A Wavelet-Galerkin Method for a 1D Elastic Continuum with Long-Range Interactions

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Keywords: Non-local elasticity, long-range interactions, weak formulation of elasticity, fractional calculus.

SUMMARY. An elastic continuum model with long-range forces is addressed in this study. The model stems from a physically-based approach to non-local mechanics where non-adjacent volume elements exchange mutual central forces that depend on the relative displacement and on the product between the interacting volume elements; further, they are taken as proportional to a material dependent and distance-decaying function. Smooth-decay functions lead to integro-differential equations while hypersingular, fractional-decay functions lead to a fractional differential equation of Marchaud type. In both cases the governing equations are solved by the Galerkin method with different sets of basis functions, among which also discrete wavelets are used. Numerical applications confirm the accuracy of the Galerkin solution as compared to finite difference solutions.

1 INTRODUCTION

In the last decades experimental results that cannot be explained by classical local continuum mechanics have forced scientists and engineers to formulate alternative theories which may better fit to observed phenomena. These include shear bands in tensile specimens, acoustic wave dispersion in granular materials, softening phenomena and smoothing effects of concentrated stress at crack tips.

It is generally believed that most of these phenomena may be given an exhaustive explanation at a micro-structural level and then, since the end of the fifties, a first approach to this problem has been framed in the context of atomic theory and lattice mechanics. However, the strong computational effort involved by the use of such theories have soon motivated an increasing interest towards continuum formulations where microstructural effects are accounted for by properly modified constitutive relations, including non-local terms as weighted integrals [1,2] or gradients [3,4]. These approaches enjoy the beauty of a constitutive relation that does not involve additional state variables of the elastic problem. On the other hand, approaches involving non-local weighted integrals lead to non-convex potential energy functions, while approaches involving non-local gradients may experience inherent difficulties in deriving the boundary conditions. As an alternative to modified constitutive relations, microstructural effects have been accounted for in the equilibrium equation (i) by including non-local forces in an integral form [5,6]; (ii) by the so-called continualization, where a continuum model is built based on higher-

order differential operators ensuring that the continuum behavior approximates the behavior of the discrete lattice [7-9].

Recently, a non-local continuum model has been proposed for a 1D bar using a physically-based approach [10,11]. The 1D bar has been modelled as the continuum limit of a discrete ensemble of distinct volume elements. Adjacent elements exert mutual classical contact forces while non-adjacent elements exert mutual, central and distance-decaying forces. The latter are taken to be proportional to the interacting volumes and to their relative displacement. As the size of the volume elements reduces to zero, the resulting 1D continuum is found to be governed by an integro-differential equation for long-range forces with a smooth decay or by a fractional differential equation for long-range forces with a fractional decay. In both cases either mechanical or kinematic boundary conditions may be consistently enforced. It may be also shown that the physically-based approach enjoys all the features of the elasticity theory since the pertinent elastic potential energy is convex and positive definite.

The solution to the integro-differential equation has been built based on a standard finite difference (FD) method, suggested by the underlying physical model of distinct volume elements itself [11]. Similarly, a fractional finite difference (FFD) method [12] has been adopted to solve the fractional differential equation [10]. However, in both cases all the advantages of the continuum representation are lost since, depending on the problem at hand, a relevant number of volume elements may be required to attain convergence and at the expense, obviously, of an increasing computational effort. This may be typically the case not only of statics but also of dynamics applications where, for instance, constructing the eigensolution of large size matrices does involve significant computational costs.

In this study the authors aim to show that the solution for the non-local bar proposed in ref. [10,11], when long-range forces feature either a smooth or a fractional decay, may be constructed by a well-known approximate method of classical elasticity theory such as the Galerkin method, formulated based on principle of virtual displacements. The results prove that accurate solutions to the non-local bar may be built in a continuum setting, without resorting to a back-discretization of the governing equations.

The mechanics of the non-local bar is described in Section 2. The formulation of the Galerkin method is given in section 3. Numerical results are presented in Section 4, where the FD and the FFD solutions are used as benchmark solutions.

2 THE MODEL

Let us introduce a discrete model of the bar consisting of n small finite volumes $V_j=A\Delta x$, where A is the cross sectional area, $\Delta x=L/n$ and L is the length. Any volume V_j is in equilibrium under the external body force $f_jA\Delta x$, where $f_j=f(x_j)$, being $x_j=(2j-1)\Delta x/2$ (j = 1,2,…, n), N_j-1 and N_j are the axial contact forces exerted by the adjacent volumes V_{j-1} and V_{j+1}, respectively. Further, within the theoretical framework of continuum mechanics with long-range forces, it may be consistently assumed that any volume V_j is acted upon by the resultant Q_j of long-range forces due to surrounding, non-adjacent volume elements. Specifically, Q_j is taken as the resultant of long-range central forces applied to the centroid of the volume elements (see Fig. 1), given by:

$$Q_j = \sum_{h=j+1}^{n} Q^{(h,j)} + \sum_{h=1}^{j-1} Q^{(h,j)} \tag{1}$$

where $Q^{(h,j)} = q^{(h,j)} V_h V_j = q^{(j,h)} V_h V_j$, being $q^{(h,j)}$

$$q^{(h,j)} = \left[u\left(x_h\right) - u\left(x_j\right) \right] g\left(x_h, x_j\right), \quad \text{for } g\left(x_h, x_j\right) = g\left(\left| x_h - x_j \right|\right). \tag{2}$$

Specifically, $g(x_h,x_j)$ is an appropriate material-dependent and distance-decaying positive function, taken to be monotonically decreasing.

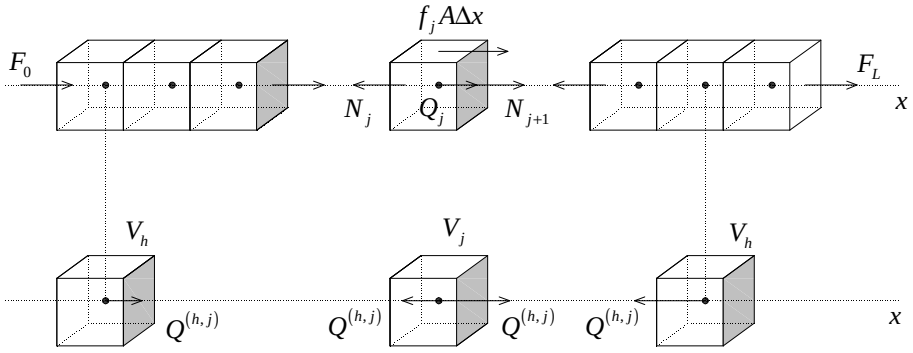

Figure 1: Equilibrium of the volume element V_j in the discretized non-local bar.

The static equilibrium equation of the volume element V_j in Fig. 1 is then written as

$$\Delta N_j + Q_j + f_j A\Delta x = \Delta N_j + \sum_{h=j+1}^{n} q^{(h,j)} \left(A\Delta x\right)^2 + \sum_{h=1}^{j-1} q^{(h,j)} \left(A\Delta x\right)^2 + f_j A\Delta x = 0 \tag{3}$$

where $\Delta N_j = N_j - N_{j-1}$. Dividing Eq.(3) by $A\Delta x$ and letting $\Delta x \longrightarrow 0$ yields the equilibrium equation of the 1D non-local bar in the form

$$\frac{d\sigma_l\left(x\right)}{dx} + A\int_0^L q\left(x,\xi\right) d\xi = -f\left(x\right), \qquad \text{for } q\left(x,\xi\right) = \eta\left(x,\xi\right) g\left(x,\xi\right) \tag{4}$$

where $\eta(x,\xi)=u(\xi)-u(x)$; $\sigma_l(x)=N(x)/A$ is the local stress due to the contact forces (i.e., the Cauchy stress) and the integral terms in Eq.(4) are the resultants (per unit volume) of the long-range forces due, respectively, to the volume elements to the right and to the left of the location x. Based on the resultant non-local stress $\sigma_{nl}(x)$, given as

$$\sigma_{nl}\left(x\right) = A\int_{\xi=x}^{L}\int_{\varsigma=0}^{x} q\left(\xi,\varsigma\right) d\xi d\varsigma \tag{5}$$

it may be proved that Eq.(4) reverts to

$$\frac{d\sigma\left(x\right)}{dx} = \frac{d\sigma_l\left(x\right)}{dx} + \frac{d\sigma_{nl}\left(x\right)}{dx} = -f\left(x\right) \tag{6}$$

where $\sigma(x)=\sigma_l(x)+\sigma_{nl}(x)$ is the overall axial stress. It has to be remarked that the resultant non-local stress in Eq.(5) is obtained by cutting the bar into two parts and evaluating the resultant of the long-range forces exchanged by the volume elements to the right and to the left of the location x.

The solution for the non-local bar is sought based on the equilibrium equation (6) along with pertinent compatibility and constitutive equations. They summarize as follows:

$$\frac{d\sigma(x)}{dx}=\frac{d\sigma_l(x)}{dx}+A\int_0^L q(x,\xi)\,d\xi=-f(x)$$
$$\frac{du(x)}{dx}=\varepsilon(x);\quad \eta(x,\xi)=u(\xi)-u(x) \tag{7a-c}$$
$$\sigma(x)=\sigma_l(x)+\sigma_{nl}(x)=\bar{E}(x)\varepsilon(x)+A\int_{\xi=x}^{L}\int_{\varsigma=0}^{x} g(\xi,\varsigma)\left[u(\xi)-u(\varsigma)\right]d\xi d\varsigma$$

Note that in Eq.(7c) the constitutive equation for the local stress $\sigma_l(x)$ in terms of the strain $\varepsilon(x)$ is taken as $\sigma_l(x)=\bar{E}\varepsilon(x)$, for $\bar{E}=\beta_1 E$, being β_1 a positive dimensionless constant introduced, as in the integral model of non-local elasticity [13], to weigh the amount of local stress. The latter Eq.(7d) represents the constitutive equation relating the local and non-local contribution to the overall stress. Also it is to be observed that the contribution provided by long-range forces at the location x is in integral form and, for this, interactions between all volume elements of the solid are accounted for (to the left and to the right of the location x). This consideration is necessary since it is to be used to specify the static boundary conditions associated to the elastic problem,

$$u(0)=u_0;\quad u(L)=u_L \tag{8a,b}$$

$$\sigma(0)A=\sigma_l(0)A=-F_0;\quad \sigma(L)A=\sigma_l(L)A=F_L \tag{9a,b}$$

where F_0 and F_L are the end forces at x=0 and x=L, respectively. Further recognize that, in Eqs.(9), $\sigma_l(0)=\sigma_{nl}(L)=0$ as it may be derived from Eq.(7c).

Based on Eqs.(7), the governing equation may be rewritten in terms of displacement as

$$\bar{E}\frac{d^2u(x)}{dx^2}+A\int_0^L\left[u(\xi)-u(x)\right]g\left(|x-\xi|\right)d\xi=-f(x) \tag{10}$$

For completeness it is noted that, based on the same reasoning followed above, Eq.(10) generalizes for an infinite bar in the form

$$\bar{E}\frac{d^2u(x)}{dx^2}+A\int_{-\infty}^{\infty}\left[u(\xi)-u(x)\right]g\left(|x-\xi|\right)d\xi=-f(x) \tag{11}$$

Now it is worth pointing out that Eq.(10) and Eq.(11) involve an integral term analogous to the integral term accounting for long-range forces in a peridynamic bar [6]. However Eq.(10) and Eq.(11) are integro-differential equations and, due to the differential term, they yield continuous displacement fields under concentrated forces. This is not the case in the peridynamic solution [6].

Next some further comments are made about the specific functional class to adopt for the distance-decaying function $g\left(\left|x-\xi\right|\right)$. It may be chosen as a smooth function without singularities (like Gaussian-type or continuous with an isolated discontinuity like the exponential decay) so that Eq.(10) is an integro-differential equation. On the other hand an attractive choice for the distance decaying function is related to the fractional power-law decay

$$g\left(\left|x-\xi\right|\right)=\frac{\beta_2 E\alpha}{A^2\Gamma\left(1-\alpha\right)}\frac{c_\alpha}{\left|x-\xi\right|^{1+\alpha}} \tag{12}$$

that may prove appropriate for materials involving long-range interactions at a molecular level such as electrostatic, long-range elastic bonds in next to the nearest next (NNN) lattices or magnetic forces as Lorentz forces. More details about such a power-law decay of the long-range interactions may be found in very recent literature [14]. Specifically, in Eq.(12) $\Gamma(\bullet)$ is the Euler-Gamma function; α is a real, material-dependent parameter ruling the decay of the interactions, being $0\leq\alpha\leq1$; c_α is a dimensional coefficient of fractional order, $[c_\alpha]=L^\alpha$ also depending on the material; $\beta_2=1-\beta_1$ is a positive dimensionless constant introduced, as in the integral model of non-local elasticity [13], to weigh the amount of non-local stress. This kind of distance-decaying function, if replaced for $g\left(\left|x-\xi\right|\right)$ into Eq.(11), yields an hypersingular kernel that coincides with the sum of Marchaud left and right fractional derivatives, leading to the second-order fractional differential equation [10]

$$\bar{E}\frac{d^2u\left(x\right)}{dx^2}-C_\alpha\left[\left(\mathbf{D}_{-}^{\alpha}u\right)\left(x\right)+\left(\mathbf{D}_{+}^{\alpha}u\right)\left(x\right)\right]=-f\left(x\right) \tag{13}$$

where $C_\alpha=\beta_2 E c_\alpha/A^2$. In Eq.(13), the left and right Marchaud fractional derivatives are defined as the convolution integrals (for details about fractional calculus see ref. [15])

$$\left(\mathbf{D}_{-}^{\alpha}u\right)\left(x\right)=\frac{\alpha}{\Gamma\left(1-\alpha\right)}\int_{-\infty}^{x}\frac{u\left(x\right)-u\left(\xi\right)}{\left(x-\xi\right)^{1+\alpha}}d\xi;\quad \left(\mathbf{D}_{+}^{\alpha}u\right)\left(x\right)=\frac{\alpha}{\Gamma\left(1-\alpha\right)}\int_{x}^{\infty}\frac{u\left(x\right)-u\left(\xi\right)}{\left(\xi-x\right)^{1+\alpha}}d\xi \tag{14}$$

For a finite domain such a correspondence between hypersingular kernels and fractional operators does not hold and the governing equation of the axial displacement is obtained in terms of the truncated Marchaud operators in the form

$$\bar{E}\frac{d^2u\left(x\right)}{dx^2}-C_\alpha\left[\left(\hat{\mathbf{D}}_{0^+}^{\alpha}u\right)\left(x\right)+\left(\hat{\mathbf{D}}_{L^-}^{\alpha}u\right)\left(x\right)\right]=-f\left(x\right) \tag{15}$$

where the truncated Marchaud operator represents the integral terms in the Marchaud fractional derivative on a finite domain, defined as

$$\left(\mathbf{D}_{0^+}^{\alpha}u\right)(x)=\frac{\alpha}{\Gamma(1-\alpha)}\int_0^x\frac{u(x)-u(\xi)}{(x-\xi)^{1+\alpha}}d\xi+\frac{1}{\Gamma(1-\alpha)}\frac{u(x)}{x^{\alpha}}=\left(\hat{\mathbf{D}}_{0^+}^{\alpha}u\right)(x)+\frac{1}{\Gamma(1-\alpha)}\frac{u(x)}{x^{\alpha}};$$

$$\left(\mathbf{D}_{+}^{\alpha}u\right)(x)=\frac{\alpha}{\Gamma(1-\alpha)}\int_x^L\frac{u(x)-u(\xi)}{(\xi-x)^{1+\alpha}}d\xi+\frac{1}{\Gamma(1-\alpha)}\frac{u(x)}{(L-x)^{\alpha}}=\left(\hat{\mathbf{D}}_{L^-}^{\alpha}u\right)(x)+\frac{1}{\Gamma(1-\alpha)}\frac{u(x)}{(L-x)^{\alpha}} \tag{16a,b}$$

3 APPROXIMATE SOLUTIONS FOR THE NON-LOCAL CONTINUUM

To the authors' best knowledge, no exact, closed-form solution can be found for the axial displacement field $u(x)$ of the elastic problem formulated in Section 2; only some approximate solutions based on the FFD method [10] and the FD method [11] have been proposed. However such numerical solutions required, for accuracy reason, a very fine discretization grid thus leading to the need of developing alternative analytical approaches to the problem, as it will be pursued in the following Section.

3.1 The Galerkin solution

The Galerkin method to solve the elastic problem with long-range forces may be formulated by resorting to the principle of virtual displacements for the continuum with long-range forces, which may be written as

$$\begin{aligned}&\int_0^L\delta u(x)\left[\frac{d\sigma}{dx}+f(x)\right]Adx+\left[F_0+\sigma_l(0)A\right]\delta u(0)+\left[F_L-\sigma_l(L)A\right]\delta u(L)=\\&=\int_0^L\delta u(x)\left[\bar{E}\frac{d^2u}{dx^2}+A\int_0^L\left[u(\xi)-u(x)\right]g(|x-\xi|)d\xi+f(x)\right]Adx+\\&+\left[F_0+\sigma_l(0)A\right]\delta u(0)+\left[F_L-\sigma_l(L)A\right]\delta u(L)=0\end{aligned} \tag{17}$$

where $\delta u(x)$ is an arbitrary, but kinematically admissible, variation of the displacement field. Let us assume that the displacement field along the bar may be represented as

$$u(x)\cong\phi_i(x)c_i\quad(i=1,2,...,m) \tag{18}$$

where $\phi_i(x)$ are trial, real-valued functions satisfying the kinematic boundary conditions and c_i are real, unknown coefficients; also, the Einstein summation convention has been used for shortness. Replacing Eq.(18) for $u(x)$ in Eq.(17) yields

$$\begin{aligned}&\int_0^L\delta u(x)\left[\bar{E}c_i\frac{d^2\phi_i}{dx^2}+Ac_i\int_0^L\left[\phi_i(\xi)-\phi_i(x)\right]g(|x-\xi|)d\xi+f(x)\right]Adx+\\&+\left[F_0+\sigma_l(0)A\right]\delta u(0)+\left[F_L-\sigma_l(L)A\right]\delta u(L)=0\end{aligned} \tag{19}$$

The approximate form in Eq.(18) adopted for $u(x)$ does not allow to satisfy Eq.(17) for every choice of the variation $\delta u(x)$ so that the coefficients c_i in Eq.(18) may be evaluated by requiring

that the functional class of the variations of the displacement field coincides with the trial function, i.e. $\delta u(x)= \phi_j(x)$ (j=1,2,…,m). Eq.(19) may be further simplified by integration by parts of the first integral, which yields the following set of m algebraic equations in the m unknown coefficients c_i

$$\begin{aligned}&\int_0^L \bar{E}A\frac{d\phi_j}{dx}c_i\frac{d\phi_i}{dx}dx+\int_0^L\int_0^L \phi_j(x)\left[\phi_i(\xi)-\phi_i(x)\right]c_i g\left(|x-\xi|\right)A^2 d\xi dx = \\ &=\phi_j(L)F_L-\phi_j(0)F_0+\int_0^L f(x)\phi_j(x)dx\end{aligned} \tag{20}$$

The algebraic system of equations in Eq.(20) is cast in the matrix for

$$\mathbf{K}^{(G)}\mathbf{c}=\left(\mathbf{K}^{(G-l)}+\mathbf{K}^{(G-nl)}\right)\mathbf{c}=\mathbf{F} \tag{21}$$

where $\mathbf{K}^{(G)}$ is the stiffness matrix evaluated via the Galerkin approximation and the coefficient vector $\boldsymbol{c}^T$=[c_1,c_2,…,c_m]. The elements of the load vector, of the local stiffness matrix $\mathbf{K}^{(G-l)}$ and of the long-range interactions stiffness matrix $\mathbf{K}^{(G-nl)}$ are, respectively,

$$F_j=\phi_j(L)F_L-\phi_j(0)F_0+\int_0^L f(x)\phi_j(x)dx \tag{22a}$$

$$k_{ij}^{(G-l)}=\int_0^L \bar{E}A\frac{d\phi_i}{dx}\frac{d\phi_j}{dx}dx\ ;\ k_{ij}^{(G-nl)}=\int_0^L\int_0^L \phi_i(x)\left[\phi_j(\xi)-\phi_j(x)\right]g\left(|x-\xi|\right)A^2 d\xi dx \tag{22b,c}$$

The global stiffness matrix $\mathbf{K}^{(G)}$ is symmetric (it is readily seen in this case since $\delta u(x)=\phi_j(x)$ (j=1,2,…,m)) and positive definite. Then it may be inverted to derive the coefficient vector $\mathbf{c}$, based on which the solution (18) may be computed.

4 NUMERICAL RESULTS

Consider a clamped bar acted upon by two self-equilibrated point forces F applied at distance d from the bar ends. As a first case, the smooth exponential decay

$$g\left(|x-\xi|\right)=C\exp\left(-|x-\xi|/\lambda\right); \tag{23}$$

is assumed for the long-range forces, where λ is the internal length, that is the influence distance beyond which the non-local effects may be neglected [16], C is a coefficient weighing the non-local effects. The solution to the integro-differential equation (11) is built by the Galerkin method devised in Section 3. For comparison, different sets of basis functions are used: (i) the harmonic functions

$$\phi_i(x)=b^{-1/2}\sin\left(2i\pi x/L\right),\quad \text{for } b=\int_{-L/2}^{L/2}\sin^2\left(2i\pi x/L\right)dx \tag{24}$$

(ii) the Meyer scaling functions, defined in the frequency domain by the following relations [17]

$$\Phi(\omega) = 2\pi^{-1/2} \qquad \text{if} \quad |\omega| < 2\pi/3$$

$$\Phi(\omega) = 2\pi^{-1/2} \cos\left(\frac{\pi}{2} v\left(\frac{3}{2\pi}|\omega| - 1\right)\right) \qquad \text{if} \quad 2\pi/3 < |\omega| < 4\pi/3 \tag{25}$$

$$\Phi(\omega) = 0 \qquad \text{if} \quad |\omega| > 4\pi/3$$

for $v(y)=y^4(35-84y+70y^2-20y^3)$.

(iii) the db3 Daubechies scaling functions [17].

Note that a few wavelet-Galerkin solutions for differential and integro-differential equations already exist in the literature [18].

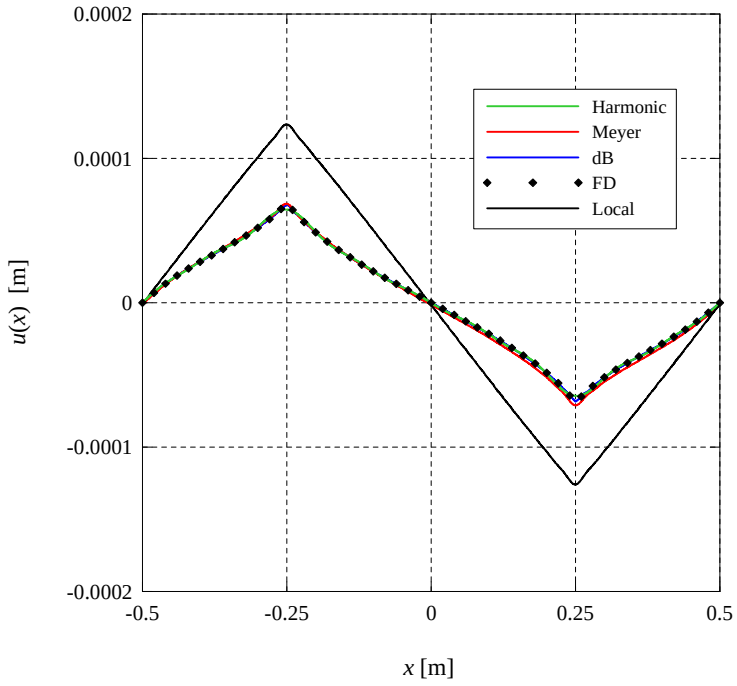

Figure 2: Displacement solution of a symmetrically-load bar.

The Galerkin solutions are compared to the FD solution constructed by discretizing the integro-differential equation (11) on a n-point grid. The Galerkin method and the FD method are all Matlab-coded and run on a Intel(R) Core(TM)2 Duo 2.10 GHz, where 0.001 sec is the CPU time resolution. Here results are presented for the following geometrical and mechanical parameters: A=1 cm^2, E=2.1×10^6 daNcm^{-2}, L=100 cm, F=10^3 daN and d=25 cm. Also, $\beta_1=\beta_2=0.5$; λ=10 cm in Eq.(23). Note that the numerical values for the above parameters are theoretical values chosen to enhance non-local effects in the response, case in which it appears more meaningful to

assess the matching between the solution strategies proposed in the paper. In general, however, they may be set based on experimental evidence.

Fig. 2 and Fig. 3 show the axial displacement and strain for $g\left(\left|x-\xi\right|\right)$ given as Eq.(23), when m=10 harmonic basis functions (24) are considered to build the Galerkin solution (i), the scale m=6 is selected for both the Meyer and Daubechies wavelet solutions, and n=4000 volume elements V_j are taken for the FD solution. In terms of displacement, it is seen that the Galerkin (i)-(ii)-(iii) and the FD solutions are in a good agreement. In terms of strain, the wavelet-Galerkin solution (ii)-(iii) prove slightly more accurate than the harmonic-Galerkin solution (i). Such result is expected due to the well-known localization properties of the wavelet functions, which appear particularly suitable when discontinuous fields as the strain field in Fig. 3 are involved. In general, it is worth remarking that the Galerkin solutions all prove more efficient than the FD solution since the required CPU times are equal to 7.1 sec for the Galerkin solution (i), 6.3 sec for the Galerkin solution (ii) 6.8 sec for the Galerkin solution (iii), and to 53.83 sec for the FD solution.

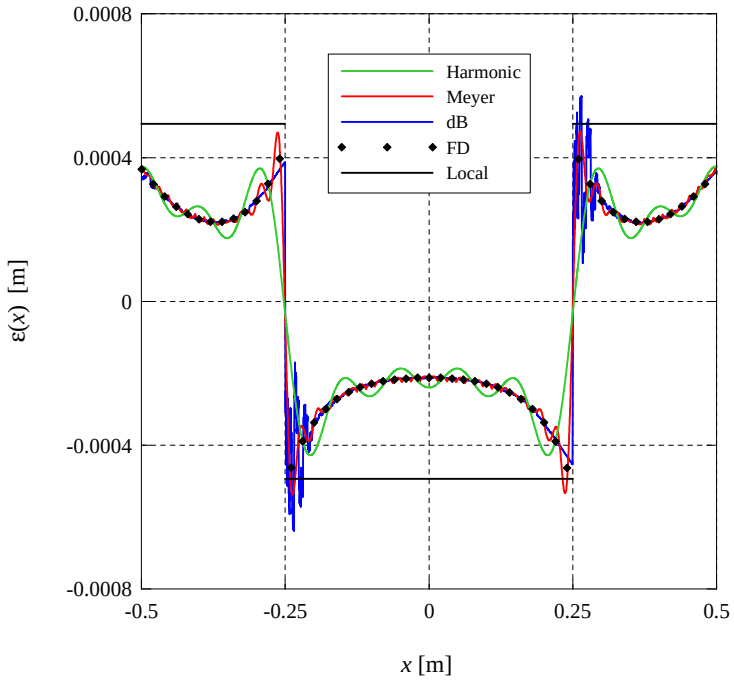

Figure 3: Strain solution of a symmetrically-load bar.

5 CONCLUSIONS

It has been shown that a classical method of linear elasticity theory, such as the Galerkin method, can be applied to solve a 1D non-local continuum bar recently proposed in the literature. In this manner accurate approximate solutions have been obtained, with a significant reduction of computational effort as compared to the numerical solutions previously built [10,11]. Among different sets of basis functions, wavelet-based Galerkin solutions have been found particularly suitable for capturing both displacement and strain fields.

It is worth remarking that the non-local elasticity model, here formulated and solved for a 1D

bar, lends itself to a straightforward generalization to 3D continua, based on the same concepts. A detailed formulation and pertinent numerical results will be presented in future self-contained studies.

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