

A MULTISCALE MESHFREE METHOD FOR THE ANALYSIS OF NANOSCALE MATERIALS

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A great challenge in terms of modeling and simulation of nanostructured materials are the extremes in the gap in terms of both length and time scales that are involved in the applications. Most of the existing simulation approaches are not well suited for analyzing these types of applications since they are typically formulated at a single time or length scale. Implementation of these single scale approaches results in either incapability in describing the physics or inability to accommodate the scales that are involved.

We have developed a bridging scale concurrent approach for the correct simulation and thus design of such hybrid devices/structures. In the current work, the coarse scale approximation is established by constructing meshfree[1] shape function in a coarse scale model. The total scale solution is obtained from the molecular dynamics equation and the difference between the total scale and coarse scale gives the fine scale part of the solution. With a defined projection operation, the multiscale decomposition ensures a seamless link between the coarse and fine scales. Compared with most of the existing multiscale methods, neither “handshake” region nor mesh refinement is required. The meshfree approximation is applied to the entire domain of the problem, and the molecular structure is embedded in selected regions of interest. Therefore, a unique feature of the proposed method is that the meshfree discretization co-exists with the molecular structure in these enriched regions. The robustness of the method will be illustrated from a few examples.

References

1. Liu, W.K., S. Jun, and Y.F. Zhang, *Reproducing Kernel Particle Methods*. International Journal for Numerical Methods in Fluids. **20**(8-9): p. 1081-1106,1995.