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DIRECT COUPLING BETWEEN MOLECULAR DYNAMICS AND CONTINUA: A THERMO-MECHANICAL APPROACH

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Multiscale models, which couple an atomistic domain (to capture realistic physical mechanisms) to a continuum region (to reduce computational cost), are today applied to a variety of physical problems including frictional contact and crack nucleation and propagation. However, most of these applications are limited to zero Kelvin. In this presentation, we begin with the application of one of the existing multiscale model known as the *Bridging Domain* method [1] to a normal contact problem at finite temperatures. The difficulty of using this method at finite temperatures is illustrated with the observation of the development of strong thermal gradients and related thermal expansion/contraction near the handshake/coupling region.

We present a new multiscale model [2] to couple molecular dynamics with finite elements at finite temperatures using spatial filters. The need of spatial filters is demonstrated by simulating a one-dimensional model at constant finite temperature. The mismatch in the dispersion relations between continuum and atomistic models leads, at finite temperature, to unwanted mesh vibrations, which are illustrated using a standard least square coupling formulation. We propose the use of spatial filters with the least square minimization to selectively damp the unwanted mesh vibrations. The restitution force from the generalized Langevin equation is modified to perform a two-way thermal coupling between the two models. Several numerical examples, including a dynamic impact test, are shown to validate the proposed coupling formulation in two-dimensional space. In particular, our reduced-model calculations match accurately full-MD simulations, and the total energy of the system is preserved at all times.

REFERENCES

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