Performance Profiling for Molecular Dynamic (MD) Codes

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

Abstract

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 petaflop 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, NAMD, and GROMACS MD codes. Rhodopsin is the biological system that was used in these computational performance studies.

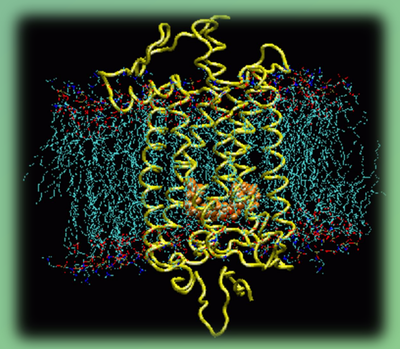
Purpose

Optimize algorithm performance to fit a given architecture

Methodology

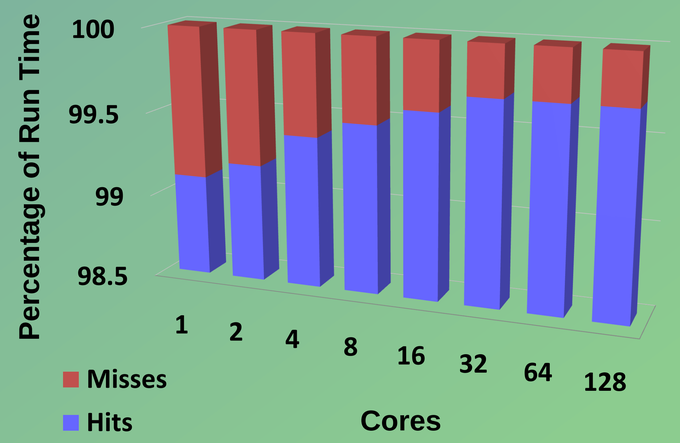
- Use UNIX operating system
  - vi editor
  - Molecular dynamic code
  - Message passing interface (MPI) programming
- Use craypat (performance tool used to profile MD codes)
- Ran programs on various numbers of cores with various profiling experiments
- Use MD codes to perform atomistic computer simulations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

Rhodopsin is a protein found in the retina. →



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

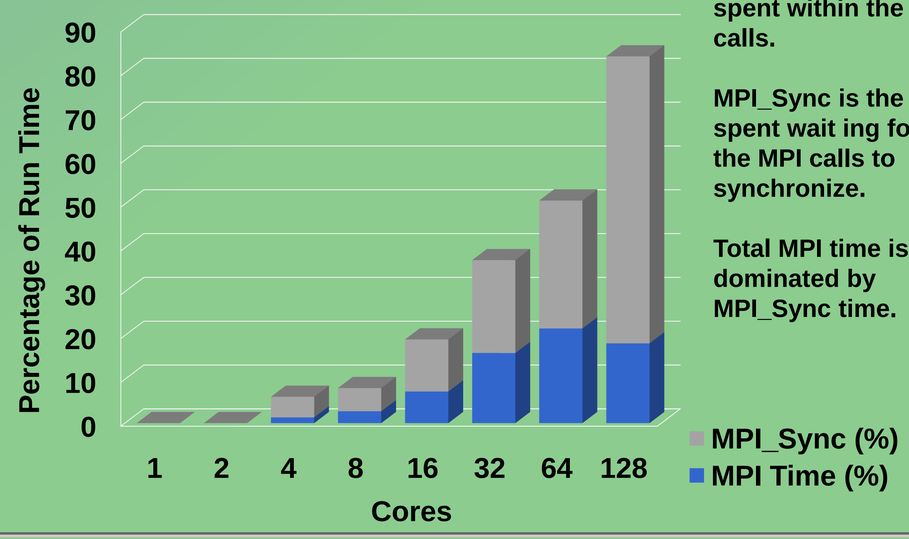
L1 + L2 Cache Hit and Miss Ratio



Information is searched in Levels 1, 2, 3, and DIMS. 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 and MPI SYNC

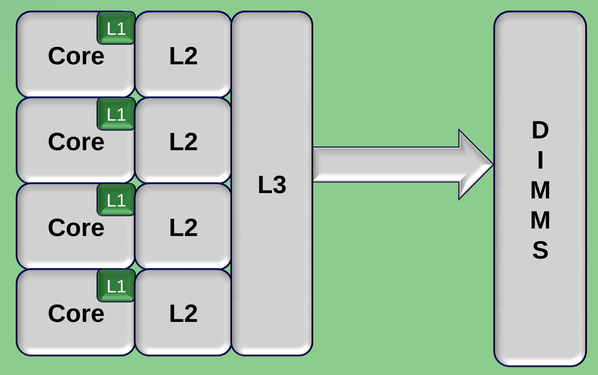


MPI time is the time spent within the MPI calls.

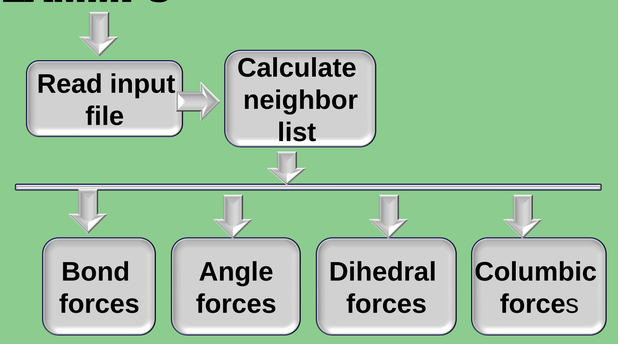
MPI_Sync is the time spent wait ing for the MPI calls to synchronize.

Total MPI time is dominated by MPI_Sync time.

AMD processor (4-core)



LAMMPS



Future Research

- Implement LAMMPS on future architecture
  - Six-core upgrade on JaguarPF (Istanbul)
  - Future hybrid graphics processing unit (GPU)

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