

Modeling and Simulation Framework at the Nanoscale

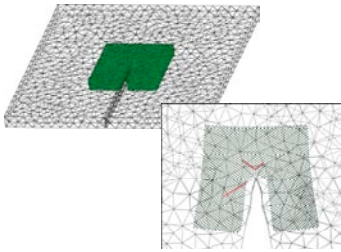
NSF Proposal Number: 0211474

PIs: J. Fish, C. Picu, K. Anderson and M. Shephard

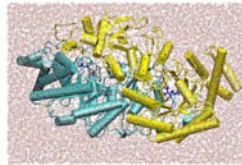
Students and Associates: Z. Yuan, W. Chen, B. Gressick, J. Critchley, A. Rakshit, M. Nuggehally, R. Mukherjee

Rensselaer Polytechnic Institute

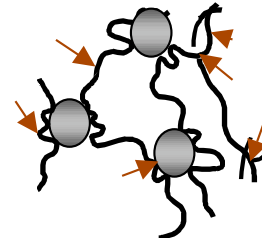
The RPI team is developing a suite of hierarchical multiscale models and scale bridging procedures aimed at analysis, design and manufacturing of nanomaterials and nanodevices. We are in the process of validating the capabilities developed for three applications including nanocomposites¹, lattice structures² 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 methods⁵ 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 nanoparticles¹.

References

¹ Picu, R.C., Ozmusul, MS., "Structure of linear polymeric chains confined between spherical impenetrable walls," J. Chem. Phys., 118, 11239, (2003).

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).

³ J. Fish and W. Chen, "Generalized Mathematical Homogenization of Discrete Locally Periodic Medium," in preparation.

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).

⁶ J. Fish and Z. Yuan, "Multiscale Enrichment based on the Partition of Unity," International Journal for Numerical Methods in Engineering, in print, (2004).