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Multiscale Topology Optimization using Atomic Finite Element Method (AFEM)

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Abstract
In this research, the applicability of Atomic Finite Elements to topology optimization is analyzed. To do this, a structural atomic simulation based on the AFEM is developed and analyzed, and then used to implement a molecular level topology optimization software.

Key words:
AFEM, topology, optimization

Introduction

Topology optimization is a computational method used to determine the structure that best responds to an engineering application, given some restrictions. The model used to represent the structure analyzed is often based on multiscale simulation, in which critical parts are described by atomic models, while other parts are described by Continuum Mechanics.

This method, however, is limited by the model used to simulated the structure and by the corresponding computational cost. This restriction is even more important in the atomic simulation, in which the cost grows with the number of atoms, and, thus, with the size of the structure. In that sense, AFEM rises as an alternative of atomic modeling with order O(N).

In this research, the atomic simulation using AFEM is developed and analyzed, to determine the most efficient version. Later, this method is applied to topology optimization, in order to determine the effectiveness of the combination, when compared to other methods.

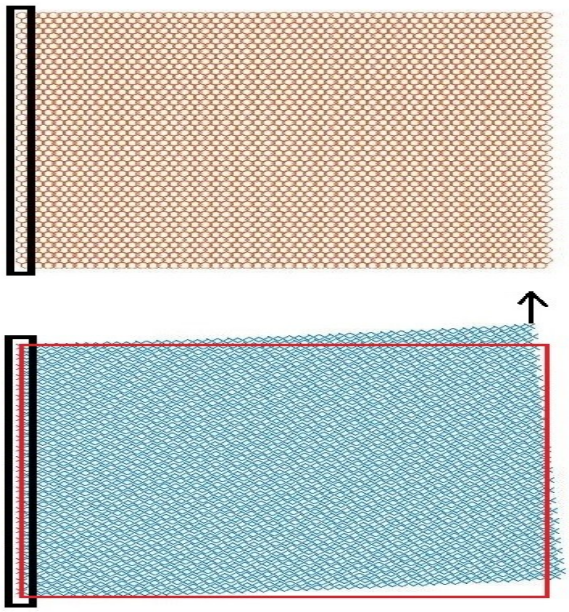

Image 1. Two dimensional structure subjected to external force. On top, original shape and below, deformed shape after application of force. The red box in the second figure indicates the original shape, for comparison

Results and Discussion

At the present stage, the atomic simulation using AFEM is being developed. The current program is capable of simulating 2D structures with external forces acting on them, with up to 40.000 atoms. It's expected that this number can grow to up to 1.000.000.

Furthermore, recent advancements in the code have reduced the execution time in 90% when compared to previous implementations. Greater reductions are being analyzed.

Conclusions

The results obtained so far, indicate that quality of the code is critical to efficiency. Further improvements in the implementation must be pursuit, to achieve a program capable of dealing with bigger structures in a shorter amount of time.

DAMASCENO, Daniela Andrade. Nonlinear atomic-scale finite element method for the modeling of nanomaterials and nanostructures. 2017. 1 recurso online (110 p.). Tese (doutorado) - Universidade Estadual de Campinas, Faculdade de Engenharia Mecânica, Campinas, SP.