Paper ID: 4797
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MATERIALS AND STRUCTURES SYMPOSIUM (C2)
New Materials and Structural Concepts (4)

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PROPOSING NODAL POSITION FINITE ELEMENT METHOD APPLICABLE TO MODELING OF NEW SPACE MATERIALS

Abstract

The exploration of the universe from space is one of the most challenging and controversial issues for international space community from feasibility and financial point of view. Constructing spacecrafts, satellites, space launch vehicles and other space products in an affordable way have been many scientists' favourite topic. To achieve these goals, developing new materials with desirable density and toughness applicable for space product structure can be a promising way. In order to develop new space materials with suitable physical and mechanical properties and to avoid empirical methods as well as time-consuming and costly prototype testing, a multiple-scale modeling and characterization of materials like cross-linked aerogel is suggested.

The reason for choosing multiple-scale modeling is that the traditional continuum mechanics models cannot accurately describe the influence of the nanostructure upon the mechanical properties of the newly developed materials. On the other hand, full atomistic description is capable but unrealistic, since even the use of state-of-the-art parallel supercomputers can only handle a limited number of atoms (109), corresponding to less than one cubic micron.

The multi-scale modeling leads to a coupled system of equations of finite element (FE) method in continuum and molecular dynamics (MD) in atomistic domain. This promising approach increases the efficiency of the simulations substantially and connects the atomistic to the continuum regions without compromising accuracy. However, the description of the Hamiltonian of the traditional FE is based on the nodal displacement field and it is inconsistent with the MD description that uses the position vector of the atoms. To overcome this inconsistency and unify the description, the new Nodal Position Finite Element Method (NP-FEM) is proposed.

The new NP-FEM formulation uses nodal positions as basic variables instead of nodal displacements, which allows the direct coupling of the FE and MD Hamiltonians used in multi-scale modeling. In addition, the new NP-FEM addresses the limitations of the existing FEM in dealing with large rigid body motion coupled with the small elastic deformation. As a result, it eliminates the need to decouple the elastic deformation from the rigid-body motion and consequently the errors caused by approximation in kinematics relationship and the accumulated numerical errors arising from the incremental solution procedure of existing FEM.

This presentation consists of full description of the newly proposed nodal position finite element method and its application in multi-scale modeling of new nanostructured space materials like cross-lined aerogel.