Coupling of Finite Elements and Molecular Dynamics at Finite Temperature

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ABSTRACT

Behavior of many materials shows effects that cannot be modelled on the macroscopic scale. These effects require micro-scale modeling and often quite different computational methods compared to those on the macro scale are used for this purpose (e. g. discrete methods instead of continuous methods). Particularly for design of new materials, for which the lack of experimental data excludes development of purely phenomenological material laws, predictive modeling of effects on the micro-scale may be crucial. Therefore, it is attractive to combine different computational models within one framework. This is the goal of multi-scale modeling of materials.

Many methods have been developed in the past to bridge the huge gap between molecular dynamics and classic continuum mechanics (e.g. the quasicontinuum method [1]). One important challenge is the modelling of atomistic effects at non-zero temperature. Many multiscale methods treat temperature as a modification of the atomic potential by assuming some simplification (e.g. quasi-harmonic approximation). Therefore, these theories basically represent a zero Kelvin multiscale simulation with a modified atomistic potential.

However, these simplification fails to recover some effects, which arise from the increasing vibration of the atoms at higher temperature (e.g. change of lattice). Therefore, although the aforementioned concepts provide useful results in many applications, it is also interesting to investigate multiscale theories that directly treat atomic vibrations in a different way.

Multiscale-simulation requires some kind of coarse-scaling technique. The fine-scale is molecular dynamics and the coarse scale is finite elements, so there needs to be some kind of coupling mechanism. In this work a new approach to couple molecular dynamics and finite element discretizations of non-linearly elastic continua at finite temperature is introduced, which has been implemented into the simulation software NumPro, developed at the institute. In addition, a number of test cases have been calculated and results are presented.

REFERENCES

[1] E. B. Tadmor, R. E. Miller: *Modeling Materials*, Cambridge University Press, 2011