

Performance Profiling for Molecular Dynamic (MD) Codes

Justin Vaughner

Alabama Agriculture and Mechanical University
Research Alliance in Math and Science

National Center for Computational Sciences, Oak Ridge National Laboratory
Arnold Tharrington, PhD

https://info.ornl.gov/sites/rams09/j_vaughner/Pages/default.aspx



Molecular Dynamics (MD) is a widely used technique for computational studies of biological and material systems. Key users of the National Center of Computational Sciences (NCCS) Cray XT5 petaflops Supercomputer use MD codes to perform computational research on biological systems. Consequently, it is important to understand the performance of these MD codes on the XT5. The goal is to compare performance profiles between LAMMPS, SNAMD, and GROMACS MD codes. Rhodopsin is the biological system used in these computational performance studies.

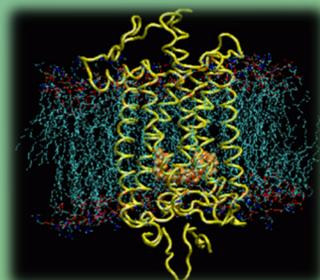
Purpose

Optimize algorithm performance to fit given architecture

Methodology

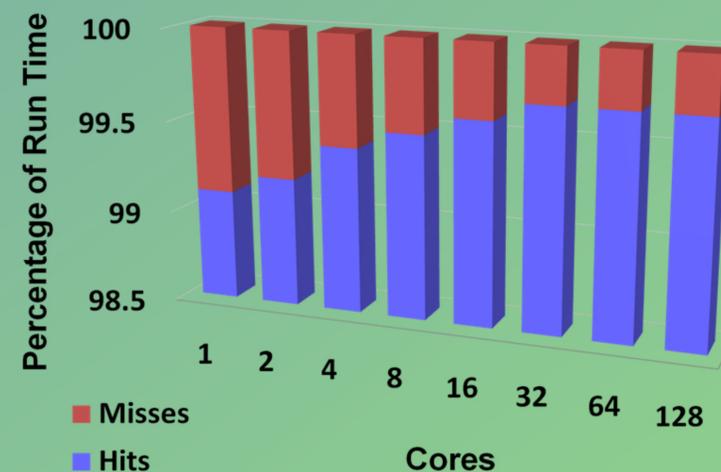
- Use UNIX operating system
 - vi editor
 - molecular dynamic code
 - message passing interface (MPI) programming
- Use craypat (performance tool to profile MD codes)
- Run programs on various numbers of cores with various profiling experiments
- Use MD codes to perform atomistic computer simulations
 - materials
 - biological systems

Rhodopsin is a protein found in the retina.



K. Palczewski et al., *Science* 289, 739 (2000)

L1 and L2 cache hits and misses



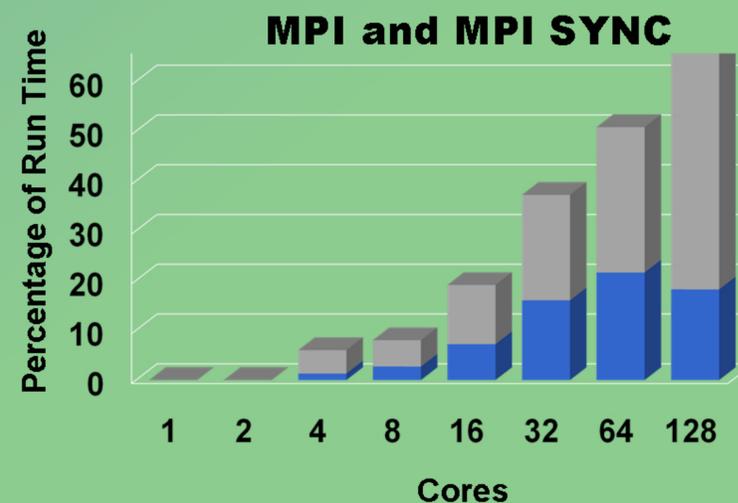
Information is searched in Levels 1, 2, 3, and DIMMS. If information is not found in one level, it misses and goes to the next level.

LAMMPS cache hit and miss ratio remains constant with the number of cores while running on JaguarPF.

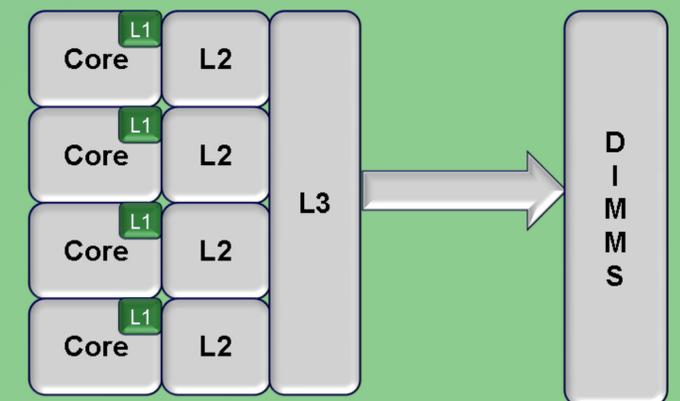
MPI time is the time spent within the MPI calls.

MPI_Sync is the time spent waiting for the MPI calls to synchronize.

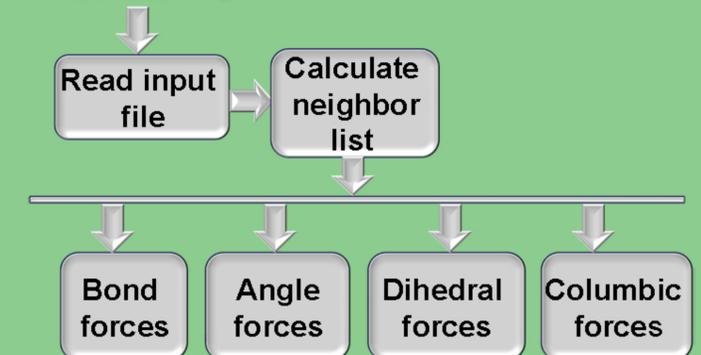
Total MPI time is dominated by MPI_Sync time.



AMD processor (4-core)



LAMMPS



Future Research

- Implement LAMMPS on future architectures
 - Six-core upgrade on JaguarPF
 - Future hybrid graphics processing unit