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PREFACE

The Conferences in Boundary Element Techniques are devoted to fostering the continued involvement of the research community in identifying new problem areas, mathematical procedures, innovative applications, and novel solution techniques in both boundary element methods (BEM) and boundary integral equation methods (BIEM). Previous successful conferences devoted to Boundary Element Techniques were held in London, UK (1999), New Jersey, USA (2001), Beijing, China (2002), Granada, Spain (2003), Lisbon, Portugal (2004), Montreal, Canada (2005), Paris, France (2006), Naples, Italy (2007), Seville, Spain (2008) and Athens, Greece (2009).

The present volume is a collection of edited papers that were accepted for presentation at the Boundary Element Techniques Conference held at the Maritim Hotel Berlin, Germany, during 12th-14th July 2010. Research papers received from 18 counties formed the basis for the Technical Program. The themes considered for the technical program included solid mechanics, fluid mechanics, potential theory, composite materials, fracture mechanics, damage mechanics, contact and wear, optimization, heat transfer, dynamics and vibrations, acoustics and geomechanics.

A symposium “Recent Advances in Theory and Application of BEM” was organized at the conference in honor of Professor Zhenhan Yao (Tsinghua University, Beijing, PR China), who is working on BEM for many years and has made many significant contributions to the Computational Mechanics especially to BEM. We would like thanks the organizers of the symposium (Prof. Ch. Zhang, Prof. C.Y.Dong and Prof. Y.H.Liu) for their effort.

The conference organizers would also like to express their appreciation to the International Scientific Advisory Board for their assistance in supporting and promoting the objectives of the meeting and for their assistance in the form of reviews of the submitted papers.

Editors
July 2010
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Three-dimensional eigenstrain formulation of boundary integral equation method for spheroidal particle-reinforced materials

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Keywords: eigen-strain, Eshelby tensor, spheroidal particle, boundary integral equation, iteration

Abstract. A computational model is presented using the proposed three-dimensional eigenstrain formulation for modeling the spheroidal particle-reinforced materials. The model and its solution procedure is based on the concept of equivalent inclusion of Eshelby while the eigenstrains in each inhomogeneity embedded in the matrix are determined using an iterative scheme. With the proposed model, the solution scale of the inhomogeneity problem can be significantly reduced as the unknowns are on the boundary of the solution domain only. Using the algorithm, the stress distributions and the overall elastic properties are identified using the boundary element method (BEM) for spheroidal particle-reinforced inhomogeneous materials over a representative volume element. The performance and efficiency of the proposed computational model are assessed through several examples.

1. Introduction

The determination of elastic behaviour of an embedded inclusion is of considerable importance in a wide variety of physical and engineering problems. Since the pioneer work of Eshelby [1], inclusion and inhomogeneity problems have been a focus of solid mechanics for several decades. Following Eshelby’s idea of equivalent inclusion and eigenstrain solution, quite a diverse set of research work has been reported analytically [2-5] and/or numerically [6-13] in the literature. The eigenstrain solution can represent various physical problems where eigenstrain may correspond to thermal strain mismatches, strains due to phase transformation, plastic strains or fictitious strains arising in the equivalent inclusion problems, overall or effective elastic, plastic properties of composites, quantum dots, microstructural evolution, as well as the intrinsic strains in the residual stress problems [14].

The analytical models available in the literature can be the basis for understandings to predict the stress/strain distribution either within or outside the inhomogeneity and for further research of the inclusion problem. However, these analytical solutions were obtained generally for problems with simple geometries only, such as single ellipsoidal, cylindrical and spheroidal inclusion in an infinite domain. Therefore, numerical simulations with finite element methods (FEM), volume integral methods (VIM) or BEM have been used in the analysis of inhomogeneity problems with various shapes and materials. The FEM may produce results for the whole composite materials, including results inside the inhomogeneity [7], but the solution scale would be large since both the matrix and every inhomogeneity should be discretized. The VIM and the BEM seem to be more suitable for the solution of the inhomogeneity problems in comparison with the FEM. In the VIM [8-10], the zones of inhomogeneity are represented by the volume integrals, which will essentially simplify the construction of the final matrix of the linear algebraic system to which the problem is reduced to some extent after the discretization. However, as the interfaces need to be discretized in the VIM, it is suitable only for small scale problems with a few inhomogeneities. The situation in the application of BEM to inclusion problems, often coupled with the VIM [11,12], is much the same with that of the VIM in
which the problems of simple arrays of inclusions were solved in small scales owing to the reason similar
to that in the VIM, i.e., the unknown appearing in the interfaces. For large scale problems of inhomogeneity
with BEM [13], special techniques of the fast multipole expansions [15] should be employed, which leads to
complexity of the solution procedure.

To the authors’ knowledge, Eshelby’s idea of equivalent inclusion and eigenstrain solution has not yet
been fully utilized in the area of numerical study of the inhomogeneity problems [16]. Based on the
Eshelby’s idea, the authors recently proposed the eigenstrain formulation of the BIE for modeling
particle-reinforced materials in two-dimensional elasticity [17]. In the present work, the computational
model is extended to the three-dimensional case for modeling spheroidal particle-reinforced materials at this
initial stage and solved by the BEM [18].

2. Eigen-strain formulation of BIE

In the present model, The particle and matrix are assumed to be isotropic and bonded perfectly so that the
displacement continuity and the traction equilibrium remain along their interfaces. The problem domain
considered is a bounded region \( \Omega \) filled with the matrix and the inclusions surrounded by the outer boundary
\( \Gamma \). The inhomogeneous zones in the domain are denoted by \( \Omega_1 \), with the boundary \( \Gamma_1 = \Omega_1 \cap \Omega \). The
displacement and the stress fields of the problem can be expressed by the eigenstrain formulations of the BIE
[17] as follows:

\[
\begin{align*}
C(p)u_\alpha(p) &= \int_{\Omega} u^\alpha(q) (p,q) d\Omega(q) - \int_{\Gamma} \tau^\alpha(q) (p,q) d\Gamma(q) + \sum_{\Omega_1} \left( \int_{\Omega_1} \sigma^\alpha_{pq}(p,q) d\Omega(q) \right) \\
C(p)\sigma_{ij}(p) &= \int_{\Omega} \sigma_{ij}(q) (p,q) d\Omega(q) - \int_{\Gamma} \tau_{ij}(q) (p,q) d\Gamma(q) + \sum_{\Omega_1} \left( \int_{\Omega_1} \sigma_{ij}^{\alpha}(p,q) d\Omega(q) \right) + \delta_\alpha (p) \sigma_\alpha^0 \tag{1}
\end{align*}
\]

where \( \sigma_\alpha^0 \) represent the eigenstrains of particles, which are determined in an iterative manner
to be described in the next section. Obviously, the eigenstrains in each particle depend on the applied stresses
or strains, the geometries as well as the material constants of the particle and matrix. Following the idea of
Eshelby [1], the eigenstrains, or the stress-free strains, in a particle with material being identical to matrix, or
the so called equivalent inclusion, without applied stress correlate the constrained strains \( \sigma^0 \) by the
Eshelby tensor \( S_{ijkl} \) as follows if the deformed particle has been placed back into the matrix:

\[
\sigma^0_{ij} = S_{ijkl} e^0_{kl} \tag{3}
\]

The Eshelby tensor is only geometry dependent and generally takes the form of integrals. For simple
geometries, the components of \( S_{ijkl} \) can be given explicitly and are available in literatures [3,19].

For inhomogeneity problems, by defining the Young’s modulus ratio \( \beta = E_I/E_M \), where the subscripts I and
M represent the inhomogeneity and matrix, respectively, a particle under applied strains \( \sigma^0 \) to be replaced by
an equivalent inclusion without altering its stress state, the following relation should hold true according to
Hooke’s law:

\[
(1 - \beta) \sigma^0_{ij} + \beta \delta_\alpha e^0_{kl} = -\frac{YM}{1-2\nu_M} S_{ijkl} e^0_{kl} = -(1 - \beta) e^0_{ij} - \beta \delta_\alpha e^0_{kl} \tag{4}
\]
where $\beta_i = (1 + \nu_0)/(1 + \nu_i)$, $\beta_3 = (1 - 2\nu_0)/(1 - 2\nu_3)$, and $\nu$ is Poisson's ratio. Combining eqs (3) and (4), the
eigenstrains in each particle can be predicted from the given applied strains.

3. Solution procedures

The present computational model for spheroidal particle-reinforced materials is solved by the BEM.
However, the domain integrals in eqs (1) and (2) need to be transformed into the boundary-type integrals [20]
before discretization:

$$\int_{\Omega_i} \sigma_{ijkl} d\Omega = \int_{r_i} \nu_{ij} \tau_{ijkl} dT \quad \text{(5a)},$$
$$\int_{\Omega_i} \sigma_{ijkl} d\Omega + \sigma_{ijkl} = \int_{r_i} \xi_{ijkl} dT \quad \text{(5b)}$$

In eq (5) the assumption that the eigenstrains in each particle are constant has been used. It is known that the
generalized applied strain or the applied stress at each particle will be disturbed by other particles, especially
those in the adjacent zone surrounding the concerned particle. As a result, the applied strains so as to the
eigenstrains should be corrected in an iterative way in the solution procedure. After discretization and
incorporated with the boundary conditions, eq (1) can be written in the matrix form as:

$$Ax = b + Be$$

where $A$ is the system matrix, $B$ the coefficient matrix for eigenstrains, $b$ the right vector related to the
known quantities on the outer boundary, $x$ the unknown vector, $\varepsilon$ is the eigenstrain vector of all the particles
to be corrected in the iteration. It needs to be pointed out that the coefficients in $A$, $B$ and $b$ are all constants
so that they need to be computed only once. At the starting point, the vector $x$ is assigned by initial values
with the applied strains via the equations (2) at each position of the particles at the elastic state computed
irrespective of particles. Then the unknown vector $x$ can be computed by the following iterative formulae:

$$x^{(k+1)} = A^{-1}\left[b + Be^{(k)}\right]$$

where $k$ is the iteration count. Define the maximum iteration error $e_{\text{max}} = \max |e^{(k+1)} - e^{(k)}|$, which is the
maximum difference of eigenstrain components between the two consecutive iterations. The convergent
criterion in the present study is chosen as $E_{\text{max}} \leq 10^{-3}$. It should be addressed here that for the evaluation
of applied stresses of certain particle at $\Omega_i$, eq (2) should be reformed by excluding the current particle as

$$\sigma_{ij}(p) = \int_{\Omega_i} \varepsilon_{ijkl}(p,q)\cdot I_{ijkl}(q) dT(q) + \int_{r_i} \xi_{ijkl}(p,q)\cdot I_{ijkl}(q) dT(q) + \sum_{j=1}^{N_i} \varepsilon_{ijkl}^{(h)}(p,q) \int_{r_i} \xi_{ijkl}(p,q)\cdot I_{ijkl}(q) dT(q), \quad p \in \Omega_i$$

because the stress state at the due place are generated, in addition to the applied load, by the disturbances of
all other particles in the solution domain, where $N_i$ is the total number of particles. The flow chart of the
algorithm is shown in Fig. 1.

4. Numerical examples

A cube is chosen as the representative volume element (RVE) as shown in Fig. 2 with triply periodically
spaced spheroidal particles. The particle spacing is defined in Fig. 3a. The discretization is shown also in Fig. 3 for the outer boundary (b) and the interface in one octant (c), respectively. However, it needs to be pointed out that the interface discretization has no contribution to the degree of freedom of the problem for the present algorithm since the purpose of it is only for the numerical evaluation of domain integrals in eq (1) by boundary-type quadrature using eq (5) when the distances between \( p \) and \( q \) are relatively small. Otherwise, the one-point computing [21] can achieve enough accuracy as follows if the distances are relatively large:

\[
\int_{\Omega} \sigma_{ij}^* d\Omega = V \sigma_{ij}^* \quad (9a),
\]

\[
\int_{\Omega} \sigma_{ij}^* d\Omega = V \sigma_{ij}^* \quad (9b)
\]

where \( V \) stands for the volume of \( \Omega \) and \( O_{ij}^* = 0 \) if \( p \in \Omega \cup \Gamma \).

In order to assess the model with the eigenstrain formulation, the stresses across the interface of a single spheroidal particle in the RVE in triaxial tension are computed and compared with the exact solutions. The results are presented in Fig. 4 to show the validity and accuracy of the algorithm. It is interesting to see from Fig. 4 that the tangential stresses on the interface computed using the eigenstrain formulation take just the average values of the two sides, the particle and matrix. In the stress computation, the technique of distance transformation [22] is employed when the point \( p \) is very close to the interface. Nevertheless, the same problem with single particle can also be solved using the traditional BEM with the domain decomposition or sub-domain technique. The degree of freedom and CPU time of the two algorithms are listed in Table 1. The results are obtained by running the program on a desk-top computer (Intel Pentium Dual CPU, 1.60GHz), showing the efficiency of the eigenstrain formulation.

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Figs. 5a and 5b present the computed overall properties of the RVE and the CPU time, respectively, as a function of the total particle number, \( N_t \), while the relative particle sizes, \( r_0/s \) (Fig. 2a) are kept constant. It is
seen from Fig. 5a that the computed overall properties become stable when \( N_i \) reaches \( 10^4 \) and above. The degree of freedom for the eigenstrain formulation holds constant, say 492 in the calculation (Table 1), independent of \( N_i \). In contrast, the same problem is difficult to be solved using the domain decomposition algorithm on the desk-top computer.

Figure 5: Overall properties of the RVE (a) and the CPU time (b) as a function of total particle number, \( N_i \)

The effect of the relative particle size, \( r_p/s \), and the modulus ratio, \( E_i/E_{M0} \), on the overall properties of the RVE are presented in Figs. 6a and 6b, respectively. It can be seen from Fig. 6a that the moduli increase monotonically with \( r_p/s \) for hard particles but decrease for soft particles as expected. The elastic behavior of the overall properties with the variation of \( E_i/E_{M0} \) in Fig. 6b are similar to those in the two-dimensional case [17] that the most effective range of \( E_i/E_{M0} \) to the overall properties is between 0.1 and 10 while the stagnancy of properties are observed in ranges when \( E_i/E_{M0} \) is very small or very large.

Figure 6: Overall properties as a function of relative particle size, \( r_p/s \) (a) and the modulus ratio, \( E_i/E_{M0} \) (b)

The convergence behavior of the algorithm are presented in Fig. 7, showing that the iteration times varies with a number of factors such as the size of particles or volume fractions, the ratio of modulus as well as the loading manners, etc., which is considered to reflect the effects on the stress states at locations among

Figure 7: The convergence behaviors of the algorithm with respect to relative particle size, \( r_p/s \) (a) and the modulus ratio, \( E_i/E_{M0} \) (b)

The convergence behavior of the algorithm are presented in Fig. 7, showing that the iteration times varies with a number of factors such as the size of particles or volume fractions, the ratio of modulus as well as the loading manners, etc., which is considered to reflect the effects on the stress states at locations among
particles. However, the convergence can be generally achieved with a few iterations. The two principal factors need to be considered which influence the convergence behavior in the present algorithm. The first would be the mutual disturbances of the stress states among particles while the second would be the mismatches between particles and the matrix.

5. Conclusion

The novel computational model and solution procedure are presented for particle-reinforced composites using the proposed three-dimensional eigenstrain formulation of the BIE and solved by the BEM in the present study. As the unknowns appear only on the boundary of the solution domain, the solution scale of the problem with the present model remains fairly small in comparison with the traditional algorithm using FEM or BEM. The tangential stresses on the interface computed using the eigenstrain formulation take just the average values of the two sides, the particle and matrix. The effectiveness and efficiency of the proposed model as well as the convergent performance of the solution procedure are assessed by several numerical examples.

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References