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Nonlocal finite element modeling of the tribological behavior of nano-structured materials

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Abstract. A nonlocal finite element model is developed for solving elasto-static frictional contact problems of nanostructures and nanoscale devices. A two dimensional Eringen-type nonlocal elasticity model is adopted. The material is characterized by a stress-strain constitutive relation of a convolution integral form whose kernel is capable to take into account both the diffusion process of nonlocal elasticity and the scale ratio effects. The incremental convex programming procedure is exploited as a solver. Two examples of different nature are presented, the first one presents the behavior of a nanoscale contacting system and the second example discusses the nano-indentation problem.

Keywords: nonlocal finite element; nano-structured materials; nano-indentation; contact mechanics.

1. Introduction

The field of nano-scale systems and devices has expanded considerably over the last decade. The length scale and large surface to volume ratio of that type of devices result in high friction and adhesion forces that seriously affect the performance and reliability of the devices. Therefore, these nano-tribological phenomena need to be studied and understood at nano-scale level.

To study and predict the details of any physical phenomenon, we have to choose the convenient theory for investigation. All physical theories possess a certain domain of applicability outside of which they fail to predict the physical phenomena with reasonable accuracy. The domain of applicability of any field theory is a function of some internal characteristic length scales of the media for which the theory is constructed. When these internal length scales is sufficiently small as compared to the corresponding external length scales, then the field theory gives sufficiently accurate results, otherwise it fails to apply.

To investigate any mechanical or tribological phenomenon for nanoscale systems, we have to be equipped with a field theory capable to account for the scale ratio of the internal and external characteristic lengths. However all elastic materials possess internal structure in molecular and atomic scale, but unfortunately the classical theory of elasticity does not account for the scale ratio. Obviously, the lengths scale ratio associated with nanoscale systems, where the external length scale is comparable to the internal length scale, is out of the applicability domain of the local elasticity

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theory. Thus, there is an expectation that classical local elasticity theory ceases to be valid at nanometer length scale, Eringen (1987).

The question arising here is: should we give up the classical local elasticity theory and rely only on the atomic theories? The decision depends on the characteristic scale ratio; if the motion of each atom in a body is essential for the description of a physical phenomenon, then the lattice dynamics is the only choice. If, on the other hand, the collective behavior of large numbers of atoms is adequate for the description, then continuum theory offers much simpler and practical methodology.

Nonlocal elasticity represents a powerful extension of the classical continuum approach to account for the small length scale and retaining most of the advantages of the continuum approach.

Linear theory of nonlocal elasticity, which had been proposed independently by many authors, Kroner (1967), Edelen *et al*. (1971) and Eringen (1972, 1983, 1987, 2001), incorporates important features of the lattice dynamics and yet it contains classical elasticity in the very small scale ratio. Therefore the theory is capable of addressing small as well as large scale ratio phenomena. In the nonlocal elasticity theory, the stress state at a given point is regarded as being determined by the strain state of all points in the body. While the constitutive equations of classical elasticity is an algebraic relationship between the stress and strain tensors that of the nonlocal elasticity involves spatial integral which represents a weighted average of the contributions of the strain tensors of all points.

Eringen (1972, 1983, 1987, 2001), developed a simplified nonlocal elasticity theory of integral type for linear homogeneous isotropic continuum. This nonlocal theory differs from the classical local elasticity theory only for the stress-strain constitutive relations. According to Eringen's model, the continuum can be conceived as an aggregate of material particles, linked to one another by cohesive bonds between adjacent particles and long forces or ligaments between the nonadjacent particles. Precisely, the nonlocal strain at a field point x, namely $\varepsilon(x)$ can be represented as the sum of two contributions: one is arising at x itself and the other one is the strain at x induced by strains arising or acting at all $x \neq x$ in the volume of the continuum. This second contribution, expressible through a convolution integral, represents the diffusion part of the nonlocal elastic behavior of the material. Therefore, the model of nonlocal elasticity is accounting for both the material properties and the geometry of the domain occupied by the material.

Application of nonlocal elasticity to investigate the mechanical behavior of nanoscale devices and nanostructured materials, where scale ratio effect become prominent and has to be accounted for, is one of the important applications. Recently, many researchers such as Peddieson *et al*. (2003), Wang and Vandan (2006), and Reddy (2007), have applied the nonlocal elasticity to analyze the mechanical behavior of nanoscale structures. Most of these articles focused only on one dimensional structure as beams and nanotubes. Many other articles focused on two dimensional structures such as thin film elements, Freund and Suresh (2003); graphine sheets, He *et al*. (2005); Kitiporchi *et al*. (2005). Very few articles are dealing with the mechanics of interacting bodies in relative motion, which includes many tribological aspects of solids in contact such as friction, wear, lubrication, etc.

Most of these tribological aspects depend basically on analyzing and modeling of the contact problems between the interacting deformable bodies where the modeling of contact in solids poses mathematical and computational difficulties. With application of loads to the bodies in contact, the actual contact area which is not known a priori, changes nonlinearly and the stresses at contact interface are complex to determine. Various factors such as the inequality constraints of non-interpentration, the stress singularities caused by sharp-edged indenters and the transition from stick to slip conditions complicate the analysis of contact problems, Mahmoud *et al*. (1998, 2005), Meguid *et al*. (2005).

Unfortunately, analytical formulations for two and three dimensional problems in the context of nonlocal elasticity are cumbersome and hard to solve. Therefore, numerical procedures which are general and effective are quite reliable. The nonlocal finite element method is one of the most reliable methods to investigate the mechanical and tribological behavior of nanoscale systems and devices.

The main objective of the present work is the development and implementation of a variational nonlocal finite element model to investigate the mechanical and tribological behavior of elasto-static frictionless/frictional contact of nanoscale systems .The model is equipped with an incremental convex programming solver, developed by Mahmoud *et al*. (1998, 2005), to match with the variational inequality nature of contact problems. Two problems of different nature are studied. The first problem, which is considered as a typical example of nanoscale devicedeals with the study of the frictional contact of an elastic cylinder pressed against an elastic substrate coated with a hard layer. The lengths of the cylinder and the elastic substrate are of nanoscale dimensions. The second problem discusses the nanoindentation of metals by a flat-ended cylindrical punch.

2. Formulation of the problem

Consider two isotropic and homogeneous elastic bodies of nanoscale dimensions, shown in Fig. 1, being subjected to static loads. Each of the two bodies occupies a bounded domain Ω in two dimensions. The boundary Γ of each body is assumed to consist of three disjoint portions, Γ_D, Γ_F, Γ_C, where Γ_D and Γ_F are the portions of the boundary on which the displacements and tractions are prescribed, respectively, and Γ_C is the candidate contact interface; i.e. Γ_C is a portion of the boundary that contains the adjacent surfaces interface which may come into contact upon application of the loads.

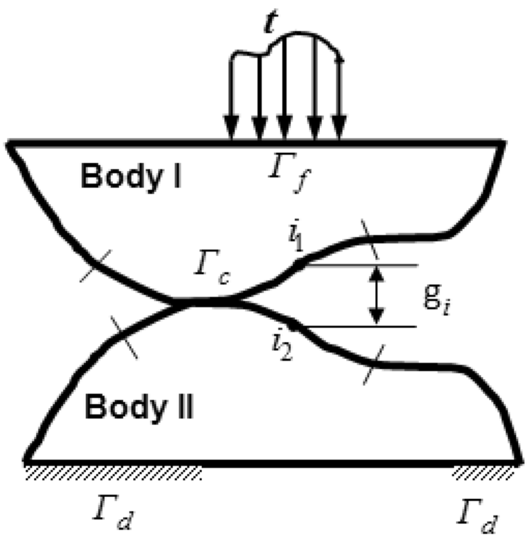

Fig. 1 Contact of two elastic bodies

The formulation of the contact problem in the framework of nonlocal elasticity is given as follows
• Equilibrium equations

$$\sigma_{ij,j} + f_i = 0 \qquad \text{in } \Omega \tag{1a}$$

• Kinematic and kinetic boundary conditions

$$u_i = U_i \qquad \text{on } \Gamma_d \tag{1b}$$

• Contact conditions

$$U_n < g$$
$$\sigma_n = \sigma_{ij} n_i n_j \le 0 \qquad \text{on } \Gamma_c$$
$$(u_n - g)\sigma_n = 0$$
$$\sigma_\tau = -\mu\sigma_n\left(\frac{u_\tau}{\lfloor u_\tau \rfloor}\right) \tag{1c}$$

• Constitutive equations of Eringen nonlocal elasticity

$$\sigma_{ij} = \int \alpha(|X' - X|) E_{ijkl} u_{k,l} dV(X') \tag{1d}$$

where **X**, **X'** are field points into the material domain Ω, **u** is the admissible displacement vector, σ_n is the normal stress component, f is the body force vector, g is the normal gap between the nodes of a contact pair along the local the contact interface Γ_C, t is the surface traction, and E_{ijkl} is the local elastic coefficients. Eq. (1c) represents the only difference between the formulation of nonlocal elasticity problem, and the equation that corresponds to classical local elasticity. Finally, $\alpha(|X' - X|)$ is a positive scalar attenuation function which assigns a weight to the nonlocal effect induced at field point **X** by a strain acting at the source point **X'**. The attenuation function $\alpha(|X' - X|)$ decays rapidly with increasing the distance $|X' - X|$. The distance is qualifiable if only compared with the internal characteristic length "l". Therefore the attenuation function α being a function of the ratio $|X' - X| \,/\, l$.

Meanwhile, the attenuation function should take into account the scale ratio between the internal characteristic length 1 and the external characteristic one L. In the present work we adopt the following attenuation function proposed by Eringen (1983), for two dimensional domains

$$\alpha(|X'|) = (\pi c l^2)^{-1} \exp(-X.^X / c l^2) \tag{2}$$

where $c = e_0 l/L$ and e_0 is a constant of value 0.39. The influence distance of the attenuation function, beyond which the diffusion process is vanishing, is $L_R = 6l$. The classical formulation (1a-d) is equivalent to the dual formulation of minimizing the functional of total potential energy

$$F(u) = \frac{1}{2}a(u, u) - f(u) \tag{3a}$$

subject to

$$u_n \le g \qquad \text{on } \Gamma_F \tag{3b}$$

where

$$a(u, u) = \int_\Omega [\int_\Omega \alpha(|X' - X|) E_{ijkl} u_{k,l} dV(X')] u_{i,j} dX' \tag{3c}$$

and

$$f(u) = \int_\Omega f.u dX + \int_{\Gamma_F} t.u dX \tag{3d}$$

The equivalent Lagrangian formulation of the above constrained minimization model (3a-d) is

$$\text{Min} L(u, \lambda) = \text{Min}\left[F + \int_{\Gamma_C} \lambda.(u_n - g)_+ ds\right] \tag{4}$$

Where $(u_n - g)_+$, is the violation vector of the contact constraints and λ is the Lagrange multiplier vector corresponding to this violation. We have to notice that both the functional F and the contact constraints are convex functions.

3. The discretized model

By the finite element discretization scheme, the functional F defined by Eq. (3a), would take the following form

$$\text{F}(\mathbf{u}) = ½\, \mathbf{u}^t\, \mathbf{K}(\mathbf{u})\, \mathbf{u} - \mathbf{u}^t \mathbf{p} \tag{5a}$$

The contact constraints of Eq. (3b) may be reformulated in a discretized form as follows

$$C^T u - b \le 0 \tag{5b}$$

Therefore, the equivalent discretized form of the Lagrangian formulation given by Eq. (4), would take the following form

$$\text{Min} L(u, \lambda) = \frac{1}{2} u^T K(u) u + \lambda(C^T u - b) - u^T P \tag{6}$$

where K is the nonlocal global stiffness matrix which accounts for the nonlocal elasticity and the scale ratio effect, u is the displacement vector, λ is the Lagrange multiplier vector, b is the gap vector of contact pairs, P is the total force vector, $C = [c_1 c_2 \ldots c_i \ldots c_m]$, where c_i is the constraint vector corresponding to the constraint pair "*i*". The global stiffness matrix K is derived according to the procedure given by Polizzotto (2001) and Pisano *et al*. (2009).

Since the problem defined by Eq. (6) is a convex one, then Kuhn-Tucker (K-T) necessary conditions are also sufficient and any local minimum is also a global one. The global minimum point (u^*, λ^*) should satisfy the following (K-T) necessary and sufficient conditions

$$Ku^* + C\lambda^* = P \tag{7a}$$

$$\mathbf{C}^T \mathbf{u}^* \le \mathbf{b} - \mathbf{s} \tag{7b}$$

Where $\mathbf{s}$ is a non-negative vector representing the violation of the contact constraints and λ^* is the non-negative Lagrange multiplier vector.

The set of contact constraints may be divided into active and inactive subsets: the inactive subset consists of non-contacted pairs, while the active one consists of contacted pairs. Therefore Eq. 7 may be rewritten as follows

$$\begin{bmatrix} K & C_A & C_N \\ C_A^T & 0 & 0 \\ C_N^T & 0 & 0 \end{bmatrix} \begin{Bmatrix} u^* \\ \lambda_A^* \\ \lambda_N^* \end{Bmatrix} = \begin{Bmatrix} P \\ b_A \\ b_N - s \end{Bmatrix} \tag{8}$$

where λ_A^* is the Lagrange multiplier vector of the active constraints which have positive values, λ_N^* is the inactive constraints multipliers which should have zero values, and b_A and b_N are the gap vectors for active and inactive constraint sets. It should be noticed that the members of both sets are not known a priori. The state of each constraint may be changed from an active to an inactive one and vise versa according to the level of the applied vector *P*. Accordingly, the incremental value of the active multiplier λ_A of a contact pair may be positive or negative as the contact pressure of the pair is increasing or decreasing respectively. The incremental solving procedure of convex model is given in details by Mahmoud *et al.* (1998, 2005).

4. Numerical examples

The NL-FEM contact model is used to solve two contact problems of different natures. The first one presents the frictional behavior of an elastic cylinder of nanodimensions pressed against an elastic substrate coated with a hard layer.

The second problem is the nanoindentation for a flat ended cylindrical punch of nano scale acting on elastic half space with a normal central force.

Example 1: Contact of an elastic cylinder pressed against an elastic substrate coated with a hard layer

Friction and wear have been recognized as limiting factors to numerous applications and many areas of technology. Thus, there has been significant interest in understanding and controlling these processes. Recently, research has focused on nanoscale devices with moving parts which motivate the study of frictional contact and wear of this type of devices. Therefore, the first problem is the contact of an elastic cylinder which is pressed against an elastic substrate coated with a hard layer. The dimensions, material properties, loading and boundary conditions are shown in Fig. 2, where *L* and *F* are typical units of length and force respectively. Assuming the material of the cylinder and substrate follows Eringen's nonlocal elasticity model with the following parameters:

$e_0 = 0.39$, Eringen (1983),
Radius of the indenter "*R*" = 10(L),
Internal characteristic length "*l*" = 0.14 nm,
External characteristic length = "*R*",
Influence length of the attenuation function "L_R" = 6l.

The space domain is modeled by four nodes isoparametric quadrilateral nonlocal finite

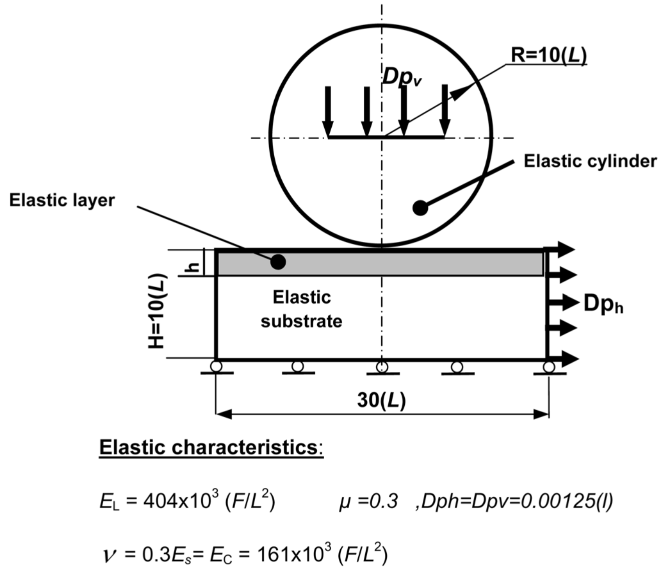

Fig. 2 Contact of an elastic cylinder and a coated elastic substrate

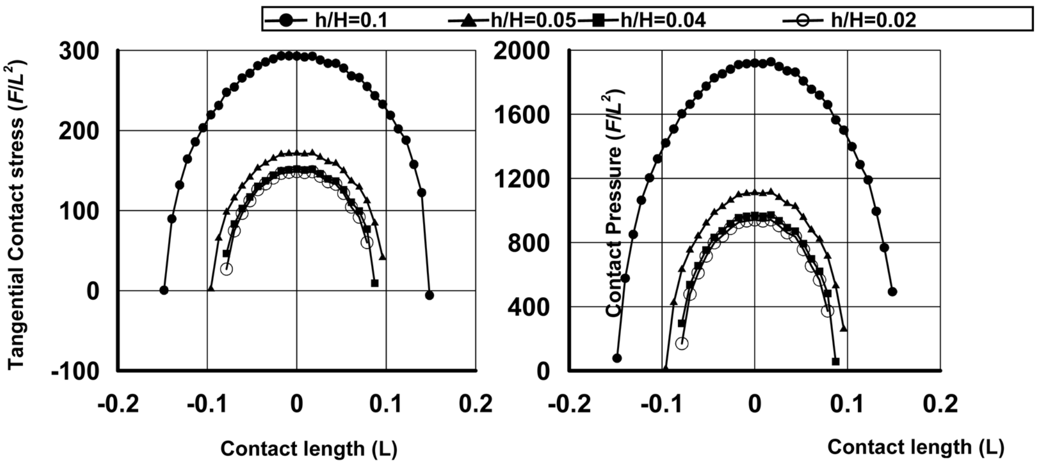

Fig. 3 Contact pressure distribution for different h/H

elements.The grid consists of 885 elements and 938 nodes for the cylinder, 1024 elements and 990 nodes for the coated substrate. The potential contact interface is modeled by 55 nodes.

The contactpressure and the tangential contact stress distributions along the contact interface are shown in Fig. 3 for different values of h/H.

Example 2: Nanoindentation of elastic half space by a flat ended cylindrical punch

Nanoindentation is commonly used to measure hardness, elastic modulus, and wear resistance of materials, Guidry *et al*. (2009), Qi *et al*. (2009), Bhushan (2005). Hardness and elastic modulus are

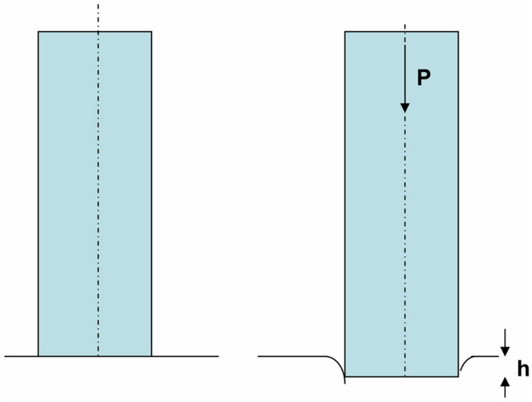

Fig. 4 Nanoindentation by a flat ended cylindrical punch

calculated from load-displacement data given by the indentation process. When a nanoscale indentation test is operated, the scale ratio would affect the mechanical properties of the tested materials.

In the context of classical local elasticity, Sneddon (1965) derived load–displacement relations for arbitrary shaped axisymmetric punch. The solution of Sneddon for indentation without friction of an elastic half space by a flat ended cylindrical punch, Fig. 4 in the context of local elasticity can be given as follows.

For a penetration of value "*h*", the mean value of the contact pressure distribution along contact interface, P_m, is given as follows

$$P_m = \frac{2Eh}{\pi\alpha(1-2\upsilon)} \tag{9}$$

where "α" is the indenter tip radius. The distribution of contact pressure under the punch $\sigma_1 z(r \le a, z = 0)$, is given by the following equation

$$\sigma_z(r, 0) = \frac{P_m}{2\left(1 - \frac{r^2}{\alpha^2}\right)^{\frac{1}{2}}} \tag{10}$$

and the shape of the deformed boundary, $u_z(r > a, z = 0)$ is given by the following function

$$u_z(r, 0) = \frac{2h}{\pi}\sin^{-1}\left(\frac{\alpha}{r}\right) \tag{11}$$

The previous solution of Sneddon is only limited to local elasticity materials and the solution has a singularity at the boundary of the contact interface.

The nonlocal finite element has been performed for a typical frictionless indentation problem, shown in Fig. 4, and the material having a scale ratio parameter "$c = e_0.l/L$" which is assumed to be 0.005 and the position and contact pressure along contact interface are normalized as "r/a" and "$\sigma z/E$".

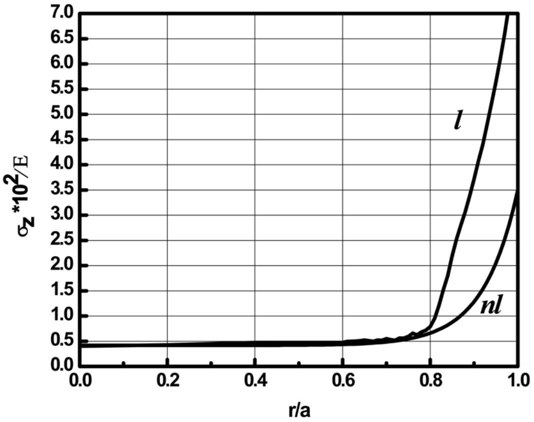

Fig. 5 Normalized indentation pressure distribution along contact interface

The distributions of contact pressure along contact interface for a normalized penetration value $h/a = 0.1$ are shown in Fig. 5 for both the nonlocal elasticity model and that derived by Sneddon.

By comparing the results, we can notice that while the local contact pressure tends to infinity value at the boundary of the contact interface, the nonlocal one is finite inside and on the boundary of the interface, which is consistent with the experimental results. The maximum value of the nonlocal pressure distribution occurs very close to the boundary of contact domain but not at the boundary itself.

5. Conclusions

A nonlocal finite element model (NL-FEM), has been developed in the context of two dimensions nonlocal elasticity to solve frictionless/frictional contact problems of nanoscale systems and devices. The contact problem is formulated into a variational inequality form and solved by an extended incremental convex programming procedure developed by Mahmoud *et al*. (1998, 2005).

The stress-strain constitutive relations are characterized by Eringen convolution integral form whose kernel plays the role of the attenuation function for the nonlocality effects. A bi-exponential attenuation function is adopted and the scale ratio of the internal and external characteristic lengths is taken into account.

The NL-FEM model is used to solve two contact problems of different nature; the first one is a frictional contact of an elastic cylinder of nano dimensions, resting on an elastic substrate coated with a hard layer .The contact length and the contact pressure distribution are determined and compared with those of local elasticity. Contact length of nonlocal elasticity model is less than that of the local model while the peak contact pressure is slightly higher.

The second problem discusses the nanoindentation of flat ended punch acting on an elastic half space with normal central force. The results are compared with the analytical local elasticity solution of Sneddon. As a main finding, none of the classical singularities exists in the nonlocal elasticity solution. Consequently, nonlocal contact pressure is finite along the contact interface. The maximum nonlocal contact pressure occurs close to the boundary of the interface and the contact pressure distribution is slightly higher for the interior points.

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