

Hierarchical-ACA DBEM for Anisotropic Three-Dimensional Time-Harmonic Fracture Mechanics

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Abstract. A hierarchical BEM solver for the analysis of three-dimensional anisotropic time-harmonic fracture mechanics problems is presented. A thorough investigation on the relations and interactions between the numerically computed anisotropic fundamental solutions and the algorithm used to approximate the blocks of the hierarchical matrix, namely Adaptive Cross Approximation, is carried out leading to the employed computational strategy. The use of the hierarchical matrices and iterative solvers is proved as an effective technique for speeding up the solution procedure and reducing the required memory storage in time-harmonic three-dimensional anisotropic fracture mechanics problems.

Introduction

Boundary element techniques have proved successful especially in fracture mechanics and elastodynamics, mainly due to the simplification of the modeling as well as the accuracy in the representation of the involved fields. However, rather poor attention has been devoted to 3-*D* fracture dynamic problems in anisotropic materials, especially for solids with finite dimensions. This is essentially due to the lack of closed form expressions for the 3-*D* anisotropic elastodynamics fundamental solutions with the consequent increase in the required computational time. This occurrence and the features of the BEM resolving matrix, which is non-symmetric and fully populated, represent an important limitation for the usage of the method in large scale simulations. Recently, investigations have been carried out to improve boundary elements solution methods and different techniques have been developed among which those based on hierarchical matrices appear very promising for anisotropic problems [1]. In the present paper a fast BEM (HBEM) for the time-harmonic analysis of 3-*D* cracked anisotropic bodies, based on hierarchical matrices and the use of the Adaptive Cross Approximation algorithm (ACA) for their efficient computation, is investigated. This approach has been already successfully used for isotropic dynamic fracture mechanics [2]. However, the analogous anisotropic problem presents additional complexities related to the oscillatory behaviour of the problem fundamental solutions and the need to compute them numerically [3]. Actually, the ACA algorithm convergence and performances are theoretically established for asymptotically smooth kernels and thus, for kernels which do not satisfy this condition, like the anisotropic 3-*D* time-harmonic elastodynamics ones, ACA should be interpreted as a rank-revealing decomposition whose applicability and efficiency have to be heuristically verified. This couples with the use of numerical integration schemes for the fundamental solution computation, which is expected to affect ACA, and consequently the performances of the method. So the hierarchical representation coupled with ACA for anisotropic 3-*D* time-harmonic fracture mechanics BEM deserves investigation to assert its effective application.

Hierarchical dual boundary element method for anisotropic time-harmonic elastodynamics

Boundary integral equations and standard collocation dual BEM. The integral equations needed in the Dual Boundary Element Method for fracture mechanics are obtained by: i) collocating the boundary integral representation for the displacements on the external boundary of the body and on one of the crack surfaces, ii) collocating the boundary integral representation for the tractions on the second crack surface

[1]. Accounting for the decomposition of the time-harmonic fundamental solution into the static and the frequency dependent contributions [4], the displacement boundary integral equation for a point \mathbf{x}_0 belonging to the external boundary of the body subjected to a load with circular frequency ω is written as

$$c_{ij} u_j(\mathbf{x}_0) + \oint_{\Gamma} T_{ij}^S u_j d\Gamma - \int_{\Gamma} U_{ij}^S t_j d\Gamma + \int_{\Gamma} T_{ij}^R u_j d\Gamma - \int_{\Gamma} U_{ij}^R t_j d\Gamma = 0 \quad (1)$$

where c_{ij} are the free term coefficients and the symbol \oint stands for Cauchy principal value integral due to the $|\mathbf{r}|^{-2}$ singularity of the of the T_{ij}^S kernel. For a point belonging to one of the crack surfaces, namely the lower surface, the displacement integral equation specializes as

$$c_{ij}^- u_j(\mathbf{x}_0^-) + c_{ij}^+ u_j(\mathbf{x}_0^+) + \oint_{\Gamma} T_{ij}^S u_j d\Gamma - \int_{\Gamma} U_{ij}^S t_j d\Gamma + \int_{\Gamma} T_{ij}^R u_j d\Gamma - \int_{\Gamma} U_{ij}^R t_j d\Gamma = 0 \quad (2)$$

where \mathbf{x}_0^- and \mathbf{x}_0^+ are the two coincident crack points belonging to the lower and upper crack surfaces. The traction integral equation collocated at the point \mathbf{x}_0^+ belonging to the second crack surface, namely the upper one is written as

$$\frac{1}{2} [t_j(\mathbf{x}_0^+) - t_j(\mathbf{x}_0^-)] + \oint_{\Gamma} S_{ijk}^S n_j u_k d\Gamma - \oint_{\Gamma} D_{ijk}^S n_j t_k d\Gamma + \int_{\Gamma} S_{ijk}^R n_j u_k d\Gamma - \int_{\Gamma} D_{ijk}^R n_j t_k d\Gamma = 0 \quad (3)$$

where n_j are the components of the outward normal at \mathbf{x}_0^+ , again the symbol \oint denotes the Cauchy principal value integral associated with the $|\mathbf{r}|^{-2}$ singularity of the of the D_{ijk}^S kernel and \oint stands for Hadamard principal value integral, originating from the presence of the $|\mathbf{r}|^{-3}$ singularity of the S_{ijk}^S kernel. The boundary element discretization of these integral equations and the standard collocation procedure lead to a resolving system of linear equations of the form

$$\mathbf{A} \mathbf{X} = \mathbf{Y} \quad (4)$$

where the vector \mathbf{X} contains the unknown boundary displacements or tractions and the crack unknown displacements and the right-hand-side \mathbf{Y} is obtained considering the prescribed displacements and tractions

Hierarchical Dual BEM. Grouping the collocation points and the the elements involved in the boundary element model, namely eq. (4), in a hierarchical way leads to so-called hierarchical matrix, which allows to build a data-sparse approximation \mathcal{A} of the DBEM resolving matrix \mathbf{A} [5, 6]. The hierarchical representation \mathcal{A} of a boundary element matrix consists of a collection of hierarchically ordered matrix blocks. Some blocks, corresponding to sets of collocation nodes and integration elements which are sufficiently far apart from each other, admit a special compressed low-rank representation associated with their approximation by separable expansions of the corresponding kernels. The subdivision of the BEM collocation matrix into blocks is based on a *hierarchical partition* of the mesh nodes aimed at grouping subsets of nodes corresponding to contiguous collocation nodes and integration elements, on the basis of a geometrical criterion. For the problem in hand, this partition has to take into account that different boundaries (external and cracks) and different integral operators are involved (displacements and tractions integral equation) [1]. The built partition is stored in a tree structure of index subsets, called *cluster tree*. The cluster tree is used to recursively form pairs of clusters so as to define the *block tree*, which provides the hierarchical block subdivision of the matrix. The blocks generated from the hierarchical partition can be classified into: i) *non-admissible blocks*, which need to be represented entirely; ii) *admissible blocks*, which admit a compressed low-rank approximation. The admissibility of a *block* is checked against a suitable geometrical condition, depending on a separation parameter $\eta > 0$, which controls the trade-off between the number of admissible blocks and the the quality of the approximation [1]. The low-rank approximation of the admissible blocks is computed by the Adaptive Cross Approximation algorithm (ACA), which appears to be very efficient [7]. The low-rank approximation of the admissible blocks through ACA provides remarkable computation and storage memory savings, because only few entries of the original matrix blocks need to be computed and stored. Moreover, the hierarchical representation of the resolving BEM system accelerates the matrix-vector product, which is the core operation when iterative solvers are used. This can provide significant reduction in the solution time. In the present paper, the hierarchical BEM computational scheme employed is based on the following features. Eight-node super-parametric constant elements with central collocation node and iso-parametric discontinuous eight-node quadratic elements are

used in the discretization of the external boundary and crack surfaces, respectively. The binary *cluster tree* is built by bisection, and the hierarchical representation of the matrix is stored in the associated quaternary *block tree*. The block admissibility condition is implemented by using the *bounding boxes* technique for the nodes and elements clusters [6]. Finally, the admissible blocks are approximated by employing the Adaptive Cross Approximation algorithm that allows to compute adaptively the approximation, according to an intrinsic stopping criterion related to a pre-set required accuracy ε_c [1]. The fundamental solution kernels are numerically computed according to the scheme proposed by Wang and Achenbach [4]. Once the hierarchical representation has been set up, the system solution is computed by using a preconditioned *GMRES* iterative solver. An *LU* hierarchical preconditioner built from a coarse approximation with accuracy ε_p of the original collocation matrix is used. Further details on the computational scheme can be found in Ref. [1].

Fundamental solution and low-rank blocks numerical investigation

The essential aspect for the application of the hierarchical matrices and ACA to collocation BEM models when closed-form analytical fundamental solutions are not available is the influence of the computational scheme employed for the numerical evaluation of the involved kernels. For anisotropic time-harmonic 3-D problems this issue couples with the oscillatory behaviour of the kernels, which implies the heuristic verification of ACA applicability, efficiency and performances. To investigate the low-rank approximation through ACA of the admissible blocks in the anisotropic time-harmonic 3-D collocation BEM, some representative results are here presented and discussed. They are obtained with reference to the problem of an anisotropic bar made of a trigonal material (sapphire), whose material properties are given in Ref. [1]; however, it is emphasized that the drawn conclusion are general and were verified also for other configurations and materials. The fundamental solution computation accuracy is at first ascertained. The displacements kernels and their derivatives are computed according to the scheme proposed by Wang and Achenbach [4] by mapping the original integration spherical domain over the $[0, 1] \times [0, 2\pi]$ domain where standard Gauss quadrature of order $M \times N = 3J \times 6J$ is applied. Fig. 1 shows graphically the dependency of the U_{ij} , $\partial U_{ij}/\partial x_3$ and $\partial^2 U_{ij}/\partial x_3^2$ kernels accuracy from the integration order J and the spatial oscillatory index $\xi = \omega r/c_{min}$, where r is the maximum distance occurring between the field and source point in the problem and c_{min} is the minimum phase velocity. Similar results are obtained also for the other kernels. The kernel accuracy is measured by introducing the error index $err(\mathbf{K}_{ref}, \mathbf{K}) = \|\mathbf{K}_{ref} - \mathbf{K}\| / \|\mathbf{K}_{ref}\|$ where $\mathbf{K} = [K_{ij}]$ is the considered kernel, \mathbf{K}_{ref} is its converged value and $\|\cdot\|$ denotes the Frobenius norm. The analysis of the data shows that to obtain a desired accuracy of the computed kernels, the requested quadrature order grows with the excitation frequency. Additionally, it was also found that the requested quadrature order grows with the degree of anisotropy of the material. This behaviour influences the approximation of the low-rank blocks through ACA. Indeed, the ACA algorithm computes the approximating low-rank block by using some entries of the original block, which are obtained by integrating the fundamental solution kernels. Therefore, the accuracy in the computation of the fundamental solution kernels affects the performance of ACA. The effect is shown in Figs. 2 and 3 where the convergence study in terms of block rank and memory ratio (low-rank memory storage over full rank

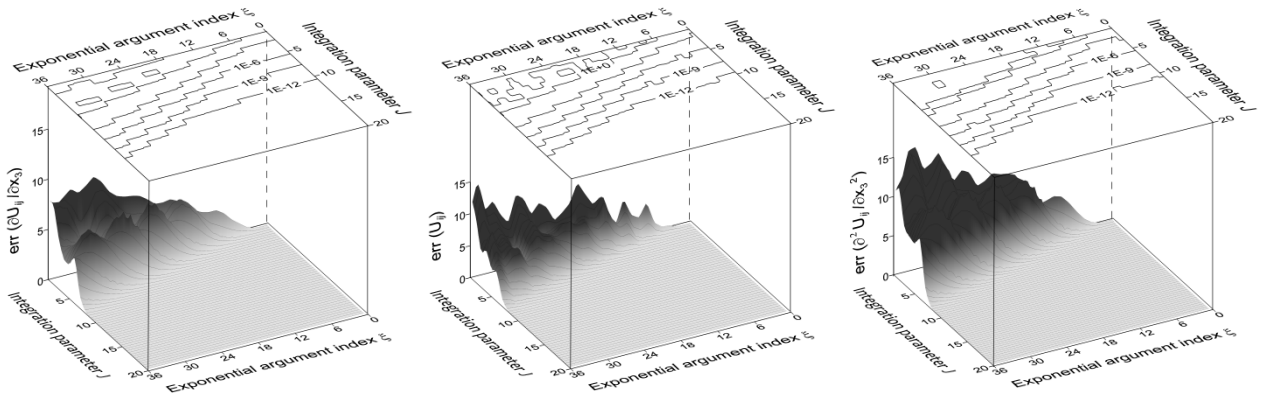


Figure 1. Error index for the U_{ij} , $\partial U_{ij}/\partial x_3$ and $\partial^2 U_{ij}/\partial x_3^2$ kernel.

memory storage) for low-rank blocks involving the displacement and traction boundary integral equations, respectively, is presented. The geometrical configuration and the mesh employed are shown in the figures where the element clusters are indicated by gray colour and the nodes of the collocation points clusters are evidenced by circles. The considered node and element clusters belong to the hierarchical representation of the BEM collocation matrix built by setting the admissibility parameter $\eta = 2.0$ and the minimum number of nodes belonging to the cluster tree leaves equal to 72. Convergence was investigated with respect to the fundamental solution integration order for (i) different dimensionless circular frequencies $\bar{\omega} = \omega L/c$, where c and L are reference phase velocity and length (taken as the corresponding maximum in the considered problem), and (ii) different values of the ACA accuracy parameter ϵ_c . The results obtained show that the convergence of the block approximation built through ACA requires adequate accuracy in the kernel numerical computation, which depends on the circular frequency. The convergence threshold depends on: (i) the circular frequency, as the higher the frequency the higher the convergence rank and memory storage; (ii) the degree of anisotropy, as the convergence rank and memory storage grows with respect to this; (iii) the accuracy required to ACA, as the higher the accuracy the higher the convergence rank and memory storage. The presented data refer to the single block but a similar behaviour is found for each low-rank block and then for the overall hierarchical matrix. Thus, there is a link between the ACA convergence and effectiveness and the integration scheme employed to compute the fundamental solution kernels. Actually, to ensure a successful and effective approximation of the low rank block, the integration order used for the computation of the fundamental solutions has to be set so as to guarantee an error in their computation sufficiently smaller than the selected ACA accuracy. At this point the guidelines for a computational strategy to apply the elastodynamic hierarchical dual boundary element method with ACA blocks approximation to anisotropic time-harmonic elastodynamic fracture mechanics can be drawn.

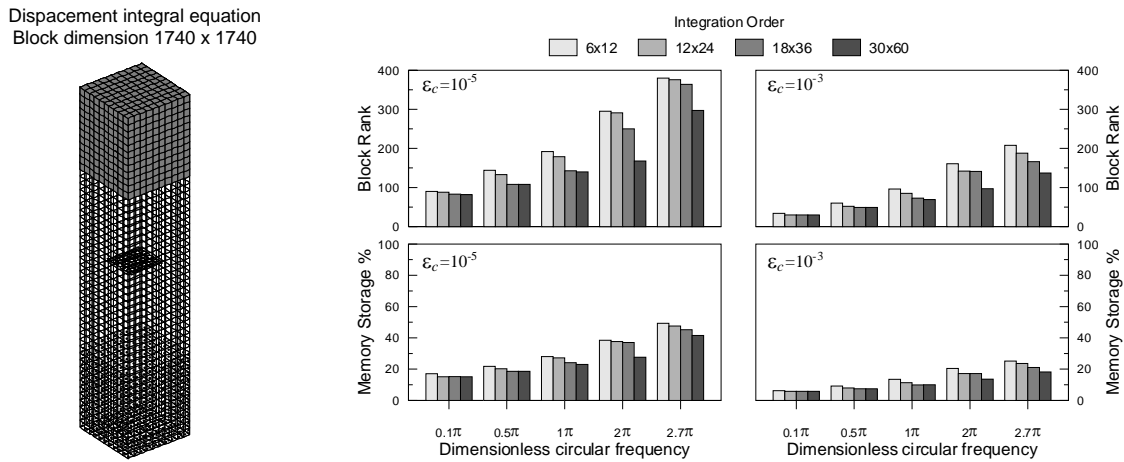


Figure 2. Low rank blocks performance analysis for displacement boundary integral operator.

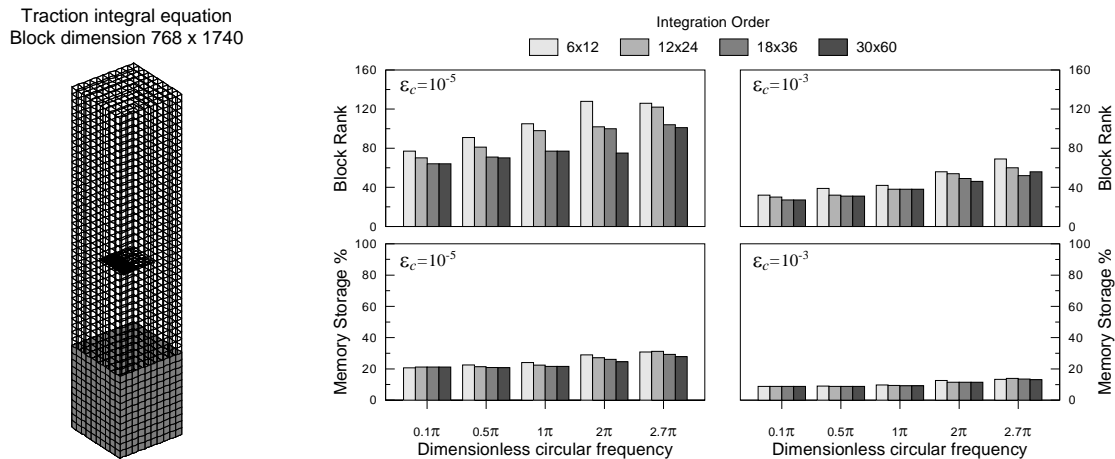


Figure 3. Low rank blocks performance analysis for traction boundary integral operator.

First a preliminary assessment of the accuracy requirements for the fundamental solution numerical evaluation is performed by determining the integration order J required to achieve a selected kernel accuracy as a function of the spatial oscillatory index ξ . This allows to obtain a relation between intervals of ξ and the integration order J , which gives a prescribed accuracy of the fundamental solution. At this point, the strategy for the computation of the blocks of the matrix hierarchical representation can be deployed. The fundamental solutions required accuracy, that is the defined kernel error, is selected sufficiently lower than the prescribed ACA accuracy ε_c . The computation of the hierarchical matrix blocks is then performed by using an integration order for the fundamental solutions evaluation which is adaptively determined according to the stated $\xi - J$ relationship. It is observed that the adaptive integration scheme essentially improves the efficiency of the full-rank blocks computation, which are not well separated and then give rise to a quite wide variation of ξ leading fundamental solutions integration order with J varying from low to higher values. On the other hand, the low rank blocks are well separated and they generally do not present meaningful variations of ξ , whose values vary around those computed by using the clusters distance. Accordingly, the fundamental solution integration order used in low-rank blocks actually comes out from the clusters distance and remains practically constants. It is relatively high due to the clusters separation. In this sense it can be stated that the adaptive integration scheme do not influence the efficiency of low rank blocks computation through ACA.

Elastodynamic hierarchical dual boundary element method performances

The effectiveness of the method is ascertained by analyzing the following method performances: i) assembly time, ii) solution time, iii) memory storage, which are compared with the corresponding quantities of the standard collocation BEM. The results presented here refers to the analysis of a clamped bar, made of trigonal material (sapphire), with length $L = 1m$ and square section of side $W = 0.2m$. A centered square crack is considered with side length $a = 0.1m$. The bar is subjected to time-harmonic tractions applied at its free end. Both the uncracked and cracked configuration have been analyzed by using different meshes with increasing number of degrees of freedom. Fig. 4 shows the results for the HBEM performances obtained considering two values of the ACA accuracy parameter ε_c and two values of the exciting frequency $\bar{\omega}$. It is observed that the HBEM reduces both assembly and solution time as well as memory storage for all of the considered configurations. Its efficiency improves with the problem size, namely the number of degrees of freedom, and for lower accuracies, when ACA uses a lower number of the collocation matrix coefficients to approximate the low-rank blocks. It is worth to note that the efficiency of the method appears better for the uncracked configuration. This is related to the use in the uncracked case of constant elements only. Actually the crack discretization scheme employs eight node discontinuous elements, which can affect the hierarchical matrix construction efficiency because some nodes of an element can belong to different blocks. It is observed that the excitation frequency slightly influence the method performances. In particular, as the excitation frequency grows the HBEM performance indexes grows as a consequence of the ACA behaviour. Analysis of the performed numerical examples allows also an estimate of the numerical complexity for the assembly time, solution time and memory storage. It was found a complexity of order $N^a \ln N$ for the solution time and memory storage with the parameter a slightly depending on ε_c and growing with it; for the solution time the assessed complexity is of order $N^2 \ln N$. It is finally remarked that this conclusions here drawn and discussed with reference to a specific problem have been verified for other configurations and materials.

Conclusions

A time-harmonic fast BEM based on hierarchical matrices has been presented for the analysis of anisotropic three-dimensional elastodynamic fracture mechanics problems. The ACA algorithm is used to approximate the admissible low-rank blocks and an iterative GMRES solver is employed for the solution in conjunction with the hierarchical representation of the collocation matrix. The crucial effects of the numerical computation of the anisotropic time-harmonic fundamental solutions on the low-rank block approximation by ACA have been addressed, and it was found that the method performances severely depend on the accuracy of the scheme used to compute the kernels. Provided that adequate fundamental solution computational scheme is employed, the analyses have also shown the efficiency of the approach, with

respect to the conventional collocation BEM, in terms of assembly time, solution time and storage memory. Indeed the proposed technique allows remarkable savings in the context of very computationally intensive problem and its efficiency grows with the size of the problem. An estimate of the method computational complexity, based on the numerical experiments carried out, has also been presented to assess the computational resources required by a problem of a given size.

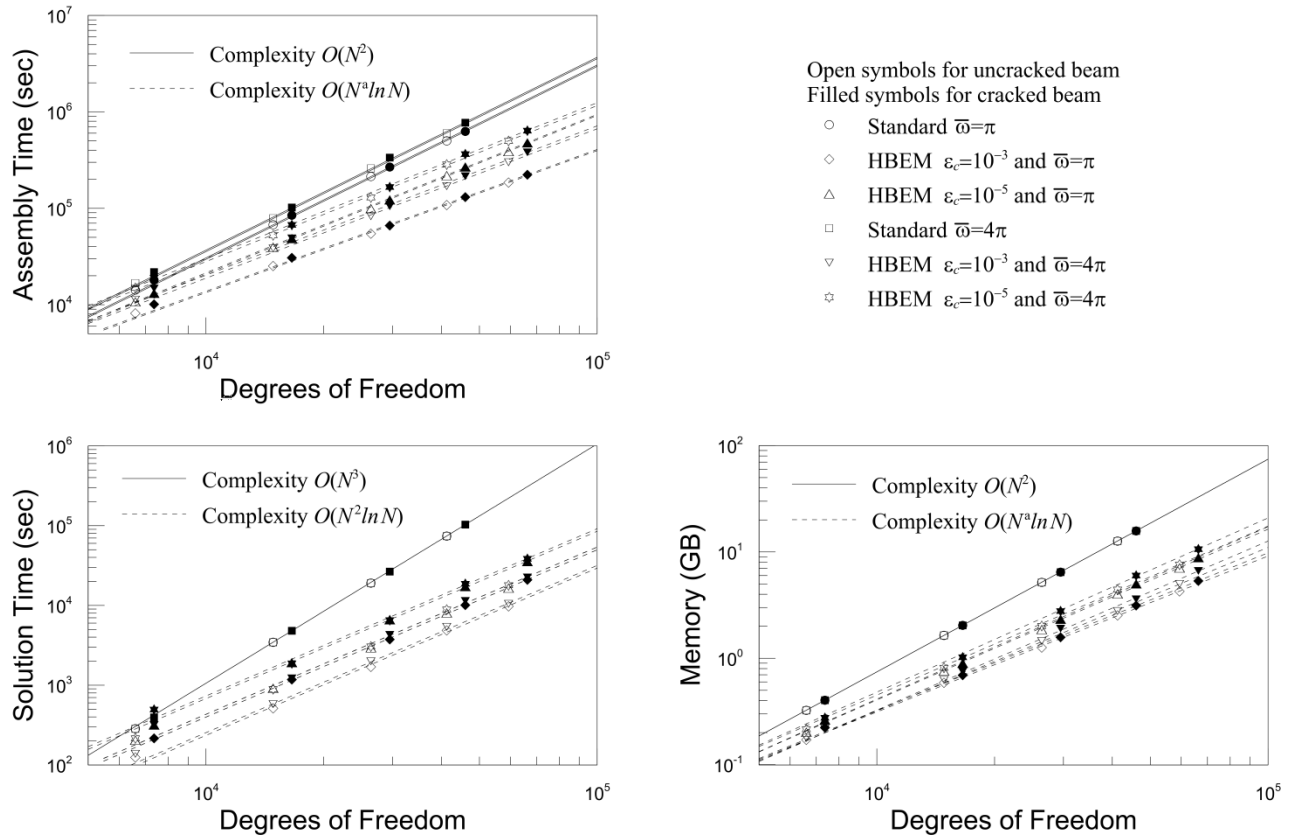


Figure 4. Complexity analysis.

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