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SBFE analysis of nano-scale elastic layer with consideration of surface energy effects

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Abstract. This paper presents an efficient and accurate numerical technique for determining the mechanical response of an infinite elastic layer under surface loading and surface stress effects. The governing equation of the bulk is formulated from the classical linear elasticity theory via a SBFE technique whereas that of the material surface is obtained from a complete version of Gurtin-Murdoch surface elasticity theory. By enforcing the continuity at the interface of the material surface and the bulk, it leads to a system of linear non-homogenous ordinary differential equations governing the nodal functions. A general solution of the resulting system of ODEs is constructed via standard procedures and then used together with the boundary conditions to form a system of linear algebraic equations governing nodal degrees of freedom. To investigate the accuracy and convergence of the proposed method, selected scenarios are solved and obtained numerical results are reported and discussed.

1. Introduction

In the early of 21st century, a nano-layer surface coating has been commonly utilized to enhance both surface and overall properties of components such as the energy harvested reflective color filter, surface wear resistance complex metal boron-carbide, and invisible carbon nanotube coating. Although experimental studies and theoretical simulations based on discrete models [1, 2] provide a profound understanding reflecting the real response of surface coatings, they result in the prohibitive cost and large computational effort, respectively. Modified continuum-based models, with the incorporation of Gurtin-Murdoch surface elasticity theory [3, 4]with the classical linear elasticity, are considered promising in that they can provide the first approximation of the response prediction of nano-size problems requiring relatively cheap computational effort.

In the past studies, the complete version of Gurtin-Murdoch model has been widely adopted to investigate the surface energy effect of various nano-size problems under prescribed loading by various analytical solution methods such as Fourier integral transform for buried load in an infinite elastic layer [5]; Hankel integral transform with Love's representation for an infinite rigid-based elastic layer under axisymmetric surface load [6] and a layered elastic half-space under axisymmetric surface load [7]; and a technique based on Boussinesq potential for an elastic half-space subject to surface circular shear traction [8]. Although those employed solution procedures are successful in predicting the response of nano-size problems via the Gurtin-Murdoch model such as the size-dependency behavior, the issue of computational efficiency arises when more practical and large scale problems become of interest.

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The present study aims to implement an alternative solution procedure, based upon the framework of a scaled boundary finite element method (SBFEM), to obtain response of nano-size problems via a continuum model enhanced by integrating Gurtin-Murdoch surface elasticity theory to treat the influence of surface energy. In particular, a problem associated with two-dimensional, infinite, rigid-based, elastic layer under surface loading is chosen as the representative case to demonstrate the capability of the proposed technique.

2. Problem formulation

Consider a two-dimensional, infinite, elastic layer of thickness h resting on a rigid foundation and subjected to arbitrarily distributed normal traction p over the length $2a$ as shown schematically in Fig. 1. The bulk of the layer is made of a homogeneous, isotropic, linearly elastic material whereas a thin layer on the top of the layer (termed here the surface) is made of a different homogeneous, isotropic, linear elastic material with the presence of initial residual surface tension. In the present study, the layer is assumed to be free of body force.

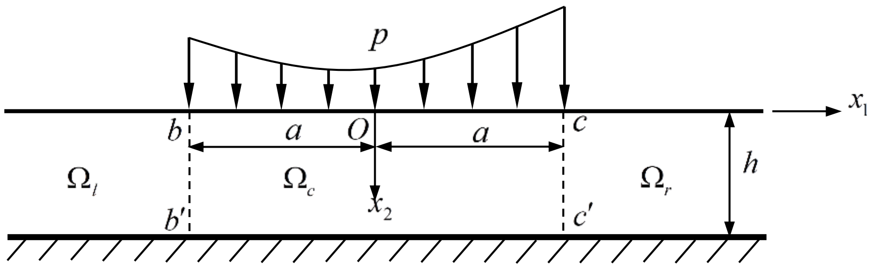

Figure 1. Two-dimensional, elastic layer subjected to arbitrary vertical pressure

The elastic layer can be divided into three sub-domains along the lines bb' and cc' and they are referred to the left part Ω_l, the center part Ω_c, and the right part Ω_r. In the formulation presented further below, a representative domain $\hat{\Omega}$ with a similar shape as that of the center part Ω_c is considered. The left, right, top and bottom boundaries of this representative domain $\hat{\Omega}$ are denoted by $\partial\hat{\Omega}^l$, $\partial\hat{\Omega}^r$, $\partial\hat{\Omega}^t$, and $\partial\hat{\Omega}^b$, respectively. Once the formulation is achieved on $\hat{\Omega}$, it can be readily applied to all subdomains Ω_l, Ω_c, and Ω_r. For instance, Ω_l is obtained from $\hat{\Omega}$ by taking the boundary $\partial\hat{\Omega}^l$ to infinity and removing all loading on the boundary $\partial\hat{\Omega}^t$.

From the classical theory of elasticity, the equilibrium equations, the constitutive laws, and the infinitesimal strain-displacement relationship of the bulk material can be expressed in a concise form, for a two-dimensional body subjected to plain-strain condition and zero body force, as

$$\boldsymbol{L}^T\boldsymbol{\sigma}^b = \boldsymbol{0} \;;\; \boldsymbol{\sigma}^b = \boldsymbol{D}\boldsymbol{\varepsilon}^b \;;\; \boldsymbol{\varepsilon}^b = \boldsymbol{L}\boldsymbol{u}^b \tag{1}$$

where $\boldsymbol{\sigma}^b, \boldsymbol{\varepsilon}^b, \boldsymbol{u}^b, \boldsymbol{D}$ and $\boldsymbol{L} = \boldsymbol{b}_1\partial/\partial x_1 + \boldsymbol{b}_2\partial/\partial x_2$ are a vector containing independent in-plane stress components, a vector containing independent in-plane strain components, a vector containing in-plane displacement components, a modulus matrix involving material constants, and a two-dimensional, linear differential operator with $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ denoting Boolean matrices, respectively; the superscript " T " denotes the matrix transpose operator; and the superscript " b " is used to emphasize field quantities associated with the bulk material. By applying the standard weighted residual technique together with the integration by parts to the basic governing equations (i.e., Eq. (1)), the alternative weak statement governing the bulk material can be expressed as:

$$\int_{\hat{\Omega}} (\boldsymbol{L}\boldsymbol{w})^T \boldsymbol{D}(\boldsymbol{L}\boldsymbol{u}^b)\,dA = \int_{\partial\hat{\Omega}} \boldsymbol{w}^T \boldsymbol{t}^{b(\partial\hat{\Omega})}\,ds \tag{2}$$

where $\boldsymbol{w}$ denotes a sufficiently smooth weighted function; $\partial\hat{\Omega} = \partial\hat{\Omega}^l \cup \partial\hat{\Omega}^r \cup \partial\hat{\Omega}^t \cup \partial\hat{\Omega}^b$; and $\boldsymbol{t}^{b(\partial\hat{\Omega})}$ is the traction acting to the boundary $\partial\hat{\Omega}$ of the bulk. Now, let one introduce the scaled boundary finite element approximation of the displacement $\boldsymbol{u}^b$ and weighted function $\boldsymbol{w}$ such that

$$\boldsymbol{u}^b = \boldsymbol{u}^b(x_1, x_2) = \sum_{i=1}^{p} \phi^i(x_2) u^i(x_1) = \boldsymbol{NU} \quad ; \quad \boldsymbol{w} = \boldsymbol{w}(x_1, x_2) = \sum_{i=1}^{p} \phi^i(x_2) w^i(x_1) = \boldsymbol{NW} \tag{3}$$

where $\boldsymbol{N}$, $\boldsymbol{U}$, and $\boldsymbol{W}$ represent, respectively, a matrix containing the basic functions ϕ^i, a vector containing the nodal displacement functions u^i, and a vector containing the nodal weighted functions w^i. By substituting the approximations of $\boldsymbol{u}^b$ and $\boldsymbol{w}$ into Eq.(2) together with the integration by parts of terms involving the first derivative of the weighted function, and by invoking the arbitrariness of the vector $\boldsymbol{W}$, we obtain the scaled boundary finite element equation of the bulk material and the corresponding boundary conditions as follows:

$$\boldsymbol{E}_2^b \boldsymbol{U}'' + [\boldsymbol{E}_1^b - (\boldsymbol{E}_1^b)^T]\boldsymbol{U}' - \boldsymbol{E}_0^b \boldsymbol{U} + \boldsymbol{T}^{bt} + \boldsymbol{T}^{bb} = \boldsymbol{0}\,; \boldsymbol{Q}^{bl} = \boldsymbol{Q}^b(x_{1l}) = -\boldsymbol{P}^{bl}\,; \boldsymbol{Q}^{br} = \boldsymbol{Q}^b(x_{1r}) = \boldsymbol{P}^{br} \tag{4}$$

where $\boldsymbol{T}^{bt} = \boldsymbol{N}^T(0)\boldsymbol{t}^{bt}(x_1)$, $\boldsymbol{T}^{bb} = \boldsymbol{N}^T(h)\boldsymbol{t}^{bb}(x_1)$, $\boldsymbol{P}^{bl} = \int_0^h \boldsymbol{N}^T \boldsymbol{t}^{bl} dx_2$, $\boldsymbol{P}^{br} = \int_0^h \boldsymbol{N}^T \boldsymbol{t}^{br} dx_2$, $\boldsymbol{B} = \dfrac{\partial \boldsymbol{N}}{\partial x_1}$

$$\boldsymbol{E}_2^b = \int_0^h \boldsymbol{B}^T \boldsymbol{b}_2^T \boldsymbol{D} \boldsymbol{b}_2 \boldsymbol{B} dx_2\,, \quad \boldsymbol{E}_1^b = \int_0^h \boldsymbol{N}^T \boldsymbol{b}_1^T \boldsymbol{D} \boldsymbol{b}_2 \boldsymbol{B} dx_2\,, \quad \boldsymbol{E}_0^b = \int_0^h \boldsymbol{N}^T \boldsymbol{b}_1^T \boldsymbol{D} \boldsymbol{b}_1 \boldsymbol{N} dx_2\,,$$

$\boldsymbol{t}^{bt}, \boldsymbol{t}^{bb}, \boldsymbol{t}^{bl}, \boldsymbol{t}^{br}$ are tractions on the boundaries $\partial\hat{\Omega}^t$, $\partial\hat{\Omega}^b$, $\partial\hat{\Omega}^l$, and $\partial\hat{\Omega}^r$, respectively, $x_1 = x_{1l}, x_1 = x_{1r}$ denote the coordinates associated with the left and right boundaries, respectively, and $\boldsymbol{Q}^b$ is termed the internal nodal flux of the bulk material defined by

$$\boldsymbol{Q}^b = \boldsymbol{E}_1^b \boldsymbol{U} + \boldsymbol{E}_2^b \boldsymbol{U}' \tag{5}$$

For the material surface, its response is modeled by the complete version of Gurtin-Murdoch surface elasticity theory [3, 4]. In particular, the in-plane and out-of-plane equilibrium equations of the surface in terms of the surface displacements, for the one-dimensional case, and the corresponding boundary conditions are given explicitly by

$$\boldsymbol{E}^s \boldsymbol{U}^{s\prime\prime} + \boldsymbol{t}^0 + \boldsymbol{t}^{sb} = \boldsymbol{0}\,; \boldsymbol{Q}^{sl} = \boldsymbol{Q}^s(x_{1l}) = -\boldsymbol{t}^{sl}\,; \boldsymbol{Q}^{sr} = \boldsymbol{Q}^s(x_{1r}) = \boldsymbol{t}^{sr} \tag{6}$$

where the superscript "s" is used to designate quantities associated with the surface; $\boldsymbol{t}^0$ is the prescribed loading on the surface; $\boldsymbol{t}^{sb}$ denotes the traction exerted to the surface by the bulk; $\boldsymbol{t}^{sl}$, $\boldsymbol{t}^{sr}$ are tractions on the left and right boundaries of the surface;

$$\boldsymbol{E}^s = \begin{bmatrix} (2\mu^s + \lambda^s) & 0 \\ 0 & \tau^s \end{bmatrix}, \; \boldsymbol{U}^s = \begin{Bmatrix} u_1^s \\ u_2^s \end{Bmatrix} \tag{7}$$

in which μ^s and λ^s are surface Lame constants, τ^s is the residual surface tension, and u_1^s, u_2^s are components of the surface displacement; and, similar to the bulk material, $\boldsymbol{Q}^s$ denotes the internal flux within the material surface defined by $\boldsymbol{Q}^s = \boldsymbol{E}^s \boldsymbol{U}^{s\prime}$. By enforcing the continuity along the interface between the bulk and the material surface, it leads to the final system of governing differential equations of the whole system and the corresponding total nodal internal flux

$$\boldsymbol{E}_2^{bs} \boldsymbol{U}'' + [\boldsymbol{E}_1^b - (\boldsymbol{E}_1^b)^T]\boldsymbol{U}' - \boldsymbol{E}_0^b \boldsymbol{U} = \boldsymbol{t}\,; \; \boldsymbol{Q} = \boldsymbol{E}_1^b \boldsymbol{U} + \boldsymbol{E}_2^{bs} \boldsymbol{U}' \tag{8}$$

where $\boldsymbol{E}_2^{bs}$ is a matrix resulting from the assembly of $\boldsymbol{E}_2^{b}$ and $\boldsymbol{E}^{s}$, $\boldsymbol{t}$ denotes a vector containing the information of the side-face tractions, and $\boldsymbol{Q}$ denotes the total nodal internal flux. By further enforcing the prescribed displacement at the bottom of the layer, the nodal displacement vector $\boldsymbol{U}$ and nodal traction vector $\boldsymbol{t}$ can be partitioned into $\boldsymbol{U} = \{\boldsymbol{U}^f \quad \boldsymbol{U}^r\}$ and $\boldsymbol{t} = \{\boldsymbol{t}^f \quad \boldsymbol{t}^r\}$ where $\boldsymbol{U}^f, \boldsymbol{t}^r$ are unknown a priori and $\boldsymbol{U}^r, \boldsymbol{t}^f$ are fully prescribed. According to such partition, the system (8) can also be portioned to arrive at the reduced system of differential equations governing the unknown displacement $\boldsymbol{U}^f$.

3. Solution methodology

Following the standard procedure in the theory of differential equations, the general solution of the unknown displacement $\boldsymbol{U}^f$ can be readily established. In particular, the homogeneous solution, denoted by $\boldsymbol{U}^{fh}$, is obtained by the technique of assuming a solution form and this finally leads to solving a linear eigen problem. A selected efficient algorithm is adopted to accurately and efficiently determine all the eigenvalues and eigenvectors. To construct the particular solution of the unknown displacement $\boldsymbol{U}^{fp}$ for the prescribed traction on the top of the layer (which is assumed expressible in a polynomial form), a well-known method of undetermined coefficients is applied.

By using the general solution of the unknown displacement $\boldsymbol{U}^f$ together with the boundary conditions at the left and right boundaries of the layer, it results in a system of linear algebraic equations governing the unknown data on the boundaries of the layer. Such results for the representative domain can then be used to generate three sub-systems of linear equations governing the unknown data on the boundary of the left part Ω_l, the center part Ω_c, and the right part Ω_r. Finally, by enforcing the continuity of the displacement and traction along the interface between the left part and the center part (i.e., the line bb') and the interface between the right part and the center part (i.e., the line cc') and the standard assembly procedure, it yields a final system of linear algebraic equations governing the nodal displacement data along the two interfaces bb' and cc'. Once such primary unknowns are solved, the elastic field including the displacement and stress within the layer can be readily post-processed with the use of basic field equations (1) and the approximations (3).

4. Preliminary results

To verify the proposed technique, a representative case associated with an elastic half-plane subjected to a constant pressure p over the length $2a$ and without the surface stress effect is considered since the exact solution of the elastic field is available for the comparison purpose. In the numerical study, three levels of discretization across the thickness of the layer (associated with 4, 8, and 16 quadratic elements) are adopted to confirm the convergence of computed numerical solutions and the ratio $h/a = 200$ is chosen to simulate the half-plane case. Results of non-zero stress components along the x_2-axis are reported in Fig. 2(a) together with the exact solution. It is seen that the convergence of the computed numerical solutions and the excellent agreement with the reference solution are observed.

To further demonstrate the capability of the proposed technique to handle nano-scale problems with the surface stress effects, consider an elastic layer of the thickness $h = 8\Lambda$ (where Λ is an intrinsic length scale of the material defined in [5, 6]) under the constant pressure p over the length $a = 2\Lambda$. The material properties for the bulk and the surface used in the numerical study are taken from [6]. Converged results of the stress components along the x_2-axis obtained from the proposed technique are reported in Fig. 2(b) for the two cases (with and without surface stresses). It is apparent that the presence of the surface stresses can significantly alter the elastic response of the layer when the characteristic length of the problem is comparable to the material length scale Λ.

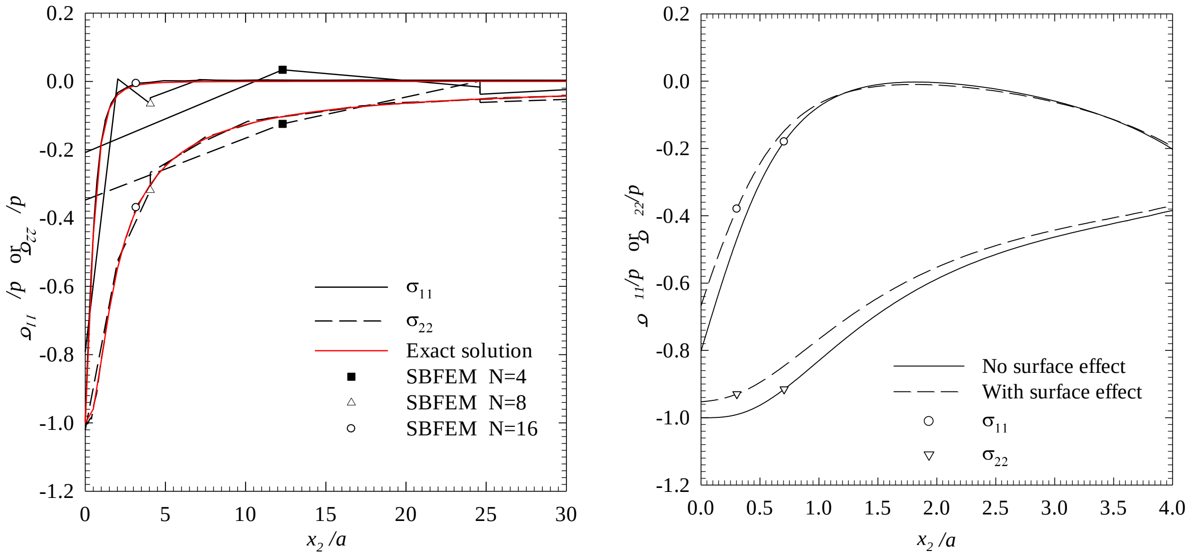

Figure 2. Non-dimensional stress field of (a) elastic half-plane and (b) elastic layer

5. Conclusion

An efficient and accurate numerical technique based on SBFEM has been successfully implemented to determine mechanical response of an elastic layer under the surface loading and surface stress effects. Based on results from a preliminary numerical study, the proposed technique has been found promising and computationally robust. The proposed technique will be used to solve more complicated problems including nano multilayer media and functionally graded material.

Acknowledgments

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