NANO HIGHLIGHT
Modeling and Simulation Framework at the Nanoscale

NSF NIRT Grant 0303902

PIs: **J. Fish, C. Picu, K. Anderson, M. Shephard**
Rensselaer Polytechnic Institute

Research has focused on the development of adaptive information-passing and concurrent multiscale methods and application of the technologies developed to hierarchical polymeric systems. In this regard a Generalized Mathematical Homogenization (GMH) theory for finite temperatures has been developed [**Error! Bookmark not defined.**]. The theory is based on the introduction of fast temporal scales (in addition to multiple spatial scales) and correlation of fast time derivatives of atomistic displacements to the finite temperature. The coarse scale material constants (for both mechanical fields and heat flow) were derived directly from atomistic features.

A Flexible Divide-and-Conquer Algorithm (FDCA) [2] permits the seamless treatment for drastically different modeling approaches (e.g. atomistic, bead, articulated body, flexible body, and continuum models) within adjacent regions within polymer chains. The domain of each of these regions, as well as the model type used may then be adaptively adjusted as governed by internal metrics to realize accuracy requirements.

A concurrent multiscale (CM) approach based on multigrid ideas has been developed in [4] for bridging diverse spatial and temporal scales. The method consists of the waveform relaxation scheme aimed at capturing the high frequency response of the atomistic vibrations and the coarse scale solution in space and time intended to resolve the smooth features of the discrete medium. The CM approach developed has been found to provide significant speedup over classical explicit integrators used in molecular dynamics simulations in particular on parallel machines.

A synthesis of the Generalized Mathematical Homogenization and Partition of Unity methods has been developed in [**Error! Bookmark not defined.**] [7]. The so-called MEPU or Multiscale Enrichment based on Partition of Unity is developed for enriching the coarse scale continuum descriptions or coarse-grained discrete formulations. It is primarily intended to extend the range of applicability of the mathematical homogenization theory to problems where scale separation may not be valid.

References

[1] J. Fish, W.Chen and Y. Tang, “Space-Time Generalized Mathematical Homogenization of Atomistic Media at Finite Temperatures,” International Journal for Multiscale Computational Engineering, 2005.
[2] R. M. Mukherjee and K.S. Anderson, “A Logarithmic Complexity Divide and Conquer Algorithm for Multi-flexible Articulated Body Systems”, ASME Journal of Computational and Nonlinear Dynamics, 2005, accepted.
[3] K.S. Anderson, R.M. Mukherjee, J. H. Critchley, J. L. Ziegler, and S.R. Lipton “POEMS: Parallelizable Open-Source Efficient Mulitbody SOFTWARE”, Engineering with computers, 2005
[4] H. Waisman and J. Fish, “Space-Time multigrid for bridging discrete scales,” International Journal for Numerical Methods in Engineering, 2005.
[5] J. Fish and Z.Yuan, “Multiscale Enrichment based on Partition of Unity,” International Journal for Numerical Methods in Engineering, Volume 62, Issue 10, pp. 1341-1359 (2005).
[6] J. Fish and Z.Yuan, “Multiscale Enrichment based on Partition of Unity for non-periodic fields,” International Journal for Numerical Methods in Engineering, 2005.

[7] Fish J, Yuan Z. Multiscale Enrichment based on Partition of Unity for non-periodic fields. International Journal for Numerical Methods in Engineering 2005; To appear.