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MULTISCALE SIMULATION OF ATOMISTIC SYSTEMS BASED ON EXTENDED SPACE/TIME FINITE ELEMENT METHOD

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ABSTRACT

In this presentation, we present applications of extended space/time finite element method for coupled atomistic-continuum simulation of nanoscale material. Our method is motivated by the limitations of the single scale approach such as the finite element approximation in representing the fine scale physics in both the spatial and temporal scale. As such, multiscale approximations are established over the entire space-time domain based on the framework of space/time discontinuous Galerkin method and the extended finte element method. The unique features of the proposed method are as follows: By augmenting the shape function basis with enrichment function, the method does not require substantial efforts in refining the spatial mesh or time step for simulating small scale systems. With the use of physics-based enrichment, we show that the continuum and atomistic representations can be consistently linked and this naturally results in a reflectionless condition at the continuum/atomistic interface without the need to impose numerical dissipation. After an outline of the basic methodology and implementations, realization of these important properties will be illustrated through example problems.

References

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