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.

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