Physics Seminar

Wednesday 4/28/2010, 4:30 pm

Science & Engineering Building Auditorium

Andrew J. Pounds

Departments of Chemistry and Computer Science
Mercer University

Computer Data Structures for Parallel Molecular Dynamics Calculations

While many excellent programs exist for completing molecular dynamics simulations in parallel, most, if not all, experience performance bottlenecks at the point of sharing data prior to updating the force, velocity, and position vectors. Even though numerous strategies have been developed to speed up this process, techniques at the data sharing and hardware level generally target state of the art systems with multiple network pathways between processors. Such methods are generally not appropriate for installations where systems use commodity switch components and single network cards in each system.

We present here data structures and parallel programming methodologies designed to keep a constant flow of data moving between commodity computer systems in a distributed memory environment and thereby minimize the networking bottleneck common to molecular dynamics code. Performance and scalability of these techniques will be demonstrated and the ease of implementation discussed.

Please join us for light refreshments at 4:15pm outside SEB 203.