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Development of a 4-node finite element for the computation of nano-structured materials

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Abstract

The molecular structure of a material determines its mechanical, thermal and chemical properties. Thus, to better understand characteristic mechanical properties like damping behavior or softening, in principle, one just has to model the interactions of a sufficiently large number of atoms. Various force field approaches have been proposed for that purpose, which are based on molecular-dynamic simulations, or rather quantum-mechanical ab initio calculations. They provide the potential energy of a structure in dependence of sort and number of chemical and physical bonds. In general, the different energy forms can be represented by nonlinear normal, bending and torsional springs which suggests the use of a finite element code. However, standard finite elements like truss, beam or shell elements are not very applicable because of the interaction of many atoms and, considered from a mechanical perspective, the absence of rotational degrees of freedom. For example, a bending of beam elements would lead to unrealistic constraints of neighboring molecular groups. In order to overcome this disadvantage, a new 4-node finite element is introduced, which uses only translational degrees of freedom and therefore is capable of representing the different energy forms exactly.

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1. Introduction

Engineers and scientists have the common goal of better understanding and predicting the behavior of all kinds of materials. The material properties can gradually change under chemical, thermal and mechanical loads. However,

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physical-mathematical models developed for this purpose are usually not comparable with one another since they are often based on different length scales:

$$\text{quantum scale} \leftrightarrow \text{nanoscale} \leftrightarrow \text{microscale} \leftrightarrow \text{macroscale}$$

For example, on the macroscale that is frequently used by engineers, material may be regarded as homogeneous and isotropic while on the microscale cracks or other material inhomogeneities have to be considered.

Looking at the opposite end of the length scale, the Schrödinger equation [1,2] describes the movement of individual protons, neutrons and electrons and yields probability distributions for the steady state. Since electrons are much lighter and faster than nuclei, the latter are often assumed to be fixed. This assumption, known as Born-Oppenheimer-approximation, is the basis for the numerically complex "ab initio" approaches [3] which are regarded as "correct" and the numerically more efficient "semi-empirical" approaches. For the ab initio models, after estimating an initial configuration of the orbitals, the Schrödinger equation is solved explicitly.

In order to be able to examine larger molecules with the presently available computational power, findings obtained from ab initio approaches on the quantum scale must be transferred to the molecular or rather nanoscale [4]. The molecular-mechanical approaches [5] are capable of describing interactions of a larger number of atoms, but can no longer calculate the movement of single electrons. For more information about these so-called "force fields" see e.g. [6–8].

From the authors' point of view, the force field method provides a suitable interface between physically accurate quantum-mechanical approaches, on the one hand, and numerically efficient continuum-mechanical approaches, on the other hand. Force fields adequately describe the real physics which makes them attractive as a potential tool to explain many material properties like damping behavior, fatigue cracking or fracture behavior. In principle, one just needs to apply a sufficiently large number of atoms for this purpose. In addition, force fields provide an excellent theoretical basis for the application of the finite element method due to the analogy to multi-body systems with atoms as mass points and the different kinds of bonds as spring elements. Finite element programs offer comprehensive pre- and postprocessing tools as well as sophisticated solvers which allow for the modelling, computation and visualization of even more complex structures.

Up to now, mainly standard elements such as beam or shell elements have been used to calculate nano-structured materials, see e.g. [9,10]. However, an atom, as a point object, cannot have rotational degrees of freedom which complicates the application of these standard elements. For instance, the bending of a beam leads to improper constraints in adjacent molecular parts. To overcome this disadvantage, in the following a new 4-node element is introduced, which has only translational degrees of freedom and thus is capable of properly representing the different nonlinear force field potentials.

2. Force fields

The force field method utilizes nonlinear spring elements for the chemical and physical bonds. The stiffness of each individual spring element does not only depend on the nearest neighboring atoms, but also crucially on the subsequent atoms or rather parts of molecules. Therefore, in each particular case it has to be checked whether the selected force field approach contains the molecules of interest. Among the most well-known approaches are CHARMM [11], MM3 [12], MM4 [13] as well as AMBER and ECEPP [14]. The material parameters given in the following sections hold for the DREIDING force field [15].

2.1. Potential energy

The potential energy

$$E = E_{\text{val}} + E_{\text{nb}} \tag{1}$$

of a molecule or rather an entire structure consists of energies of the valence (or bonded) interac-