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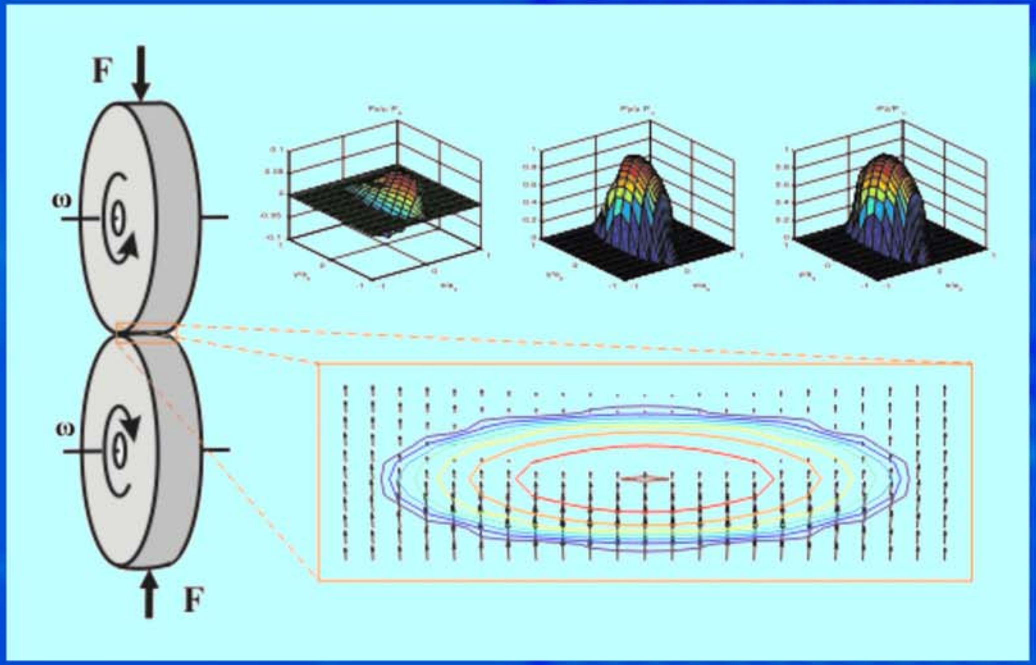

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R Abascal and M H Aliabadi

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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 techniques (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), and Montreal, Canada (2005), Paris, France (2006), Naples, Italy (2007).

The present volume is a collection of edited papers that were accepted for presentation at the Boundary Element Techniques Conference held at the Escuela Técnica Superior de Ingenieros of the Universidad de Sevilla, Spain, during 9-11th July 2008. Research papers received from 18 countries 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.

The Keynote Lectures were given by P. H. Wen, R. Gallego, O. Maeso, A. Sáez and V. Mantic.

The organizers are indebted to the University of Seville and to the Escuela Técnica Superior de Ingenieros for their support of the meeting. The 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 2008

Advances in Boundary Element Techniques

Contents

Advances in Boundary Element Techniques

Characterization of CNT-reinforced composites via 3D continuum-mechanics-based BEM

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Keywords: CNT-based composites, 3D standard BE formulations, special quadratures for singular and quasi-singular integrals, subregion-by-subregion technique.

Abstract. A continuum-mechanics-based Boundary Element Method (BEM) has been applied to estimate mechanical properties of carbon-nanotube-reinforced composites. The analyses have been carried out for three-dimensional representative volume elements (RVEs) of the composite. To model the thin-walled carbon nanotubes (CNTs), special integration procedures for calculating nearly-strongly-singular integrals have been designed, and a generic BEM substructuring algorithm allows modeling complex CNT-reinforced polymers, containing any number of nanotubes of any shape (straight or curved). Moreover, this substructuring algorithm, based on Krylov solvers, makes the independent generation, assembly, and storage of the many parts of the complete BEM model possible. Thus, significant memory and CPU-time reductions are achieved by avoiding an explicit global system of equations. Further CPU-time reduction is obtained by employing a matrix-copy option for repeated fiber reinforcement. Long and short fibers arranged according to square-packed and hexagonal-packed patterns can be considered to idealize the composite microstructure. Single-cell and multi-cell RVEs can be employed for evaluating the macroscopic material constants.

Introduction

In recent years, carbon nanotubes (CNTs) have been extensively employed to design advanced materials with improved physical properties. For example, as reported in [1] and [2], an excellent gain in the mechanical and thermal characteristics of polymeric matrices is achieved by spreading in the samples just a small portion of CNTs (about 1% of their weight). As a matter of fact, nanomaterials have developed an important role in many engineering fields as in electronics, sensors, computing, etc. Particularly in structural engineering, they have been combined with polymeric matrices to manufacture fiber-reinforced light-weight composites, actually a new generation of composites.

Available formulations for treating nanosysstems and their validity in the light of the different scales, going from atomistic to continuum models, are discussed in [3]. Considering the dimensions of nanosystems, molecular dynamics (MD) formulations should be employed to describe their physical behavior appropriately. Nevertheless, still constrained by limited computer power (even for present-day computers) to apply MD-based simulations to practical problems, attempts to assure the use of continuum-mechanics (CM) formulations to nanosystems have been made in the computational and experimental level [4-8]. Of course, because of their geometric similarity to hollow cylindrical tubes (single-walled or multi-walled), most of the CM-models for CNTs bases upon shell elements [4-7].

In [9], Chen and Liu apply a CM-based strategy to characterize CNT-reinforced composites. There, a 3D quadratic solid (brick) finite element is employed to model representative volume elements containing a single CNT (single-unit-cell RVEs), and a 2D quadratic 8-node finite element, to model multi-unit-cell RVEs (containing many CNTs). In the present work, single-unit and multi-unit cells are also considered to characterize CNT-reinforced composites, but a 3D standard boundary element technique is applied to solve the RVEs. In general, the strategy applied here comprises a robust subregion-by-subregion (SBS) technique, necessary for modeling heterogeneous materials, and efficient integration procedures, needed to evaluate the singular and nearly-singular integrals coming up in the matrix-coefficient calculations. Details of the SBS technique, based on Krylov solvers, are given in [10]. It accounts for the micromechanical modeling of composites consisting of a large number of fibers spread in a polymeric matrix. Moreover, to efficiently model composites containing geometrically and physically identical substructures, such as a number of identical fibers, a matrix-copy option is included. Thus, matrices for repeated subregions are immediately obtained simply by copy and rotation transformations. Here, just the diagonal-preconditioned biconjugate gradient solver (J-BiCG) is applied along with the SBS technique. In addition, discontinuous boundary elements [10-11] are employed to make the modeling of complex composites considerably easier.

As mentioned above, the other pillar of the strategy is the special integration schemes for coping with nearly-singular integrals resulting from either thin-walled domains or discontinuous boundary elements. In the applications here, for weakly-singular and nearly-weakly-singular integrals, numerical quadratures that combine triangle and polynomial coordinate transformations [10,12] are employed, and for the nearly-strongly-singular integrals, the line-integral approach detailed in Araújo and Gray [13], which uses closed expressions for the strongly-singular line integrals involved, is adopted.

For verifying the robustness of the strategy, 3D simulations of CNT-based RVEs derived from square-packed fiber arrays are considered. Possible future developments are also commented upon.

3D modeling of CNT-based RVEs

Provided that continuum mechanics models satisfactorily describe the mechanical behavior of CNTs, a 3D standard boundary element technique is employed to model general CNT-based composites consisting of a number of CNT fibers scattered in a material matrix (see Fig. 1). For that, the subregion-by-subregion (SBS) technique described in [10], essential to cope with heterogeneous materials, is applied. Here, structured matrix-vector products (SMVP) [10] and the special matrix-copy option for repeated substructures are considered.

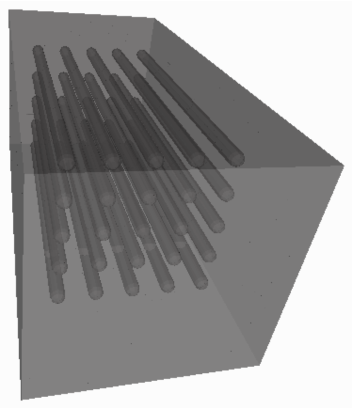


Figure 1: Fiber-reinforced composite

The SBS technique is similar to the element-by-element (EBE) technique, widely applied to solve large-order engineering problems with finite elements (FEM). Its main idea is to use an iterative solver, which allows working with smaller parts of the system of equations without explicitly assembling the global matrix. Yet, in the BE-SBS technique, contrary to EBE techniques, no data-structure optimization is further needed to reduce CPU time and memory, as coefficients belonging to edges shared by different subregions do not overlap. For n_s subregions, after introducing the boundary conditions, the BE global system of equations can be written as

$$\sum_{m=1}^{i-1}\left(\mathbf{H}_{im}\mathbf{u}_{mi}-\mathbf{G}_{im}\mathbf{p}_{im}\right)+\mathbf{A}_{ii}\mathbf{x}_i+\sum_{m=i+1}^{n}\left(\mathbf{H}_{im}\mathbf{u}_{im}+\mathbf{G}_{im}\mathbf{p}_{mi}\right)=\mathbf{B}_{ii}\mathbf{y}_i \qquad ,i=1,n_s\,, \tag{1}$$

where $\mathbf{H}_{ij}$ and $\mathbf{G}_{ij}$ denote the usual BE matrices obtained for source points pertaining to subregion Ω_i and associated respectively with the boundary vectors $\mathbf{u}_{ij}$ and $\mathbf{p}_{ij}$ at Γ_{ij} . Note that if $i \neq j$, Γ_{ij} corresponds to the interface between Ω_i and Ω_j; Γ_{ii} is the outer boundary of Ω_i. The SBS algorithm bases then on separately storing and manipulating the subsystems in Eq. (1). During the solution by means of some Krylov-type solver, the fiber-matrix interfacial conditions (here supposed to be perfectly bonded) are taken into account. In addition, for the *i*-th subregion, the following data structure for matrices $\mathbf{H}_i$ and $\mathbf{G}_i$ is adopted:

$$\begin{array}{l|ccc|c|ccc|l}
 & \multicolumn{3}{c}{\text{block 1}} & \multicolumn{1}{c}{\text{block 2}} & \multicolumn{3}{c}{\text{block 3}} & \\
\mathbf{H}_i = [& \mathbf{H}_{i1} & \cdots & \mathbf{H}_{i,i-1} & \mathbf{A}_{ii} & \mathbf{H}_{i,i+1} & \cdots & \mathbf{H}_{in} &] \\
\mathbf{G}_i = [& \mathbf{G}_{i1} & \cdots & \mathbf{G}_{i,i-1} & \mathbf{B}_{ii} & \mathbf{G}_{i,i+1} & \cdots & \mathbf{G}_{in} &]
\end{array} . \tag{2}$$

As shown by Araújo and Gray [14], using structured matrix-vector products (SMVP) increases the solver efficiency. Moreover, using discontinuous boundary elements considerably simplifies the modeling of complex CNT-based composites [10], and additional efficiency is also brought about by a "matrix-copy" option, which accounts for promptly obtaining the coefficient matrix for repeated substructures by copying and rotating a previously assembled one. Thus, matrix-assembly CPU time is considerably reduced for composites containing many physically and geometrically identical reinforcement elements (as usual).

Characterizing CNT-based composites

The material characterization of composites takes place on the micromechanical level, where the many parts compounding it (polymer and fibers) are directly modeled. In this paper, square-packed arrays are considered to idealize the smearing of fibers inside the matrix material (Fig. 2), and the BE SBS technique discussed above is applied to analyze the corresponding 3D RVEs. The macroscopic material parameters are then calculated solving the RVEs for proper loading cases [15].

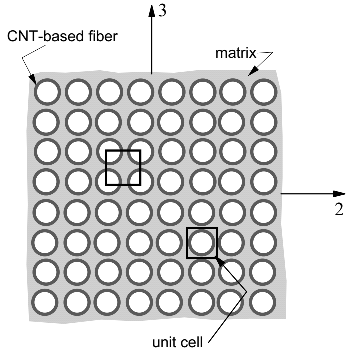
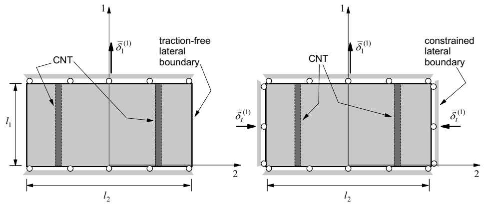


Figure 2: Square-packed array

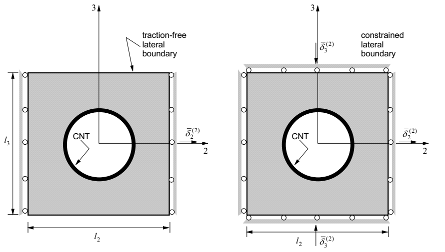
For measuring constants E_1, υ_{12}, and υ_{13}, one considers the specimen under stretching (or shortening) in the 1 principal material direction (fiber direction), and boundary conditions on the lateral surfaces perpendicular to the 2 and 3 directions, so as to simulate the surrounding medium (Fig. 3). The following expressions are employed [13]:

$$E_1 = \bar{\sigma}_1^{(1)} \left(\frac{l_1}{\bar{\delta}_1^{(1)}} \right), \qquad \nu_{12} = \nu_{13} = -\left(\frac{\bar{\delta}_2^{(1)}}{l_2} \right) \left(\frac{l_1}{\bar{\delta}_1^{(1)}} \right), \tag{3}$$



(*a*) 1st analysis (*b*) 2nd analysis

Figure 3: Boundary conditions in strain state 1



(*a*) 1st analysis (*b*) 2nd analysis

Figure 4: Boundary conditions in strain state 2

where $\bar{\sigma}_1^{(1)}$ denotes the average stress in the 1 direction of the RVE. For evaluating the constants E_2, υ_{23} and υ_{21}, strain state 2 in Fig. 4, in which $\bar{\sigma}_1^{(2)} = 0$, is considered. It turns out

$$E_2 = \bar{\sigma}_2^{(2)} \left(\frac{\bar{\delta}_2^{(2)}}{l_2} \right)^{-1} , \qquad \nu_{23} = -\left(\frac{\bar{\delta}_3^{(2)}}{l3} \right) \left(\frac{l_2}{\bar{\delta}_2^{(2)}} \right) , \qquad \nu_{21} = \nu_{12} \left(\frac{E_2}{E_1} \right) , \tag{4}$$

where $\bar{\sigma}_2^{(2)}$ is the average stress in the 2 direction of the RVE in 2nd analysis [13].

Applications and discussions

The BE SBS technique has been applied to evaluate engineering constants for square-packed CNT-based composites. In the numerical tests, a long CNT through single-unit-cell and 2×2 -unit-cell RVEs (Fig. 5 and Fig. 6) is considered. For comparison purposes, the same physical constants used by Chen and Liu [9] are adopted here: $E_{CNT} = 1{,}000 \, {}^{nN}\!/_{nm^2}$ GPa and $\nu_{CNT} = 0.30$ for the CNT, and $E_m = 100 \, {}^{nN}\!/_{nm^2}$ GPa and $\nu_m = 0.30$ for the polymer matrix. The cylindrical cross section of the CNT fibers has outer radius $r_0 = 5.0\,nm$ and inner radius $r_i = 4.6\,nm$. The RVE in Fig. 5 has dimensions $l_1 = 10\,nm$, and $l_2 = l_3 = 20\,nm$, and in Fig. 6, $l_1 = 10\,nm$, and $l_2 = l_3 = 40\,nm$.Discontinuous boundary elements, when needed, are generated by shifting the nodes interior to the elements a distance of $d = 0.10$ (measured in natural coordinates). In both analyses, an 8-node quadrilateral boundary element is adopted, and the tolerance for the iterative solver (J-BiCG) taken as $\zeta = 10^{-6}$.

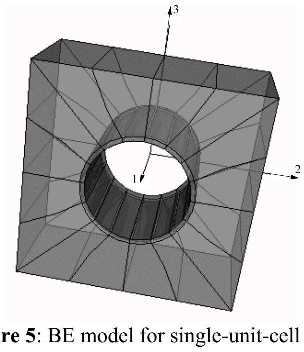


Figure 5: BE model for single-unit-cell RVE for long CNT square-packed arrays

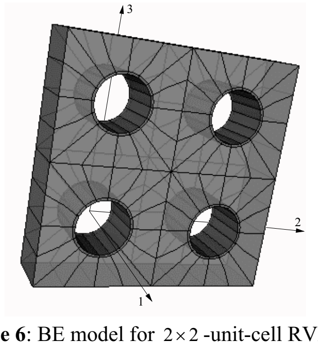


Figure 6: BE model for 2×2 -unit-cell RVE for long CNT square-packed arrays

The BE model in Fig. 5 has two subregions: one for the matrix material, one for the CNT. Both the matrix material and the CNT are modeled with 64 boundary elements, resulting in a total of 1,824 degrees of freedom for the global system. The 2×2-unit-cell RVE in Fig. 6 gives rise to a global system with 6,990 equations, the matrix material having been modeled with 224 elements (666 nodes), and each CNT, again with 64 elements (192 nodes). For the CNTs, the BE matrix is only assembled for one of them and then copied for the others. Discontinuous boundary elements are placed at the polymer-CNT interfaces in both models. The engineering constants estimated using these RVEs are shown in Tab. 1.

Table 1: Engineering constants (long CNT, square-packed array)

	single-unit-cell RVE		2×2-unit-cell RVE
	Chen & Liu (3D FE)	BE SBS	BE SBS
E_1/E_m	1.3255	1.3227	1.3225
$E_2/E_m, E_3/E_m$	0.8492	0.8323	0.8319
ν_{12}, ν_{13}	0.3000	0.2974	0.2975
ν_{23}	0.3799	0.3757	0.3597

For the single-unit-cell RVE, good agreement with the values obtained by Chen and Liu [9] using refined 3D FE models is achieved. It should also be noted that the n_{it}/n values, where n_{it} is the number of iterations for the solver and *n* the system order (*n*=1824), indicate good solver performance for both loading cases; these numbers were 0.28 for strain state 1 and 0.25 for strain state 2. The sparsity of the global matrices is 29% in both cases. For the 2×2-unit-cell RVE, no considerable changes are observed in the material constant values (see Tab. 1), which indicates that, for the determination of elastic constants, single-unit-cell-based RVEs satisfactorily represent the composite material. Moreover, these calculations highlight the computational efficiency of the matrix-copy option in case of repeated substructures (2×2-cell RVE). The n_{it}/n values once again indicate good solver performance; they are 0.21 in the strain state case 1 and 0.19 in the strain state case 2. The global matrix sparsity for this model (with 5 subregions) is 57%.

Conclusions

A 3D linear elasticity boundary-element formulation based upon a robust subregion-by-subregion (SBS) technique has been developed and proven to be very convenient to analyze representative volume elements of CNT-reinforced composites. First, the efficiency of the line-integral approach (see reference [13] for details) should be stressed: besides allowing modeling thin-walled domains, it also accounts for the reliable use of discontinuous boundary elements, so providing easier modeling of complex coupled domains by means of the SBS algorithm. The matrix-copy option also increases the efficiency of the BE SBS algorithm, avoiding the repeated calculation of matrices for identical substructures. This significantly reduces the total matrix-assembly time for fiber-/particle-reinforced composites, while the J-BiCG iterative solver has shown very good performance in general: for a stopping criterion of $\zeta = 10^{-6}$, $n_{it}/n < 0.20$ for the larger model (6,990 equations). In addition, more efficient Krylov solvers, such as the BiCGSTAB(*l*), can be applied. As a final comment regarding efficiency, note that the SBS approach effectively exploits the sparsity of the global system, usually high for many coupled models.

The computed effective material constants from the SBS algorithm compared very well with results from refined FE models [9]. Finally, a boundary element formulation is well suited to the study of composites. The determination of the effective elastic constants is dependent upon the surface stress solution, and as tractions are directly obtained from solving the boundary integral equations, this evaluation is straightforward. Moreover, for complex composites, surface meshes are simpler to generate than volume discretizations. By the way, the formulation is also adequate to simulate the matrix-fiber delamination. Non-linear interfacial constitutive laws can be readily implemented in the code. Of course, a parallel version of the SBS algorithm is straightforward.

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