Coupling atomistic models with continuous finite beam elements

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ABSTRACT

Concurrent simulations of atomistic (discrete) and continuum models are one key to perform static calculations of large atomistic structures. Occurring ghost forces at the interfaces between discrete (atomistic) and continuous regions are a major challenge for the definition of such interfaces. The so called *virtual projection method* [1] is a class of force-based a/c schemes which reduce (or even avoid) ghost forces. This class of coupling schemes is able to deal with atomistic models consisting of bonded, multi-body interactions and continuous finite elements having translational and rotational degrees of freedom. In finite element codes dealing with molecular mechanics in the way described in [2], the implementation of the *virtual projection method* is restricted to the element level by formulating a transitional finite element.

The present work uses the *virtual projection method* to perform multiscale simulations of carbon nanotubes (CNTs). Atom interactions are described by the *dreiding* potential [3] considering 2-, 3- and 4-body interactions. First a representative continuous finite beam element is developed which represents the atomistic structure of a CNT [1]. Observing the internal energy of the atomistic structure in a molecular static simulation under different deformations leads to an approximation of the correlation between the deformation and the energy. This serves as the internal energy of a finite 3D beam element. After that concurrent multiscale simulations consisting of atomistic regions and the developed 3D finite beam elements can be performed. At the interfaces the regions are coupled by the *virtual projection method*. The results are compared to molecular static simulations serving as references.

Following this procedure multiscale simulations on super CNTs of order 1 are performed to show the capability of the *virtual projection method* and the presented representative continuous finite beam elements even in the context of more complex structures.

References

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