Modeling and Simulation Framework at the Nanoscale

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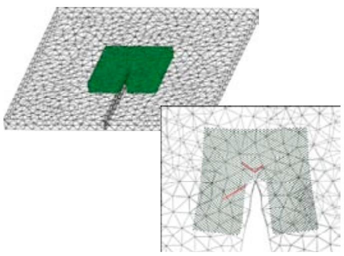
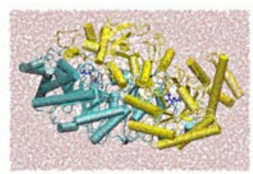
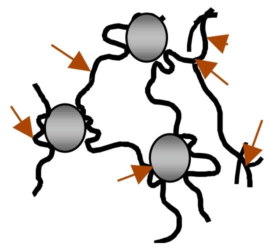
The RPI team is developing a suite of hierarchical multiscale models and scale bridging procedures aimed at analysis, design and manufacturing of nanomaterials and nanodevices. We are in the process of validating the capabilities developed for three applications including nanocomposites[1], lattice structures [2] and proteins (see Figure below).



Lattice Structures



Protein in solvent



Nanocomposites

We are focusing on both the information-passing or concurrent discrete-to-continuum multiscale bridging approaches. In the concurrent approach, both the discrete and continuum scales are simultaneously resolved, whereas in the information-passing schemes, the discrete scale is modeled and its gross response is infused into the continuum scale. Among the information-passing bridging approaches, the focus is on the generalized mathematical homogenization theory[3,4], the model reduction methods[5] and Multiscale Enrichment based Partition of Unity Method (MEPU)[6]. Using the information-passing approach we were able to predict the mechanical behavior of polymer-based nanocomposites filled with nanoparticles[1].

References

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[2] D.K. Datta, C. Picu, M. Shephard, "Composite Grid Atomistic Continuum Method: An adaptive approach to bridge continuum with atomistic analysis" to appear in International Journal for Multiscale Computational Engineering, (2004).

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[4] J. Fish and C. Schwob, "Towards Constitutive Model Based on Atomistics," International Journal of Multiscale Computational Engineering, Vol. 1 pp. 43-56, (2003).

[5] B. Gressick, J. Wen and J. Fish, "Order Reduction for Large Scale Finite Element Models," submitted to International Journal for Multiscale Computational Engineering, (2004).

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