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Finite Element Molecular Modeling: A Structural Method for Large Deformations

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Abstract : Atomic interactions in molecular systems are mainly studied by particle mechanics. Nevertheless, researches have also put on considerable effort to simulate them using continuum methods. In early 2000, simple equivalent finite element models have been developed to study the mechanical properties of carbon nanotubes and graphene in composite materials. Afterward, many researchers have employed similar structural simulation approaches to obtain mechanical properties of nanostructured materials, to simplify interface behavior of fiber-reinforced composites, and to simulate defects in carbon nanotubes or graphene sheets, etc. These structural approaches, however, are limited to small deformations due to complicated local rotational coordinates. This article proposes a method for the finite element simulation of molecular mechanics. For ease in addressing the approach, here it is called Structural Finite Element Molecular Modeling (SFEMM). SFEMM method improves the available structural approaches for large deformations, without using any rotational degrees of freedom. Moreover, the method simulates molecular conformation, which is a big advantage over the previous approaches. Technically, this method uses nonlinear multipoint constraints to simulate kinematics of the atomic multibody interactions. Only truss elements are employed, and the bond potentials are implemented through constitutive material models. Because the equilibrium bond- length, bond angles, and bond-torsion potential energies are intrinsic material parameters, the model is independent of initial strains or stresses. In this paper, the SFEMM method has been implemented in ABAQUS finite element software. The constraints and material behaviors are modeled through two Fortran subroutines. The method is verified for the bond-stretch, bond-angle and bond-torsion of carbon atoms. Furthermore, the capability of the method in the conformation simulation of molecular structures is demonstrated via a case study of a graphene sheet. Briefly, SFEMM builds up a framework that offers more flexible features over the conventional molecular finite element models, serving the structural relaxation modeling and large deformations without incorporating local rotational degrees of freedom. Potentially, the method is a big step towards comprehensive molecular modeling with finite element technique, and thereby concurrently coupling an atomistic domain to a solid continuum domain within a single finite element platform.

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