

LA-SIGMA Breakout Sessions

Large-Scale Molecular Dynamics

Science Challenge

Simulation package LAMMPS: add reactive potentials, develop for next generation supercomputers. Work with Steve Plimpton at Sandia National Labs

Hybrid MD/continuum: force field development may require modifying MD programs.

Improving sampling with the large-scale systems or computationally expensive potentials could be important to the success of projects.

Diversity, External Engagement, and Workforce Development

Perhaps better addressed through the Science Drivers?

Scientific Collaboration

MD is central to many of the applications of the proposal. Clearly, there are close links to Monte Carlo, force field development and ab initio methods.

Data storage and management are issues which need to be addressed. We need to establish a mechanism for the sharing of MD data, including simulation trajectories and topology input files. Questions to be addressed include who decides of what data to share, where is it stored, and who has access.

Teaching needs

Tutoring: have a Wiki or other webpage listing researchers and their expertise, so others will know who to go to for help. We could also use the seminar series to do this. (continued on next page)

MD/MC class: with an emphasis on the science behind simulations and explaining the types of simulations that are feasible, for new graduate students or experimental colleagues. This could be as an online tutorial or as a course for credit.