# Modeling and Simulation Framework at the Nanoscale

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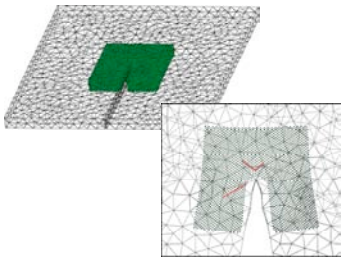
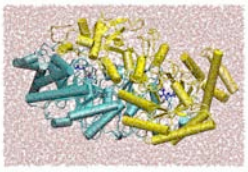
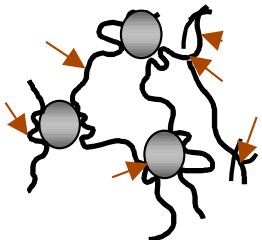
The RPI team is developing a suite of hierarchical multiscale models and scale bridging procedures aimed at analysis, design and manufacturing of nanomaterials and nanodevices. We are in the process of validating the capabilities developed for three applications including nanocomposites[1], lattice structures [2] and proteins [8] (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[5,8], 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].

The generalized mathematical homogenization theory[3] derives an equivalent continuum description directly from molecular dynamics (MD) equations. The noteworthy findings of this work are: (i) the coarse scale continuum equations (PDEs) formulated by homogenizing MD equations are identical to those obtained from the classical homogenization of the fine scale continuum, (ii) the lower order effective continuum

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properties (such as fourth order constitutive tensor) have similar characteristics to those resulting from homogenization of fine scale continuum, (iii) the higher order effective properties, such as polarization and dispersion tensors, substantially differ from those of continuum due to the *discreteness effect* medium. (Note: both the heterogeneous continuum and discrete media possess the *size effect*, but only atomistic medium has the *discreteness effect)*.

In attempt to extend the range of applicability of the generalized mathematical homogenization theory[3] to problems where scale separation may not be possible, we developed a multiscale enrichment framework based on partition of unity (MEPU)[6]. MEPU is suited for enriching the coarse scale continuum descriptions (PDEs) with fine scale features as well the quasi-continuum formulations with relevant atomistic data. Numerical results show that it provides a considerable improvement over classical mathematical homogenization theory and quasi-continuum formulations. Our current research efforts focus on extending the original periodic formulation[6] to random structures as well as to practical situations where the existence of fine scale data is confined to a limited number of sampling points.

Among the concurrent atomistic-to-continuum bridging techniques, attention is restricted to multigrid (multilevel) like methods[7,2]. We are in the process of extending the multigrid principles to space-time domain in attempt to substantially speed up MD calculations.

We had a considerable success on applying mathematically based model reduction methods to linear dynamic systems[5]. It remains to be seen how well these methods perform for atomistic systems which are inherently nonlinear. Our physically-based model reduction research efforts so far focus on two approaches: (i) Fast Molecular Dynamic (FMD) framework[8] aimed at improving multibody sub-structuring techniques, and (ii) adaptive space-time coarse graining procedures aimed adaptively selecting atomistic modes that are relevant on the coarse scale.

The FMD methods being developed have been shown to be vastly superior to those offered by the classical MBO(N)D methods for systems involving significant numbers of loops (as occurs in certain bio-molecular, and composite material systems). Additionally, the methods being employed re-cast the sequential solution offered by MBO(N)D in a form which is amenable to parallel computing. Our NIRT group has successfully transitioned the FMD framework to Sandia National Laboratory in attempt to add the necessary extensions to their LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) so that it uses the NIRT group's multibody package, and can exploit its capabilities. Thus far we were capable of reproducing the results of MBOND rigid body dynamics, and reduced order flexible body dynamics are in progress. Additionally, we are working towards improving the performance of adaptive space-time coarse graining models.

Our adaptive space-time coarse graining effort is currently focus on complex fluids. The coarse grained model can be applied to represent the deformation of filled and un-filled polymeric melts, solutions and solids close to the glass transition. The main advance here

is the bridging of temporal scales. In polymers and complex fluids, in general, the critical problem encountered when trying to probe their mechanical and dielectric properties is accounting for the large span of relevant time scales, which range from femtosecond to minutes or more. These time scales are coupled in the sense that relaxation on large scales (spatial and temporal), which is also the slowest, is driven by fast thermal fluctuations on small scales. Hence, proper prediction of the large scale response may be performed only after the fast time dynamics is captured. This development is beneficial in at least two respects: (i) the time scale linking technology developed here is applicable to model other complex systems and (ii) the model is easily transferable to nanocomposites and like heterogeneous systems.

## References


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