MOLECULAR MECHANICS SIMULATIONS OF CARBON NANOSTRUCTURES USING MULTI-SCALE BOUNDARY CONDITIONS

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Summary The method of Multi-Scale Boundary Conditions is applied to simulations of carbon nanostructures: graphite sheets and diamond. It allows simulation of a deformable boundary, thus reducing the size of computational domain and, consequently, the cost of computations. This approach is tested on model problems and results are in good agreement with the benchmark full domain solutions. The method can be useful for simulations of real-life experiments on nanoindentation of diamond and layered graphite.

INTRODUCTION

Atomistic simulation methods, such as molecular dynamics and molecular mechanics, are very important and find application in many areas of research providing information about processes happening on microscale level. However applicability and effectiveness of these methods hinge upon ability to fulfil very large scale computations. That makes these methods restricted to solving systems, which are too small even for nano scale problems. Solvable systems are of several orders of magnitude smaller than scales of real-life nanomechanical experiments. This situation is resolved with the usage of the so-called multiscale methods, when atomistic simulations are used only for a reduced domain (fine scale), and continuum finite element or meshless methods are used for the rest of the domain (coarse scale)[1]. Method of Multi-Scale Boundary Conditions (MSBCs) makes it possible to eliminate the coarse scale dimensions of freedom and simulate only the fine scale by imitating the so-called deformable boundary, when the boundary of a reduced domain behaves as if it were a part of a full domain.

MATHEMATICAL FORMULATION

The main idea of the method is based on Fourier analysis of regular atomic lattice structures [2]. For a periodic crystal lattice it is possible to derive displacements of the layer of atoms which is next to the fine scale domain (we denote it as n=1 layer) in terms of the neighboring boundary layer of the fine scale (layer n=0) and the last (boundary) layer of the full domain. We denote the last layer of the full domain as $n=a$, where a is the *coarse scale parameter*. In general form, the MSBCs can be written as $\mathbf{u}_1 = \boldsymbol{\Theta}(\mathbf{u}_0) + \boldsymbol{\Xi}(\mathbf{u}_a)$, where specific forms of operators $\boldsymbol{\Theta}$ and $\boldsymbol{\Xi}$ depend on the geometry of a crystal lattice, interatomic forces between its atoms, and a value of the coarse scale parameter. In case when the boundary of the full domain is fixed, so that displacements of atomic layer $n=a$ are zero, we have left only with the first part of this equation. In a more extended form it can be written as:

$$\mathbf{u}_{1,m} = \sum_{m'=m-m_c}^{m+m_c} \boldsymbol{\Theta}_{m-m'}\, \mathbf{u}_{0,m'} ,$$

where index m is used for numbering of atoms in the layer n (here n=0,1,a) and m_c is a truncation parameter. Typical shape of components of matrices $\boldsymbol{\Theta}_m$, called the *kernel matrices*, is given below at figure 1.

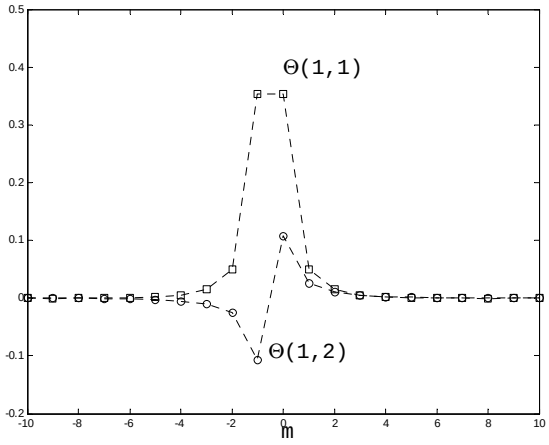

Figure 1.

It is important that the components of the kernel matrices $\boldsymbol{\Theta}_m$ decay fast with the growth of $|m|$. This allows using a small value of the truncation parameter m_c in the above equation. Also, we mention that the assumptions of regular crystal

lattice and linear deformations, which were used for MSBCs derivation, have to hold only in a small vicinity of the deformable boundary, where the MSBCs are applied. At the same time, large deformations (including plasticity) are allowed inside the reduced domain and far enough from the deformable boundaries.

SIMULATION RESULTS

We consider the following model problem (see Figure 2): a rectangular sheet of graphite is fixed at all four sides, and initial displacements are applied in several steps to one of the atoms in the middle of the domain (the loaded atom is circled at the figure) in a direction perpendicular to the plane of the sheet. Here, we apply the MSBCs at two sides – left and right. Value of the coarse scale parameter for both deformable boundaries is a=6. The whole full domain is shown at Figure 2. Filled circles – are atoms belonging to reduced domain (fine scale) and void circles – atoms of coarse scale domain, which are excluded from molecular mechanics calculations.

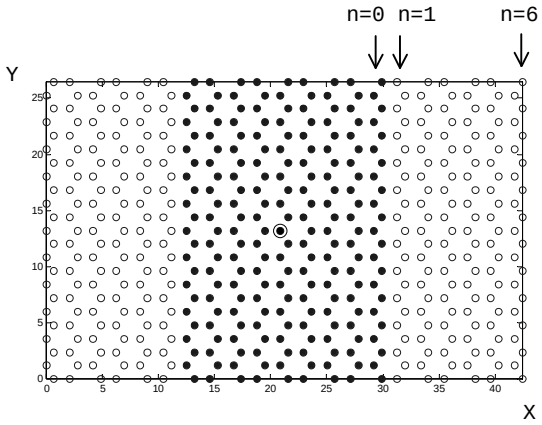

Figure 2.

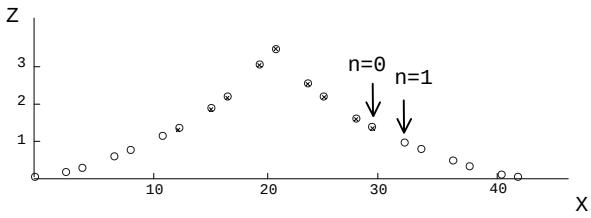

Figure 3.

Results of the computations are presented at Figure 3, where vertical displacements of atoms located along the horizontal middle line are plotted. The circles represent the exact solution for the full domain, which was obtained by regular molecular mechanics simulations. The crosses represent the approximate solution obtained for the reduced domain with the MSBCs applied. Similar results were obtained for a hexagonal domain, where all six boundaries were modeled using the MSBCs. We used hexagonal shape for reduced domain, because, in this case, all the boundaries correspond to an identical crystallographic orientation; that allows using the same kernel matrices as for the rectangular domain. This method was also applied to nanoindentation of diamond. In that case we obtain the kernel matrices for a slab-like boundary layer of atoms. Their behavior is similar to that shown at Figure 1. Application of the method to three-dimensional atomic lattice structures, such as diamond, is tractable, as soon as boundaries of the reduced domain are drawn along a limited number of crystallographic planes.

CONCLUSIONS

The method of Multi-Scale Boundary Conditions helps to overcome the limitations of atomistic simulations, regarding the size of a computational domain. By using sufficiently large values of the coarse scale parameter a it may allow simulations of real-life experiments. Current efforts are being made to apply this method to simulation of experimental results on nanoindentation of diamond and layered graphite presented in [3].

References

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