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# Lagrangian formulation of continuum with internal long-range interactions

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**Abstract** Based on a new definition of nonlocal variable, this paper establishes the Lagrangian formulation for continuum with internal long-range interactions. Distinguished from the existing theories, the nonlocal term in the Lagrangian formulation automatically satisfies the zero mean condition determined by the action and reaction law. By this formulation, elastic wave in a rod with the internal long-range interactions is investigated. The dispersion of the elastic wave is predicted.  [doi:10.1063/2.1104206]

**Keywords** nonlocal mechanics, Lagrangian formulation, long-range interactions, physically-based nonlocal model

The origin of nonlocality is due to the long-range interactions within material. This idea was first advanced by Kroner,[1] and then systematically developed into the nonlocal mechanics theory.[2–6] So far, the nonlocal mechanics theory has been applied to account for some phenomena which are not explained by the classical elasticity and plasticity, such as stress singularity at the crack tip, softening bands in tensile specimens and dispersion of acoustic waves in solids, etc. With the development of nanotechnology, considerable interests to the nonlocal mechanics are once again excited.[7–9] This is due to the advantage that nonlocal models not only involve the long-range interactions within material but also exclude the limitation of the molecular dynamics in length and time scale.

Recently, Paola et al.[10,11] proposed a physically-based nonlocal model in which the long-range interactions among non-adjacent volume elements are incorporated into the balance equation. As shown in Fig. 1, consider a rod with the internal long-range interactions. The length and cross-section area of the rod are $l$ and $A$, respectively. Imagine the rod being equally divided into $n$ elements, so that the volume of every element (e.g., the $i$th element) is $\Delta V_i = A\Delta x_i$, where $\Delta x_i = l/n$. Let $R_{ij}$ be the long-range action exerted by $\Delta V_j$ on $\Delta V_i$. In terms of the proposal advanced by Paola et al.,[10,11] $R_{ij}$ is expressed as

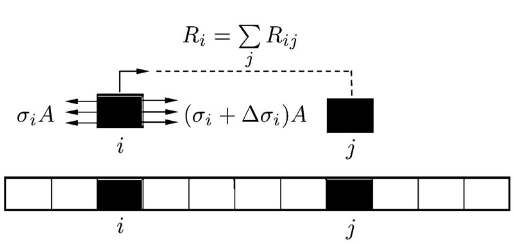


Fig. 1. A rod model with the internal long-range interactions

$$R_{ij} = g(|x_i - x_j|)(u_j - u_i)\Delta V_j \Delta V_i, \tag{1}$$

where $u_i$ and $u_j$ are the displacement of the $\Delta V_i$ and $\Delta V_j$, respectively. $g(|x_j - x_i|)$ is a weight function depending on the distance between these two elements. So the total long-range action exerted by the other elements on $i$th element can be written as

$$\begin{aligned} R_i &= \sum_{j=1}^{n} R_{ij} \\ &= A^2 \Delta x_i \sum_{j=1}^{n} g(|x_i - x_j|)(u_j - u_i)\Delta x_j. \end{aligned} \tag{2}$$

All loads applied on the $\Delta V_i$ include external body force $f_i$, the internal long-range action $R_i$ and the contact forces $\sigma_i A$ and $(\sigma_i + \triangle\sigma_i)A$ exerted respectively by the adjacent elements $V_{i-1}$ and $V_{i+1}$ on $V_i$. The Newton's law states that

$$\begin{aligned} &(\sigma_i + \Delta\sigma_i)A - \sigma_i A + \rho A \Delta x_i f_i + \\ &A^2 \Delta x_i \sum_{j=1}^{n} g(|x_i - x_j|)(u_j - u_i)\Delta x_j \\ = \ &\rho A \Delta x_i \ddot{u}_i. \end{aligned} \tag{3}$$

Let $n \to \infty$, then Eq. (3) will lead to

$$\frac{\partial \sigma}{\partial x} + \rho f + A\int_0^l g(|x-y|)[u(y) - u(x)]\mathrm{d}y = \rho \ddot{u}(x). \tag{4}$$

In Eq. (4), let

$$R = A\int_0^l g(|x-y|)[u(y) - u(x)]\mathrm{d}y, \tag{5}$$

which characterizes the long-range interactions within the rod. Clearly, If the size of representative element is far larger than the action scope of the long-range interactions, then $R$ is negligible. However, when entering

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micro/nano scale, $R$ will become one of main factors to govern the physical behaviors of materials. The effects of the internal long-range interactions have been observed in experiment.[5] Recently, the first-principle calculations also show the existence of long-range interactions within materials.[13]

According to the action and reaction law, the sum of all internal forces within a system should be zero. This is the so-called zero mean condition. It is easy to be certified by Eq. (5) that the integral of $R$ on $[0, l]$ is equal to zero. So $R$ satisfies the zero mean condition. By means of Eq. (5) and the Hooke's law ($\sigma = E(\partial u/\partial x)$), Eq. (4) becomes

$$E\frac{\partial^2 u}{\partial x^2} + \rho f + R = \rho \ddot{u}. \tag{6}$$

We find that Eq. (6) can be given by the Hamilton's principle provided by the Lagrangian density function $L$ takes the form below

$$L = \frac{1}{2}\rho(\dot{u})^2 - \frac{1}{2}E\left(\frac{\partial u}{\partial x}\right)^2 - \frac{1}{2}Ru - fu. \tag{7}$$

This idea will be expanded into a general theory latter.

Let a continuum occupy the domain $\boldsymbol{\Omega}$ in the three-dimensional Euclidean space, and every particle in the continuum be referred to a group of the orthogonal Cartesian coordinates $\boldsymbol{x} = \{x^1, x^2, x^3\}$ specifying its position in $\boldsymbol{\Omega}$. The function $\varphi = \varphi(t, x)$ denotes a field variable defined on $\boldsymbol{\Omega}$. Depending on circumstances, $\varphi$ is a scalar, vector or tensor. Similar to Eq. (5), the nonlocal variable of $\varphi$ is defined as

$$\begin{aligned}\langle\varphi\rangle \;=\; & \varphi(t,\boldsymbol{x})\int_{\boldsymbol{\Omega}} g(|\boldsymbol{x}-\boldsymbol{y}|)\mathrm{d}v(\boldsymbol{y}) - \\ & \int_{\boldsymbol{\Omega}} g(|\boldsymbol{x}-\boldsymbol{y}|)\varphi(t,\boldsymbol{y})\mathrm{d}v(\boldsymbol{y}).\end{aligned} \tag{8}$$

Let $L = L(t, x, \varphi, \dot{\varphi}, \varphi_{,k}, \langle\varphi\rangle)$ ($k = 1-3$). If necessary, the nonlocal variables $\langle\dot{\varphi}\rangle$ and $\langle\varphi_{,k}\rangle$ may be conveniently inserted into $L$. But in this case, the boundary conditions will become complicated. Then the action functional of $\varphi$ reads

$$A[\varphi] = \int_{t_0}^{t_1}\int_{\boldsymbol{\Omega}} L(t,\boldsymbol{x},\varphi,\dot{\varphi},\varphi_{,k},\langle\varphi\rangle)\mathrm{d}v(\boldsymbol{x})\mathrm{d}t. \tag{9}$$

By means of Eq. (9), the first variation of the action functional is written as

$$\begin{aligned}&\delta A[\varphi] \\ &= \int_{t_0}^{t_1}\int_{\boldsymbol{\Omega}}\left(\frac{\partial L}{\partial\varphi}\delta\varphi + \frac{\partial L}{\partial\dot{\varphi}}\delta\dot{\varphi} + \frac{\partial L}{\partial\varphi_{,k}}\delta\varphi_{,k} + \right. \\ &\left.\frac{\partial L}{\partial\langle\varphi\rangle}\delta\langle\varphi\rangle\right)\mathrm{d}v(\boldsymbol{x})\mathrm{d}t \\ &= \int_{t_0}^{t_1}\int_{\boldsymbol{\Omega}}\left[\frac{\partial L}{\partial\varphi} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\varphi}}\right) - \right. \\ &\left.\left(\frac{\partial L}{\partial\varphi_{,k}}\right)_{,k}\right]\delta\varphi\mathrm{d}v(\boldsymbol{x})\mathrm{d}t + \\ &\int_{\boldsymbol{\Omega}}\frac{\partial L}{\partial\dot{\varphi}}\delta\varphi\Big|_{t_0}^{t_1}\mathrm{d}v(\boldsymbol{x}) + \\ &\int_{t_0}^{t_1}\int_{\partial\boldsymbol{\Omega}}\frac{\partial L}{\partial\varphi_{,k}}n_k\delta\varphi\mathrm{d}s(\boldsymbol{x})\mathrm{d}t + \\ &\int_{t_0}^{t_1}\int_{\boldsymbol{\Omega}}\frac{\partial L}{\partial\langle\varphi\rangle}\delta\langle\varphi\rangle\mathrm{d}v(\boldsymbol{x})\mathrm{d}t,\end{aligned} \tag{10}$$

where $\partial\boldsymbol{\Omega}$ is the boundary surface of $\boldsymbol{\Omega}$ and $n_k$ denotes the unit normal vector on $\partial\boldsymbol{\Omega}$. It is easy to calculate that

$$\int_{\boldsymbol{\Omega}}\frac{\partial L}{\partial\langle\varphi\rangle}\delta\langle\varphi\rangle\mathrm{d}v(\boldsymbol{x}) = \int_{\boldsymbol{\Omega}}\left\langle\frac{\partial L}{\partial\langle\varphi\rangle}\right\rangle\delta\varphi\mathrm{d}v(\boldsymbol{x}). \tag{11}$$

Here, a shortened form similar to Eq. (8) is used,

$$\begin{aligned}\left\langle\frac{\partial L}{\partial\langle\varphi\rangle}\right\rangle \;=\; & \frac{\partial L}{\partial\langle\varphi\rangle}\int_{\boldsymbol{\Omega}} g(|\boldsymbol{x}-\boldsymbol{y}|)\mathrm{d}v(\boldsymbol{y}) - \\ & \int_{\boldsymbol{\Omega}} g(|\boldsymbol{x}-\boldsymbol{y}|)\frac{\partial L}{\partial\langle\varphi\rangle}\mathrm{d}v(\boldsymbol{y}).\end{aligned} \tag{12}$$

Substituting Eq. (11) into Eq. (10) leads to

$$\begin{aligned}&\delta A[\varphi] \\ &= \int_{t_0}^{t_1}\int_{\boldsymbol{\Omega}}\left[\frac{\partial L}{\partial\varphi} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\varphi}}\right) - \left(\frac{\partial L}{\partial\varphi_{,k}}\right)_{,k} + \right. \\ &\left.\left\langle\frac{\partial L}{\partial\langle\varphi\rangle}\right\rangle\right]\delta\varphi\mathrm{d}v(\boldsymbol{x})\mathrm{d}t + \int_{\boldsymbol{\Omega}}\frac{\partial L}{\partial\dot{\varphi}}\delta\varphi\Big|_{t_0}^{t_1}\mathrm{d}v(\boldsymbol{x}) + \\ &\int_{t_0}^{t_1}\int_{\partial\boldsymbol{\Omega}}\frac{\partial L}{\partial\varphi_{,k}}n_k\delta\varphi\mathrm{d}s(\boldsymbol{x})\mathrm{d}t.\end{aligned} \tag{13}$$

Let $\partial\boldsymbol{\Omega} = \partial\boldsymbol{\Omega}_1 \cup \partial\boldsymbol{\Omega}_2$, $\partial\boldsymbol{\Omega}_1 \cap \partial\boldsymbol{\Omega}_2 = \emptyset$. On $\partial\boldsymbol{\Omega}_1$, $\varphi$ takes a given value $\bar{\varphi}$. So the boundary condition on $\partial\boldsymbol{\Omega}_1$ reads

$$\varphi|_{\partial\boldsymbol{\Omega}_1} = \bar{\varphi}. \tag{14}$$

At the initial and terminal time, we have

$$\varphi|_{t_0} = \bar{\varphi}_0, \quad \varphi|_{t_1} = \bar{\varphi}_1. \tag{15}$$

Due to Eq. (14), $\delta\varphi = 0$ on $\partial\boldsymbol{\Omega}_1$. Similarly, $\delta\varphi = 0$ at the initial and terminal time because of Eq. (15). Thus, Eq. (13) reduces to

$$\begin{aligned}&\delta A[\varphi]\\&=\int_{t_0}^{t_1}\int_{\boldsymbol{\Omega}}\left[\frac{\partial L}{\partial\varphi}-\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\varphi}}\right)-\left(\frac{\partial L}{\partial\varphi_{,k}}\right)_{,k}+\right.\\&\left.\left\langle\frac{\partial L}{\partial\langle\varphi\rangle}\right\rangle\right]\delta\varphi\mathrm{d}v(\boldsymbol{x})\mathrm{d}t+\\&\int_{t_0}^{t_1}\int_{\partial\boldsymbol{\Omega}_2}\frac{\partial L}{\partial\varphi_{,k}}n_k\delta\varphi\mathrm{d}s(\boldsymbol{x})\mathrm{d}t.\end{aligned}\tag{16}$$

In terms of the Hamilton's principle, we have $\delta A[\varphi]=0$. So in Eq. (16), the fundamental lemma of variation yields the below results:

(1) Euler-Lagrangian equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{\varphi}}\right)+\left(\frac{\partial L}{\partial\varphi_{,k}}\right)_{,k}-\frac{\partial L}{\partial\varphi}=\left\langle\frac{\partial L}{\partial\langle\varphi\rangle}\right\rangle.\tag{17}$$

(2) Natural boundary condition

$$\left.\frac{\partial L}{\partial\varphi_{,k}}n_k\right|_{\partial\boldsymbol{\Omega}_2}=0.\tag{18}$$

Equation (17) is also called the nonlocal Euler-Lagrangian equation. Its right-side term is the nonlocal term, called the nonlocal traction.

According to Eq. (12), it is easy to verify that the nonlocal traction satisfies the following zero mean condition

$$\int_{\boldsymbol{\Omega}}\left\langle\frac{\partial L}{\partial\langle\varphi\rangle}\right\rangle\mathrm{d}v(\boldsymbol{x})=0.\tag{19}$$

In the existing nonlocal Lagrangian formulations,[5,12] the nonlocal term fails to satisfy the zero mean condition. So Eq. (19) represents a notable difference between Eq. (17) and the other theories. Due to Eq. (19), the integral of Eq. (17) over $\boldsymbol{\Omega}$ has the same expression as the ordinary Euler-Lagrangian equation.

Consider wave in an infinitely long rod with the internal long-range interactions. Let

$$L=\frac{1}{2}\rho\dot{u}^2-\frac{1}{2}E\left(\frac{\partial u}{\partial x}\right)^2-\frac{1}{2}\langle u\rangle u,\tag{20}$$

where

$$\langle u\rangle=\int_{-\infty}^{\infty}g(|x-y|)[u(x)-u(y)]\mathrm{d}y.\tag{21}$$

Substituting Eq. (20) into Eq. (17), we have the following wave equation

$$E\frac{\partial^2u}{\partial x^2}-\rho\frac{\partial^2u}{\partial t^2}=\int_{-\infty}^{\infty}g(|x-y|)[u(x)-u(y)]\mathrm{d}y.\tag{22}$$

Let $u=f(x)\mathrm{e}^{-\mathrm{i}\omega t}$. Then Eq. (22) reduces to

$$\begin{aligned}&E\frac{\mathrm{d}^2f}{\mathrm{d}x^2}+\rho\omega^2f(x)\\&=\int_{-\infty}^{\infty}g(|\,x-y\,|)[f(x)-f(y)]\mathrm{d}y.\end{aligned}\tag{23}$$

Taking the Fourier transform of Eq. (23), we obtain the following dispersion relation

$$\frac{\omega}{c}=\pm\sqrt{k^2+\frac{1}{E}[\bar{g}(0)-\bar{g}(k)]},\tag{24}$$

where $\bar{g}(k)$ denotes the Fourier transforms of $g(|x|)$, $k$ is the wave number, $c=\sqrt{E/\rho}$ is the wave velocity. If the internal long-range interactions within material are prescribed by the Morse potential, i.e.,

$$g(|x|)=a[\exp(-2r|x|)-2\exp(-r|x|)],\tag{25}$$

then Eq. (24) leads to

$$\frac{\omega}{c}=\pm\sqrt{k^2+6\sqrt{\frac{2}{\pi}}\frac{a}{E}\left[\frac{r^3}{(k^2+4r^2)(k^2+r^2)}-\frac{1}{4r}\right]}.\tag{26}$$

The dispersion curve determined by Eq. (26) is shown in Fig. 2, which predicts the dispersion of elastic wave due to the internal long-range interactions within material. This dispersion possibly occurs in nano-structures, but it awaits further verification.

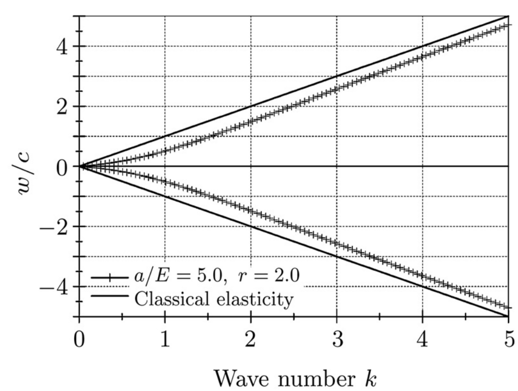


Fig. 2. Dispersion of elastic wave due to the internal long-range interactions.

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