

MULTISCALE MODELING AND SIMULATION FOR MATERIALS PROCESSING

Program Manager
Dr. Craig Hartley
Air Force Office of Scientific Research (AFOSR)

Principle Investigators
R. Komanduri, H. Lu, S. Roy, and L. M. Raff
Oklahoma State University
Stillwater, OK

PROJECT DESCRIPTION

This project focuses on some critical issues involved in multiscale, multiphenomena material modeling - theory and simulation. The primary goal is to develop scaling laws for multiscale simulations from atomistic to continuum via mesoplasticity. Various tasks involved in this project include: (1) Material response at nanolevel using MD and MD/MC simulations; (2) Scaling laws from nanolevel, via mesoplastic (micro or dislocation) level, to continuum (macro) level; (3) Integration of a novel simulation method, namely, material point method (MPM) (originally developed at the University of New Mexico with the support of Sandia National Laboratory) with MD simulation to cover a wide range of scales from continuum to nanolevel, via mesoplastic level; (4) Application of MD and MD/MC simulations of nanoindentation and nanotension using potentials developed from *ab initio* calculations using Gaussian 98 software and neural networks (NN) as well as other potentials, such as the modified embedded-atom method (MEAM); (5) Application of massive parallel processing of MD and MD/MC simulations as well as MD/MPM simulations in a distributed computing environment. Structured adaptive mesh refinement application infrastructure (SAMRAI) (developed and maintained by the Center for Applied Scientific Computing at the Lawrence Livermore National Laboratory) will be used to parallelize the serial MD/MPM algorithms for multi-processor distributed memory computation; (6) Linking the outcome of the MD/MPM simulations and the scaling laws to Computer Aided Design (CAD) so that the design engineer can utilize this tool for various materials design and processing applications.

CURRENT STATUS OF PROJECT

- We are working with Drs. Richard Harnung and Andrew M. Wissink of LLNL on linking SAMRAI with MPM. SAMRAI software is used for parallel processing of the MPM algorithm. Multiple patches at single or multiple levels are employed to simulate the material processing spanning length scales from nm to μm through parallel computation. MPM codes are being developed for simulations involving dislocations or cracks in materials.
- A coupled MD/MPM approach has been implemented to simulate material processing using a seamless coupling technique in the handshake region.
- A mesoplastic constitutive model is being developed to link MD and continuum via mesoplasticity.