# Substructure-based Block-diagonal Preconditioning for BEM Systems of Equations - Applications to the Micromechanical Analysis of General Composites

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**Abstract**. The boundary-element subregion-by-subregion (BE SBS) algorithm, developed in previous works, is employed to construct global block-diagonal preconditioners for BEM systems of equations. As the BE matrices for each BE subregion are independently assembled and stored, the block-diagonal-based preconditioners for the corresponding BE models are immediately constructed. A Krylov solver is embedded in the SBS algorithm, and this work, particularly, the Bi-CG solver is considered. The micromechanical analysis of large-order 3D representative volume elements (RVEs) of carbon-nanotube (CNT) composites are carried out to show the performance of the preconditioned iterative solver.

**Keywords**. 3D boundary-element models, subregions, Krylov solvers, block-diagonal preconditioning
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## INTRODUCTION

Fast reliable Krylov solvers have definitely contributed for the devising of efficient codes for solving large-order engineering problems [1, 2]. In these cases, in general, direct solvers present the following disadvantages: they may be exceedingly CPU time-consuming and memory-consuming. However, for general non-symmetric or indefinite matrices, like BE matrices, devising reliable iterative solvers is a still open question [3]. In these cases, Krylov solvers as the Bi-CGSTAB(*l*) [4] and the GPBi-CG (generalized product Bi-CG) [5] are among the potential good candidates. Anyway, truncating errors account for no guarantee concerning convergence reliability in practical applications. Preconditioning techniques have then been additionally employed. For BEM solvers, a series of preconditioners have been reported in the technical literature [6-8].

In this paper, the BE subregion-by-subregion (BE SBS) algorithm [9-10] is employed to construct global block-diagonal preconditioners for the BE systems of equations. The BE subsystems are independently assembled and stored, so that the global block-diagonal preconditioning can be easily formed and its **L** and **U** factors (indeed for the many on-diagonal submatrices) are easily calculated. As the Bi-CG solver, embedded in the SBS algorithm, presents a quite irregular convergence behavior, the efficiency of the preconditioner proposed will be evidenced. The microanalysis of carbon-nanotube (CNT) composites will be considered to show the performance of the preconditioning. The models contain up to several thousands of degrees of freedom

## THE BE-SBS ALGORITHM AND THE ASSOCIATED PRECONDITIONER

The boundary-element substructuring-by-substructuring (BE-SBS) algorithm [9,10] is comparable to the element-by-element (EBE) technique, developed to finite-element analysis (FEA), wherein a subregion or

substructure corresponds to a finite element. In this algorithm, the global response for a problem is obtained by working exclusively with its local full-populated subsystems of equations. No global explicit system matrix is assembled; no zero blocks are stored or handled. The boundary conditions are introduced during the matrix assembly for each subsystem, and the interface conditions (between the subdomains), given by

$$\begin{cases} \mathbf{u}_{ij} = \mathbf{u}_{ji} \\ \mathbf{p}_{ij} = -\mathbf{p}_{ji} \end{cases} \quad \text{at } \Gamma_{ij} \tag{1}$$

are directly (not iteratively) imposed in the matrix-vector products during the iterative solution process. For $n_s$ subregions, after introducing the boundary conditions, the BE global system of equations is then given by

$$\sum_{m=1}^{i-1} \left( \mathbf{H}_{im}\mathbf{u}_{mi} - \mathbf{G}_{im}\mathbf{p}_{im} \right) + \mathbf{A}_{ii}\mathbf{x}_i + \sum_{m=i+1}^{n_s} \left( \mathbf{H}_{im}\mathbf{u}_{im} + \mathbf{G}_{im}\mathbf{p}_{mi} \right) = \mathbf{B}_{ii}\mathbf{y}_i \,, \quad i = 1, n_s \,, \tag{2}$$

where $\mathbf{H}_{ij}$ and $\mathbf{G}_{ij}$ denote the regular BE matrices obtained for source points pertaining to subregion $\Omega_i$ and associated respectively with the boundary vectors $\mathbf{u}_{ij}$ and $\mathbf{p}_{ij}$ at $\Gamma_{ij}$. Note that if $i \neq j$, $\Gamma_{ij}$ denotes the interface between $\Omega_i$ and $\Omega_j$; $\Gamma_{ii}$ is the outer boundary of $\Omega_i$. $\mathbf{A}_{ii}$ and $\mathbf{B}_{ii}$ are obtained from matrices $\mathbf{H}_{ij}$ and $\mathbf{G}_{ij}$ after introducing the boundary conditions. As commented above, no explicit global system of equations is assembled, and the working subsystems are exactly those ones shown in expression (2). The matrix-vector and transpose-matrix-vector products are then calculated from the separate contributions from each subsystem, and the interface conditions are imposed in a direct way during the solver iterations. For a generic number of subregions, the diagonal blocks of the coupled system are given by

$$\mathbf{Q}_i = [-\mathbf{G}_{i1} \quad \cdots \quad -\mathbf{G}_{i,i-1} \quad \mathbf{A}_{ii} \quad \mathbf{H}_{i,i+1} \quad \cdots \quad \mathbf{H}_{in}] \,, \; i = 1, n_s \,, \tag{3}$$

where the $\mathbf{Q}_i$ matrices are straightforwardly formed having the subregion matrices for the model at hand. The construction of the global SBS-based block-diagonal preconditioner for the coupled system of equations (2) is then immediate. In the code, the BE-SBS-based preconditioner is employed to accelerate the Bi-CG iterations.

## RESULTS AND DISCUSSIONS

The performance of the SBS-based block-diagonal preconditioner is measured by analyzing the CNT-based composites shown in Fig. 1, in which representative volume elements (RVEs) based of $1 \times 1$, $2 \times 2$, and $5 \times 5$ unit

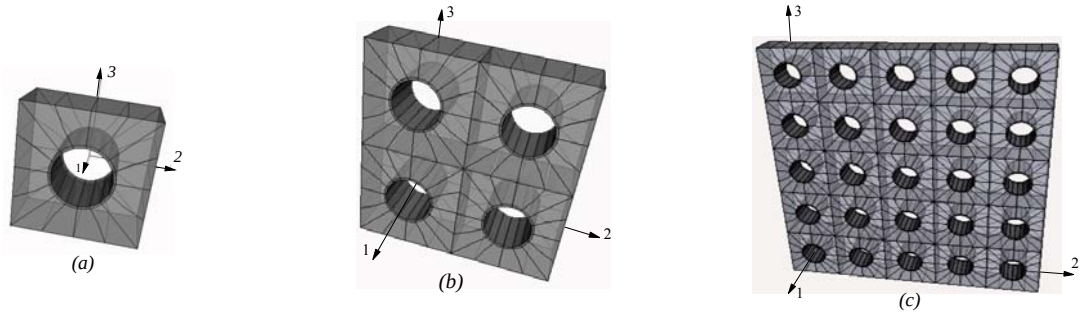



**FIGURE 1.** Square-packed long-CNT-based RVEs.

cells are employed. The long CNT fibers are geometrically defined by cylindrical tubes having outer radius $r_0 = 5.0\ nm$ and inner radius $r_i = 4.6\ nm$, and length $l_f = 10\ nm$. 8-node quadrilateral boundary elements are employed, and, in all analyses, $8 \times 8$ and 6 integration points are used for respectively evaluating all surface and line integrals involved in the special integration quadratures embedded in the code. In all (RVEs), the following pure phase constants are adopted [11]: for the CNT, $E_{CNT} = 1{,}000\ nN(nm)^{-2}$ (GPa), $\nu_{CNT} = 0.30$ , and for the matrix material, $E_m = 100\ nN(nm)^{-2}$ (GPa), $\nu_m = 0.30$ . The tolerance for the iterative solver (Bi-CG) is taken as $\zeta = 10^{-8}$, and the analyses were carried out at a notebook with dual intel 2.26GHz processor, and 3GB of random access memory. Important model data are provided in Table 1. The engineering parameters extracted from the analysis of all the RVEs shown in Fig. 1, not shown here, are in very good agreement with the results calculated by Liu and Chen [11] via finite-element analysis. In Table 2, results showing the performance of the preconditioners are presented. Compared to the Jacobi preconditioner, a considerable acceleration of Bi-CG solver is observed when the BE SBS-based block-diagonal one is applied (e.g. the Bi-CG solver becomes about 24 times faster for the $5 \times 5$ -unit-cell RVE under strain state 1). The decaying of the Euclidean residual norm, $\|\boldsymbol{\delta}\|_2$ , as a function of the iteration order for both preconditioners is also shown in Fig. 2. This graph clearly shows the superiority of the preconditioning proposed in this work.

## CONCLUSIONS

The BE SBS technique proposed in previous papers ([9], [10]) is straightforwardly used to construct block-diagonal preconditioners for BE systems of equations. The performance of this preconditioning was verified by analyzing CNT composite RVEs. Observing the Table 2, and graphs in Figure 2, we see that the BE-SBS-based

**TABLE 1.** Model data for the square-packed long-CNT RVEs

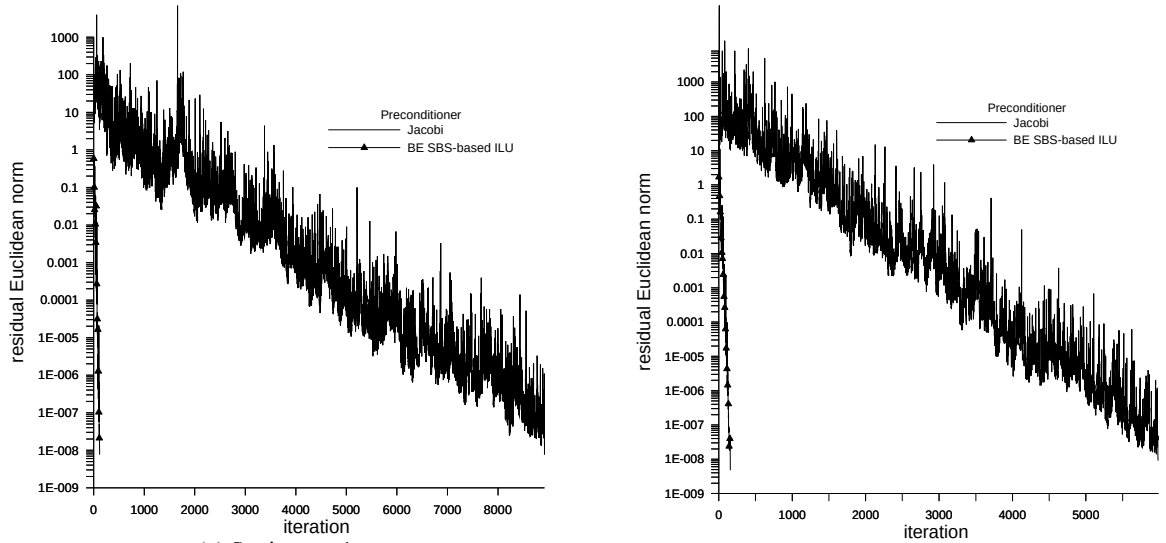
| model | nsub* | nel** | nnodes† | ndof‡ | sparsity (%) |
|---|---|---|---|---|---|
| $1 \times 1$ | 2 | 128 | 608 | 1,824 | 29 |
| $2 \times 2$ | 8 | 512 | 2,660 | 7,980 | 81 |
| $5 \times 5$ | 50 | 1,344 | 17,456 | 52,368 | 97 |

*n. of subregions; **n. of elements; †n. of nodes; ‡n. of degrees of freedom

**TABLE 2.** Performance data for the square-packed long-CNT RVEs; $\text{tol} = 1.0 \times 10^{-8}$

| **model** | **system order** | **n. of iterations (BE SBS-based ILU)** | **n. of iterations (Jacobi)** | **CPU time (*s*) (BE SBS-based ILU)†** | **CPU time (*s*) (Jacobi)** |
|---|---|---|---|---|---|
| 1x1 unit cell, strain state 1 | 1,824 | 57 | 561 | 2 | 5 |
| 1x1 unit cell, strain state 2 | 1,824 | 73 | 621 | 2 | 6 |
| 2x2 unit cells, strain state 1 | 7,980 | 81 | 2241 | 11 | 104 |
| 2x2 unit cells, strain state 2 | 7,980 | 104 | 1805 | 12 | 84 |
| 5x5 unit cells, strain state 1 | 52,368 | 116 | 8920 | 119 | 2917 |

†Including the LU decomposition CPU time




(*a*) Strain state 1




(*b*) Strain state 2

**FIGURE 2**. Residual norm vs. iteration: $5 \times 5$ -unit-cell, square-packed long CNT

block-diagonal preconditioning, compared to the Jacobi (diagonal) one, is considerably more efficient. In fact, the BE-SBS-based block-diagonal preconditioning states a transition between direct and iterative solvers, in the sense that the less the number of interfaces, the closer to the global system matrix the preconditioning matrix, $\mathbf{Q}$ , is. In addition, knowing that the global coupled system is highly sparse, we can well conclude that the preconditioner proposed will be a good approximation of the global system matrix, one of the requirements for finding good preconditioners. Generally speaking, the larger the size of the subsystems, the higher the cost for constructing the preconditioner, but a better approximation for the global system is achieved, reducing then the number of iterations. Furthermore, being this preconditioner based on the BE-SBS algorithm, its parallelization is immediate.

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