreted within that continuous framework by the presence of inertial and pseudo-dissipative post-Newtonian forces yielding a spatio-temporal blending of the inertial and elastic forces. Compared to Charlotte and Truskinovsky (2012) and the many numerical or analytical works that have dealt with the considered lattice model, this new analytical development shows two main novelties: firstly, the inertial forces of the lattice model induce an *elastodynamic normal stress field* satisfying *nonstandard Neumann-Robin's boundary conditions*, with notably *time-dependent properties* in the TN PC model; secondly, the elastodynamic normal stress field of TN PC model can be related to a *simple atomistic interpretation* at the atom level. With this pseudocontinuum modeling, the dispersion of elementary wave-functions (or phonons) generated by the singular loading pulses becomes possible and prohibits the propagation of singularities in $\mathcal{S}$ characterizing the well-known failure of the classical continuum (**CC**) theory under impact load or sudden unloading. Thus, by its salient features of memory-dependent/hereditary media (that have also been anticipated for other dispersive vibrational properties of lattices and periodic material systems such as metamaterials (Milton and Willis, 2007; Willis, 1981; Willis and Suquet, 1997) for instance), the TN PC contrast with the spatially nonlocal pseudocontinuum (**SN PC**) model proposed by Eringen (1972); Eringen and Eringen (1976); Eringen and Kim (1977), Krumshansl and Wallis (1965), Kunin (1982), Rogula (1982). Indeed that latter assumes clearly distinguishable classical inertia and a strong spatial nonlocal elasticity yielding in fact a spatial blending of the bulk and boundary forces (as will demonstrate a subsequent article on this finite chain and boundary loading effects). Additionally, by not placing any restriction on the support of the applied loading in order to deal with point impact loadings as naturally as the original discrete theory, the TN PC model manages to overcome one major drawback of the derived SN PC model, which can be both applicable and accurate only for certain types of data that make the SN model inoperable and unenforceable with concentrated loads.

This paper is organized as follows. As standard in continuum mechanics, the formulation of the TN PC model relies on a specific space-time description of the particle system displacements. Section 2 begins therefore by reminding the main properties of the discrete chain motion and how the particle displacements $\boldsymbol{u}$ can be analytically expressed in terms of the one of the two "natural" continuous interpolation fields G of the discrete impulse response of this mechanical model. To illustrate some specifities of the particle displacements $\boldsymbol{u}$, a couple of complementary tests are purposely performed, one is taken from a singular category and the other one is taken from a smooth category. Section 3 presents then the memory/history dependent continuum mechanics that can be derived from the molecular foundation to include the scale dependence of mass density and boundaries of solid bodies. The main steps of the derivation of that TN model are first discussed, based on the properties of the continuous kernel G. This yields integrodifferential equations of motion involving a generalized linear momentum field $I_1[u]$, generalized normal stress field $I_\varepsilon[u]$ and the additional inertial forces $I_p^{\text{surf}}[u]$ acting at the boundary. It is shown

[1] In *nonlocal elasticity* theories, the notion of *pseudo-continuum, i.e.*continuum theories incorporating internal space and time scales, was also called *quasi-continuum* in the sense of Krumshansl and Wallis (1965), Kunin (1982) and Rogula (1982) (see also Eringen, 1982). Historically, this concept was introduced to treat discrete and continuous elastic models in the scope of the same formalism (Kunin, 1982), what fortuitously may help multi-scale numerical methods coupling (generalized) continuous model with atomistic-lattice ones. Following partly the original idea of Kunin, the term *quasicontinuum* was later purposely borrowed and introduced in the computational mechanics by Shenoy et al. (1999); Tadmor et al. (1996) as a multi-scale numerical method coupling the *classical continuum elasticity* theory with the *nonlocal atomistic-crystal lattice* one. Developing such an averaging computational viewpoint is not however the purpose of this article.