

A CONTINUUM MECHANICAL SURROGATE MODEL FOR ROD-LIKE ATOMIC STRUCTURES BASED ON GEOMETRICALLY EXACT BEAMS

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The behavior of molecular structures can be accurately studied using Molecular Dynamics (MD). Unfortunately, these simulations modelling each atom individually usually lead to high computational costs due to the large number of degrees of freedom. One possible way to reduce these costs is to replace the atomistic description of the system under consideration with a continuum mechanical one.

In this work, we are in particular interested in rod-like structures, i.e. in slender bodies where the extension in one direction is clearly larger than in the remaining two dimensions. Well-known examples for such materials on the nanoscale are carbon nanotubes (CNT) and macromolecules such as DNA or bundles of cellulose. In these cases, the theory of geometrically exact beams introduced by Simo [1] (also referred to as Reissner-Simo beam theory) presents a promising candidate for a continuum formulation that admits setting up a suitable surrogate model that can be used to carry out computations more efficiently than it was possible using the MD model.

The essential step to establish such a surrogate model is to transfer the material-specific properties from the atomistic description to the continuous one. To this end we outline an appropriate systematic procedure that accomplishes this parameter estimation task. In particular, to set up a continuum mechanical formulation, we need to determine the initial geometry and the strain-stress relationship of the atomistic description. This procedure, in fact, turns out to be also applicable in more general situations where a classical representative volume element (RVE) cannot be defined in a straight-forward fashion.

Once such a beam characterization for the mechanical properties of the original atomic structure is obtained, certain benchmark problems can be studied both in a fully atomistic fashion using MD simulations and, on the other hand, in continuum mechanical calculations based on finite elements. The numerical results can then be checked against each other in order to determine the accuracy of the constructed surrogate model.

REFERENCES

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