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Construction of multi-dimensional isotropic kernels for nonlocal elasticity based on phonon dispersion data

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ABSTRACT

Kernels for non-local elasticity are in general obtained from phonon dispersion relations. However, non-local elastic kernels are in the form of three-dimensional (3D) functions, whereas the dispersion relations are always in the form of one-dimensional (1D) frequency versus wave number curves corresponding to a particular wave direction. In this paper, an approach to build 2D and 3D kernels from 1D phonon dispersion data is presented. Our particular focus is on isotropic media where we show that kernels can be obtained using Fourier–Bessel transform, yielding axisymmetric kernel profiles in reciprocal and real spaces. These kernel functions are designed to satisfy the necessary requirements for stable wave propagation, uniformity of nonlocal stress and stress regularization. The proposed concept is demonstrated by developing some physically meaningful 2D and 3D kernels that will find useful applications in nonlocal mechanics. Relative merits of the kernels obtained via proposed methods are explored by fitting 1D kernels to dispersion data for Argon and using the kernel to understand the size effect in non local energy as seen from molecular simulations. A comparison of proposed kernels is made based on their predictions of stress field around a crack tip singularity.

1. Introduction

Theories of classical continuum mechanics which relate local strain to work-conjugate local stress measures, provide length-scale independent solutions, and are successful in addressing a large number of physical problems. However, these theories are found to be deficient for several situations that require a characteristic length scale of the medium to enter in the physical solution. Examples include stress and strain fields around sharp crack-tips, wave dispersion, strain softening and attendant size effects (see for example, Bažant and Cedolin, 2010). The fact that atomistic calculations of material properties are necessarily non-local in their construction, upscaling from an atomistic model to a continuum model would lead to continuum stress–strain relations that display non-local character. Nonlocal theories and their implementations have been intensely researched due to their promise in capturing non-local atomistic phenomena, however, the understanding developed to-date is incomplete. Several review articles, (Bažant and Jirásek, 2002; Aifantis, 2003; Askes and Aifantis, 2011; Maugin and Metrikine, 2010) have provided important details and much insight into the types of non-local continuum theories that are at our disposal. There exists varieties of nonlocal theories depending on the strategies to incorporate additional atomistic features. The focus of the present paper is on the integral type nonlocal theory proposed in (Eringen, 1983).

In the integral type nonlocal theory, the stress at a material point is related to a weighted integral of strains over a certain finite neighborhood. The weighting function (α) is the non-local *kernel*. The nonlocal stress, $\boldsymbol{t}$, in a linear elastic body, V, can be described as,

$$t_{ij}(\boldsymbol{x}) = \int_{\Omega} \alpha_{ijkl}(\boldsymbol{x},\boldsymbol{x}')\epsilon_{kl}(\boldsymbol{x}')\,d\Omega \tag{1}$$

where $\boldsymbol{\alpha}$ is a tensorial kernel representing an attenuating elastic modulus. Here, $\boldsymbol{t}$ and $\boldsymbol{\epsilon}$ are the nonlocal stress and local strain tensors, respectively, $\Omega \subset V$ is the compact support for the kernel and $\boldsymbol{x}$ and $\boldsymbol{x}'$ are position vectors for two material points in Ω. In isotropic media, it is assumed that a unique kernel weights all entries of the stiffness tensor equally (Eringen, 2002), and the above equation becomes,

$$t_{ij}(\boldsymbol{x}) = \int_{\Omega} \alpha(\boldsymbol{x},\boldsymbol{x}')C_{ijkl}\epsilon_{kl}(\boldsymbol{x}')\,d\Omega = \int_{\Omega} \alpha(\boldsymbol{x},\boldsymbol{x}')\sigma_{ij}(\boldsymbol{x}')\,d\Omega \tag{2}$$

Here, $\boldsymbol{\sigma}$ is the Hookean (local) stress tensor, C_{ijkl} is the stiffness tensor for an isotropic material and α is a *scalar kernel function*. In

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general, the following additional properties are attributed to the kernel function, α, as described in (Eringen, 1983),

- The kernel has a peak at $\|\boldsymbol{x}-\boldsymbol{x}'\|=0$, and decays with increasing distance $\|\boldsymbol{x}-\boldsymbol{x}'\|$.
- The kernel function α reverts to a delta function as the non local zone of influence vanishes, i.e., as $\lim_{\Omega\to 0}\alpha=\delta$. As such, $\alpha(\boldsymbol{x},\boldsymbol{x}')$ satisfies the normalization condition, i.e., $\int_\Omega \alpha(\boldsymbol{x},\boldsymbol{x}')\,d\Omega=1$.
- α is bi-symmetric, i.e., $\alpha(\boldsymbol{x},\boldsymbol{x}')=\alpha(\boldsymbol{x}',\boldsymbol{x})$ and function of $\boldsymbol{x}-\boldsymbol{x}'$.

Additionally, Bažant and Chang (1984) suggested that a continuum should not yield zero energy modes for non-rigid-body deformations and should have real wave propagation velocity, which requires that the Fourier transform of α have positive values all over the reciprocal space. The same restriction on α has been reached in Polizzotto (2001) by noting that Eq. (2) is a homogeneous Fredholm integral equation of first kind and then invoking the Fredholm integral equation theory. It is noted in Bažant and Chang (1984) that some of the popular kernels do not satisfy the required conditions. Thus, it is suggested to include a dirac delta function to alleviate this problem. However, the inclusion of a delta function leads to the loss of stress regularity property of nonlocal elasticity whenever the local stress is singular. In contrast to the above mentioned restrictions on the kernel, recent research through molecular simulations have indicated that at the nanoscale, the kernel α attenuation need not be monotonous (Picu, 2002; Sundararaghavan and Waas, 2011). The reason for α to be non-monotonous is attributed to the similarity between non-local kernels and inter-atomic potentials (Picu, 2002; Sundararaghavan and Waas, 2011). The normalization condition suggests that for all $\Omega\subset V$ a uniform local strain field would produce a uniform nonlocal stress field. However, we point out that this particular restriction of nonlocal kernel is meant to be satisfied as long as Ω does not intersect the boundary ∂V of the body V. Violation of the normalization requirement leads to various problems, for instance, when Ω intersects ∂V, a uniform strain yields a non-uniform nonlocal stress. From a purely mathematical perspective, few modifications to the kernel (Polizzotto, 2001; Borino et al., 2003; Polizzotto et al., 2004) have been suggested in the past in order to satisfy the normalization requirement at domain boundaries. Notwithstanding the symmetry achieved in these papers, we note that the symmetry condition of any function is determined by symmetry of its domain and codomain. Since, near the boundary $\Omega\not\subset V$, the domain of α itself is not symmetric with respect to the center of Ω. Hence, the symmetry conditions near the boundary may need further investigation. For detailed description about the properties of the kernel function, the reader is referred to Eringen (1983), Bažant and Chang (1984), Bažant and Jirásek (2002), Polizzotto (2001) and Ghosh et al. (2013).

While various studies have focused on (mostly macroscopic) nonlocal continuum and their numerical implementations, only a few have focused on the connection of these theories to realistic materials at small scale (Lam et al., 2003; Han, 2010, and references therein). The various additional (length scale) parameters or kernels needed to capture the non-locality of the material can be obtained via molecular simulations (Picu, 2002; Maranganti and Sharma, 2007a). A systematic attempt at generating 3D kernels from molecular simulations is developed in Picu (2002). However, the 3D kernels are not defined for distances below the distance at which the *radial distribution function* goes to zero, and were constructed only for pairwise potentials. For general interatomic potentials, the nonlocality is commonly obtained via wave dispersion studies. The dispersion curves are obtained for wave modes propagating along specific wave vectors. The dispersion curves obtained in this manner are inherently one dimensional, whereas for analyzing continua (represented via integral type nonlocality) multi-dimensional kernels are needed. In this paper, a new and general procedure to obtain 2D and 3D isotropic nonlocal kernels from dispersion data is proposed. Our particular focus is on isotropic media, where we show that kernels obtained using Fourier–Bessel transform, yield axisymmetric kernel profiles in reciprocal or real space. These kernels satisfy the necessary requirements for stable wave propagation, and uniformity of nonlocal stress and stress regularization. The proposed concept is demonstrated using physically meaningful 2D and 3D kernels that should find useful applications in nonlocal mechanics.

2. Integral-type nonlocal elasticity

The equations of motion for a non-local medium is given by,

$$t_{ij,i}+\rho(f_j-\ddot{u}_j)=0 \tag{3}$$

where $t_{ij}=C_{ijkl}\int_\Omega \alpha(\boldsymbol{x}-\boldsymbol{x}')\epsilon_{kl}(\boldsymbol{x}')\,d\Omega$ for an isotropic medium. It is experimentally observed that bulk and surface waves experience wave dispersion at higher frequencies, i.e., the phase velocity depends on the wavelength. The theories of lattice dynamics can demonstrate this dispersion behavior (see Dove, 1993) but classical elasticity fails to do the same. The following steps recapitulate that nonlocal elasticity can represent wave dispersion through the kernel function. Consider a plane wave solution for an infinite nonlocal solid with no body force: $u_j(\boldsymbol{x},t)=A_j e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)}$, where $\boldsymbol{k}$ and ω are the angular wave vector and the angular frequency respectively. Substituting u_j in the equilibrium equation, Eq. (3), yields:

$$|\rho\omega^2\delta_{jk}-C_{ijkl}\hat{\alpha}(\boldsymbol{k})k_ik_l|=0 \tag{4}$$

here $\hat{\alpha}(\boldsymbol{k})$ denotes the Fourier transformed kernel. The phonon dispersion relation relating the angular frequency ω and the wave number $k=\|\boldsymbol{k}\|$ is given by Eq. (4). For isotropic case ($C_{ijk\ell}=\lambda\delta_{ij}\delta_{k\ell}+\mu(\delta_{ik}\delta_{j\ell}+\delta_{i\ell}\delta_{jk})$) in which λ and μ denote the Lame' constants, the above equation reduces to the following:

$$\rho\,\omega^2=(\lambda+2\mu)\,\hat{\alpha}(\boldsymbol{k})\,k^2 \quad \text{for longitudinal waves}$$
$$\rho\,\omega^2=\mu\,\hat{\alpha}(\boldsymbol{k})\,k^2 \quad \text{for transverse waves}$$

As described previously, in a local continuum, the kernel is a delta function ($\hat{\alpha}(\boldsymbol{k})=1$) in which case the phase velocity (ω/k) does not depend on the wave vector k. For a non-local continuum, the kernel $\hat{\alpha}(\boldsymbol{k})$ provides the means to capture the non linear dependence of phase velocity on the wave vector. In addition, for an isotropic medium, the kernel function does not depend on the mode of wave propagation. This is seen by rewriting the above equation as:

$$\frac{\rho\,\omega_{\mathrm{L}}^2}{\lambda+2\mu}=\frac{\rho\,\omega_{\mathrm{T}}^2}{\mu}=\hat{\alpha}(\boldsymbol{k})\,k^2$$

Here, the subscripts L and T demotes the longitudinal and transverse waves respectively. Phonon dispersion data can be obtained either experimentally or through molecular simulation. The following section assumes that the phonon dispersion is known and focuses on obtaining the two-dimensional (2D) and three-dimensional (3D) kernel in real space ($\alpha_{3D}(\boldsymbol{x})$) from one-dimensional (1D) kernel in reciprocal space ($\hat{\alpha}_{1D}(\boldsymbol{k})$) found by fitting Eq. (4) to the phonon dispersion data.

3. Construction of multidimensional isotropic kernels

Kernel functions needed for 1D elasticity models are even functions, hence can simply be obtained by Fourier-cosine transform of the $\hat{\alpha}_{1D}$. While in 1D, the isotropy induces merely the evenness of the kernel, in 2D and 3D it also induces rotational symmetry, i.e., the $\alpha_{2D}(\boldsymbol{x})$ and $\alpha_{3D}(\boldsymbol{x})$ should have cylindrical and spherical symmetries respectively. The most natural way to build scalar functions on a 3D