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ON NONLOCAL MODELING IN CONTINUUM MECHANICS

ABSTRACT

The objective of the paper is to provide an overview of nonlocal formulations for models of elastic solids. The author presents the physical foundations for nonlocal theories of continuum mechanics, followed by various analytical and numerical techniques. The characteristics and range of practical applications for the presented approaches are discussed. The results of numerical simulations for the selected case studies are provided to demonstrate the properties of the described methods. The paper is illustrated with outcomes from peridynamic analyses. Fatigue and axial stretching were simulated to show the capabilities of the developed numerical tools.

Keywords: solid mechanics, long-range force interactions, nonlocal theory of elasticity, nonlocal modeling

MODELOWANIE NIELOKALNE W MECHANICE KONTINUUM

W artykule dokonano przeglądu nielokalnych sformułowań dla mechaniki bryły odkształcalnej. Autor przedstawia podstawy fizyczne nielokalnych teorii mechaniki kontinuum oraz dokonuje przeglądu technik analitycznych i numerycznych stosowanych w modelach matematycznych. W pracy przedyskutowano charakterystyki oraz zakres praktycznych zastosowań wspomnianych technik modelowania. Ocena własności nielokalnych modeli została przeprowadzana na podstawie wyników symulacji numerycznych dla wybranych typów analiz z zastosowaniem perydynamiki. Przedstawiono wyniki symulacji zmęczeniowych oraz jednoosiowego rozciągania, uzyskane przy użyciu opracowanych narzędzi analiz symulacyjnych.

Słowa kluczowe: mechanika ciała stałego, nielokalne siły interakcji, nielokalne sformułowanie teorii sprężystości, modelowanie nielokalne

1. INTRODUCTION

Foundations for the classical mechanics of continuum solid media refer to the theory of linear elasticity, which is governed by locally formulated relationships between stresses and strains. Although consequently applied for decades, this theory suffers from several incapacabilities with regards to the completeness of its description of the physical behavior of deformable solids observed at various length scales. To name a couple of such-related physical phenomena, shear bands while stretching and the dispersion of waves were unexpectedly discovered during the experiments, which cannot be derived from the classical formulations of solid mechanics (Eringen, Edelen 1972; Kaliski *et al.* 1992; Di Paola *et al.* 2010). Hence, alternative theories emerged to aim at avoiding the inconsistency between the theory and experiments, which made successful attempts to use the nonlocal formulation of elasticity (Kröner 1967; Kunin 1967; Eringen 1972).

Nonlocal components, which are considered in the governing equations, allow for the unique properties of an analytical or numerical model (Eringen 1972). First, a length scale can be explicitly introduced to ensure a more-physical behavior of the model. This property of the model applies to the phenomena, which manifest their presence at different geometric scales. Due to the

involved nonlocality, it is therefore feasible to address the contribution of microstructure in the resultant macro-scale continuous model (Kunin 1983; Chen *et al.* 2004; Di Paola *et al.* 2010). Second, the phenomenon of elastic wave propagation in deformable solids can be handled more accurately via the nonlocal approach without the need for a further increase of mesh density (Eringen 1972). Having introduced nonlocal interactions into a modeled structure, one can conveniently form the shape of the dispersion curves and surfaces (Martowicz *et al.* 2015a). Effectively, the model is considered as a periodic structure being investigated within the first Brillouin zone (Martowicz *et al.* 2014a). The theory of generalized continua also reflects the nonlocal properties of solids modeled as granular media at the micro-scale and nano-scale (Ostoja-Starzewski 2013). A similar approach was also adapted for upscaling techniques (Seleson *et al.* 2009).

The nonlocal modeling technique was extensively investigated in different research areas and for various physical domains. As reported, the nonlocal approach may efficiently reduce numerical dispersion, which is crucial for the proper determination of physical dispersion (Ghrist 2000; Tam, Webb 2011; Yang *et al.* 2012). Moreover, nonlocality opened up new perspectives for modeling evolving damages (Rodriguez-Ferran *et al.* 2004; Gunzburger, Lehoucq 2010), studying vibro-acoustic

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wave interaction (Martowicz *et al.* 2014c), and allowing us to regularize boundary value problems (Bazant, Jirasek 2002). Introducing nonlocal interactions increases the quality of a mesh by allowing for the more-spontaneous growth of a modeled crack (Hu *et al.* 2012). The nonlocal theory of elasticity was successfully applied to model graphene, via both the nonlocal finite element method (FEM) (Arash *et al.* 2012) and peridynamics (Martowicz *et al.* 2015b), piezoelectricity (Eringen 1984; Zhang *et al.* 2014), and shape memory alloys (Badnava *et al.* 2014), taking into account superelasticity (Duval *et al.* 2010). Nonlocal formulations for thermoelasticity are addressed in (Eringen 1974; Balta, Suhubi 1977), including some recent works (Chang, Wang 2015). The paper is organized as follows. After the introduction (which is given in the present section), Section 2 provides the physical foundations for nonlocal modeling, followed by both analytical and numerical methods (which are briefly described in Section 3). The results of numerical studies are presented and discussed in Section 4. Final conclusions are drawn in Section 5.

2. PHYSICAL FOUNDATIONS

The classical theory of elasticity does not make any references to the granular nature of physical matter. Hence, it prevents real long-range interactions, which are present at the nano-scale and micro-scale. A common and convenient approach within the classical approach is to homogenize the properties of the material over a finite domain and provide the resultant macro- and possibly meso-scale model, which is considered valid when subjected to long wave propagation (Eringen, Edelen 1972). The description of such a model involves local stress-strain relationships. However, the experimental works regarding dispersion curves for phonons propagating in metallic structures clearly state the necessity of introducing nonlocal formalisms into the governing equations (Eringen 1972).

If more-accurate (i.e., physical) descriptions are demanded in a model, and the phenomena observed at the nano- and micro-scales are expected to be accounted for, an alternative nonlocal theory should be adapted and used, as it reflects potential-based reactions (which are nonlocal by nature). This requirement seems crucial, especially for the studies on crack growth, fatigue, and acoustic emission. Ultimately, a modeled solid acts like a periodic granular media at the micro- and nano-scales (Martowicz *et al.* 2015b). The size effect may be effectively handled by a nonlocal model as well, and various shapes of the dispersion relationships may be recreated when the

model is subjected to the propagation of elastic waves of different lengths. The size of a neighboring area for the interacting pieces of a deformable body is tuned to assure the proper representation of the phenomena present at different length scales. This approach allows the microstructure's mechanisms to be included into the resultant behavior of a meso- or macro-scale model. The nonlocal modeling is accomplished by nonlocal formulations introduced into constitutive models, allowing us to handle the real deviations observed in the experiments due to the above-mentioned inner microstructure (Di Paola *et al.* 2010).

Nonlocality is a critical issue also in the case of modeling shape memory alloys. Only the proper selection of a neighboring area for long-range interactions during the martensitic phase transformation enables the modeling strain instabilities observed during the experiments (Duval *et al.* 2010). The size effect again plays an important role and should be considered in the modeling. In the following section, examples of nonlocal modeling approaches are briefly presented to show how the long-range interactions are considered.

3. ANALYTICAL AND NUMERICAL MODELING

There have been various approaches proposed to account for the nonlocality in the models of a solid body. Depending on the formulation of a given kernel function (which is used to introduce constitutive relationships), the following types of nonlocal governing equations – based on spatial integro-differential-based expressions – are considered in contrast to the classical local Cauchy problem:

- integro-differential-based function composition (Duruk *et al.* 2010):

$$\frac{\partial^2 u(x,t)}{\partial t^2} = \frac{\partial^2}{\partial x^2} \int_{\mathfrak{R}} \beta(x-\hat{x})g(u(\hat{x},t))d\hat{x} \quad (1)$$

where β is an integrable kernel function and g denotes a nonlinear function of displacement u for the considered one-dimensional case. x and \hat{x} are, respectively, the actual central and neighboring localizations for the interacting portions of a solid;

- integro-differential expression with a nonlocal formulation of the Cauchy problem (Eringen 1992):

$$\rho(x) \frac{\partial^2 \mathbf{u}(\mathbf{x},t)}{\partial t^2} = \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}(\mathbf{x},t)) + \mathbf{b}(\mathbf{x},t) \quad (2)$$

with a nonlocal formulation for stress tensor $\boldsymbol{\sigma}$; ρ and \mathbf{b} denote mass density and external body force, respectively;

- integro-differential expression proposed for a generic volume element in a one-dimensional case (Zingales 2011):

$$\rho(x)A(x)\frac{\partial^2 u(x,t)}{\partial t^2} - \frac{\partial}{\partial x} \left[E_{nl}(x)A(x)\frac{\partial u(x,t)}{\partial x} \right] + \int_a^b g(x,\xi)\eta(x,\xi,t)d\xi = A(x)f(x,t) \quad (3)$$

where A and E_{nl} are the cross-sectional area and Young's modulus, respectively; g is the kernel, which depends on a distance-decaying function; function η is the relative displacement determined at coordinates x and ξ , f denotes the external body force field;

- nonlocal integral formulation for peridynamics (Silling 2000):

$$\rho \frac{\partial^2 \mathbf{u}(\mathbf{x},t)}{\partial t^2} = \int_H \mathbf{f}(\mathbf{u}(\hat{\mathbf{x}},t) - \mathbf{u}(\mathbf{x},t), \hat{\mathbf{x}} - \mathbf{x}) dV_{\hat{\mathbf{x}}} + \mathbf{b}(\mathbf{x},t) \quad (4)$$

with pairwise force \mathbf{f} , which acts within finite domain H and depends on both the relative position $\hat{\mathbf{x}} - \mathbf{x}$ in the reference coordinate system and the relative displacement $\mathbf{u}(\hat{\mathbf{x}},t) - \mathbf{u}(\mathbf{x},t)$.

All of the above-mentioned expressions introduce nonlocal components that allow for an extended range of interacting forces within the modeled body. Hence, this approach makes a direct reference to the potential-based interactions for granular media as experimentally identified at the nano- and micro-scales. The similarity of these expressions to those applied for the nano- and micro-structures enables us to introduce specific, experimentally proven behavior that cannot be derived from the classical local Cauchy problem description for solids.

It should be noted that the peridynamics does not introduce spatial partial derivatives (in contrast to the remaining nonlocal approaches), which helps us avoid numerical inconveniences at the geometric discontinuities. Hence, spontaneous crack growth may be modeled more physically. It is also worth mentioning that higher-order spatial partial derivatives are a common approach used to introduce a length scale into a governing equation, which is necessary for modeling phenomena at different geometric scales (Seleson *et al.* 2009). Capturing nonlocality via domain decomposition and variational calculus techniques is shown in (Di Paola *et al.* 2010; Aksoylu, Parks 2011).

To complement the above-listed nonlocal analytical approaches, various discrete and numerical methods

should also be considered. The best-known techniques are molecular dynamics (Seleson *et al.* 2009) and cellular automata with extended interaction regions; i.e., a secondary von Neumann neighbor, as reported in (Leamy, Springer 2011). The micropolar and Cosserat theories (Chen *et al.* 2004), extensions of FEM (Polizzotto 2001; Arash *et al.* 2012), and finite difference method (FDM) (Sguazzero, Kindelan 1990; Fornberg 1998) were also proposed to address nonlocal descriptions for solid mechanics.

In the case of numerical simulations, there are two important aspects that should be taken into account in the context of accuracy and computational time. First, when a reliable numerical model is built, a convergence analysis is required. For nonlocal models, however, both the average distance between the degrees of freedom (DOF) and horizon for nonlocal interactions are required to be determined simultaneously (Bobaru *et al.* 2009). Second, nonlocality opens the perspective of parallel processing since, by its nature, a number of contributing forces or their equivalent quantities must be independently found for the entire interaction region for each simulation time step. Data processing using a graphics processing unit (GPU) naturally suits the numerical algorithms developed for nonlocal methods.

4. NUMERICAL CASE STUDIES

Various applications of numerical algorithms based on nonlocal methods have been proposed over the past few decades. One of the most-recent (i.e. peridynamics) is especially worth mentioning, as it gives us the opportunity to accurately model wave-based phenomena, including the regions of geometric discontinuities. The applications of peridynamics (which were used to solve problems regarding acoustic emission), clapping phenomenon, higher order harmonic waves generations, and propagation and reflection of Lamb's waves can be found in (Martowicz *et al.* 2014b). A vibro-acoustic wave interaction solution using the nonlocal approach is presented in (Martowicz *et al.* 2014c). The results of simulations for strain wave propagation in composite materials are reported in (Hu *et al.* 2012). A recent overview on the practical applications of peridynamics can be found in (Madenci, Oterkus 2014). Below, the outcomes for a two-dimensional (2-D) peridynamic model of an aluminum plate undergoing uniaxial stretching and fatigue are shown.

Numerical simulations were used to analyze the behavior of the models made of a homogeneous, isotropic material. The governing equation used to describe a 2-D numerical model is derived from Equation (4) and takes

the following form for the i -th particle (Martowicz *et al.* 2014c):

$$\begin{cases} \rho \frac{\partial^2 u_i(t)}{\partial t^2} = \sum_{j \in H_i} \left((\xi_{X_{i,j}} + u_j(t) - u_i(t)) F_{i,j}(t) c A_{i,j} T \right) + b_{X_{i,j}} \\ \rho \frac{\partial^2 v_i(t)}{\partial t^2} = \sum_{j \in H_i} \left((\xi_{Y_{i,j}} + v_j(t) - v_i(t)) F_{i,j}(t) c A_{i,j} T \right) + b_{Y_{i,j}} \end{cases} \quad (5)$$

where $u_i(t)$ and $v_i(t)$ are the in-plane displacements of the particles along the $0X$ and $0Y$ axes. Horizon H_i determines the population of the j -th neighboring particles interacting with the i -th actual central one. $\xi_{X_{i,j}}$, $\xi_{Y_{i,j}}$, $b_{X_{i,j}}$ and $b_{Y_{i,j}}$ stand for two pairs of relative particle positions and the components of the external body force. $A_{i,j}$ determines the area of the j -th particle covered by horizon H_i . The thickness of the model is defined with parameter T . Contributing factor function $F_{i,j}(t)$ takes the following form:

$$F_{i,j}(t) = \frac{1}{\sqrt{\xi_{X_{i,j}}^2 + \xi_{Y_{i,j}}^2}} - \frac{1}{\sqrt{(\xi_{X_{i,j}} + u_j(t) - u_i(t))^2 + (\xi_{Y_{i,j}} + v_j(t) - v_i(t))^2}} \quad (6)$$

The elastic properties of the plate are defined with micromodulus function c :

$$c = \frac{6E}{\pi \delta^3 (1-\nu) T} \quad (7)$$

which is found based on Young's modulus E , Poisson's ratio ν , and the radius of circular horizon δ . Having introduced Equation (5) to govern the behavior of an aluminum plate, a peridynamic model was prepared (with dimensions of 4×10.125 mm), as shown in Figure 1. Its thickness equals 1 mm.

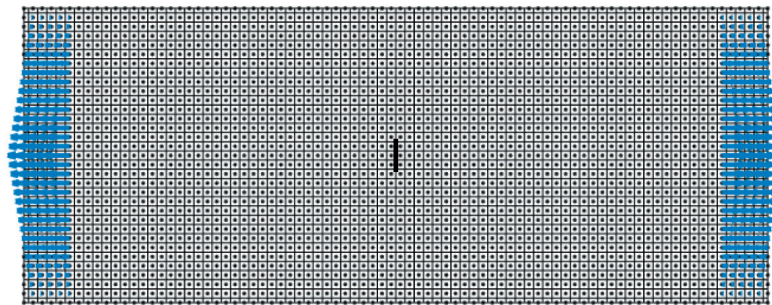


Fig. 1. Peridynamic model of aluminum plate used for stretching and fatigue analysis. Model considers centrally localized vertical crack and two areas of exciting forces

The model satisfies a free-free condition. The forces, which are used to initiate an axial deformation of the plate, are spread within the two areas, each consisting of five columns of contributing vectors, and localized at the vertical edges of the model to prevent nonphysical point concentrations in the external body excitation. A single 0.37-mm-long vertical crack is introduced in the model. The material properties are as follows: $E = 70$ GPa, $\nu = 0.3$, $\rho = 2100$ kg/m³. The model considers both the breaking of links between the particles when the ultimate stress (40 MPa) is exceeded as well as the contact mechanism, which allows for the temporal recovery of the force reactions when the edges of the developing crack approach each other. This model's formulation leads to a bilinear stiffness, which is observed for fatigue analysis. The temporal and spatial discretizations used in the model are determined with parameters $\Delta t = 20$ ns and $\Delta x = 0.125$ mm, respectively. The radius of the horizon corresponds to a distance of $\delta = 4\Delta x = 0.5$ mm (Hu *et al.* 2012). An implicit time integration scheme was applied to determine the consecutive particle displacement. A criterion based on the maximum error regarding the displacements (i.e., 0.1 nm) was used to terminate the iteration procedure for each time step.

Two case studies were investigated to track the path of the developing crack; these are shown in Figure 2.

- 1) Axial stretching with the time rise factor for force amplitude $\Delta F_0/\Delta t = 1$ MN/s. The final value of the amplitude equals $F_0 = 100$ N.
- 2) Fatigue with force amplitude $F_0 = 35$ N and frequency $f = 200$ kHz. The corresponding force amplitude's time rise factor equals $\Delta F_0/\Delta t = 28$ MN/s. The simulation assumes that the amplitude of the sinusoidal force gradually rises within period $\tau = 4$ ms after the simulation is initiated. Hence, this determines that value F_0 is effectively achieved and then kept until the simulation terminates (within one-fourth of the period of a sinusoidal force excitation).



Fig. 2. Evolution of crack's path shown for central part of model, undergoing two types of force excitations: a) straight path observed for axial stretching, captured at 100 μ s; b) skew paths for fatigue observed at 7 μ s. For better visualization, displacements shown are scaled by 50 with respect to actual ones

The exemplary results of the peridynamic simulations that are shown in the paper reflect the mechanisms of the growing and branching cracks (crack bifurcation) identified for various excitation regimes (Hu *et al.* 2012). Depending on both the increase ratio and nominal value of amplitude of the force acting on a deformable body, different physical behaviors of an emerging crack may be found. This observation refers to the experimental results, as in the case of high-strain deformations for composites described in (Haque, Ali 2005; Meyers, Chawla 2009). Since the definition of a peridynamic model allows for integral and potential-based formulations (i.e., a more-physical description of the interactions in an elastic body at the micro- and nano-scales), it is expected to model the crack's growth reliably and the phenomenon of its bifurcation employ more-realistic scenarios. The present work shows the straight and skew paths for a growing crack in a model with ongoing slow axial stretching as well as the fatigue where the different rise factors for the amplitudes of the forces are applied.

5. CONCLUDING REMARKS

Over recent decades, a rapid growth of interests regarding nonlocal methods for continuum mechanics has been observed. Among other applications of nonlocal formulations for solid mechanics, the modeling of crack and crack-wave simulations are of particular interest, since the above-mentioned methods characterize unique properties. As shown in the work, the capability of convenient modeling geometric discontinuities results in more physical paths (i.e., spontaneous paths) of emerging cracks not explicitly governed by any direction in a structured mesh. The potential-based problem description reflects the physical force dependencies between the pieces of a deformable solid body in a more-realistic way, which is demanded in reliable simulations of the crack's growth (e.g., in fatigue analyses).

The paper presents examples of the results of axial stretching and fatigue obtained with a peridynamic model. Different types of force excitations, varying in the time increase ratio and the nominal value of amplitude, lead to different paths of the crack's growth. Either the straight or skewed propagation's directions are successfully identified in the work to refer to already-published works, including the conducted experiments. From a practical point of view, it should be highlighted that the nonlocal methods are by their nature capable of applying the multi-threading technique. The numerical algorithms that have been developed for the nonlocal methods for continuum mechanics can be effectively implemented in a GPU. The calculations required for each time step can be easily dispatched for each DOF undergoing many parallel non-local interactions. New values of nodal quantities can be found solving independent tasks simultaneously.

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