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MATERIALS AND STRUCTURES SYMPOSIUM (C2)
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DEVELOPMENT OF NEW MD/FE COUPLING METHOD FOR MULTISCALE MODELING OF NANOSTRUCTURED SPACE MATERIALS

Abstract

A better understanding of the universe leads human to explore the space, the newest realm of discoveries. Everyday, larger number of science and technology disciplines getting involved in space applications. Material science along with traditional continuum mechanics and molecular physics play an important role in developing desired innovative materials applicable for constructing economical spacecrafts, satellites and other space products. Multiple-scale modeling and characterization of new nanostructured materials has introduced as a significant approach to reduce empirical, time-consuming and costly prototype testing. Multiple-scale methods have become not only popular but also necessary in the past decade because of the following reasons. Firstly, this class of simulation methods has important and useful application in nanotechnology research and developing nanoscale materials. Another factor is the existence of connection between microscale physics and macroscale deformation which is confirmed by experiments. Finally, the ongoing explosion in computational power has made the linking of disparate length scale feasible. One major category of multiscale models couples a region described with full atomistic detail interacting with another region using continuum mechanics concepts which simultaneously and continually transfer information from one domain to the other and so called concurrent methods. Critical segment of the model is transition area where the two domains overlap and should interact and transfer boundary conditions in a smooth and seamless fashion. Quasicontinuum (QC) is one of the most successful concurrent atomistic/continuum coupling models which apply Molecular Dynamic simulation for microscale and Finite Element Method for macroscale. However, this method has some limitations and two major approximations; the use of representative atoms and implementation of Cauchy-Born (CB) rule. The new formulation couples atomistic domain simulated by Molecular Dynamic (MD) with continuum domain modeled by Nodal Position Finite Element Method (NP-FEM) based on quasi-nonlocal Quasicontinuum method in order to avoid above approximations and address existing method limitations. The advantage of using NP-FEM is that the description of Hamiltonian in this model is based on nodal positions instead of nodal displacements and this is consistent with the description of Hamiltonian in MD. The proposed method is suitable to model and characterization of new nanostructured materials. This presentation consists of detailed description of the newly proposed method and its application in modeling novel space materials like cross-linked silica aerogel.