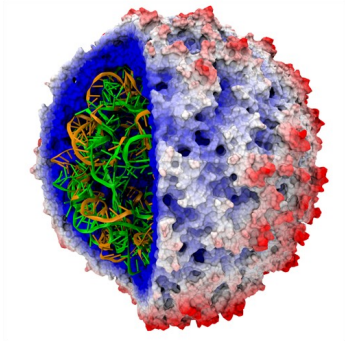
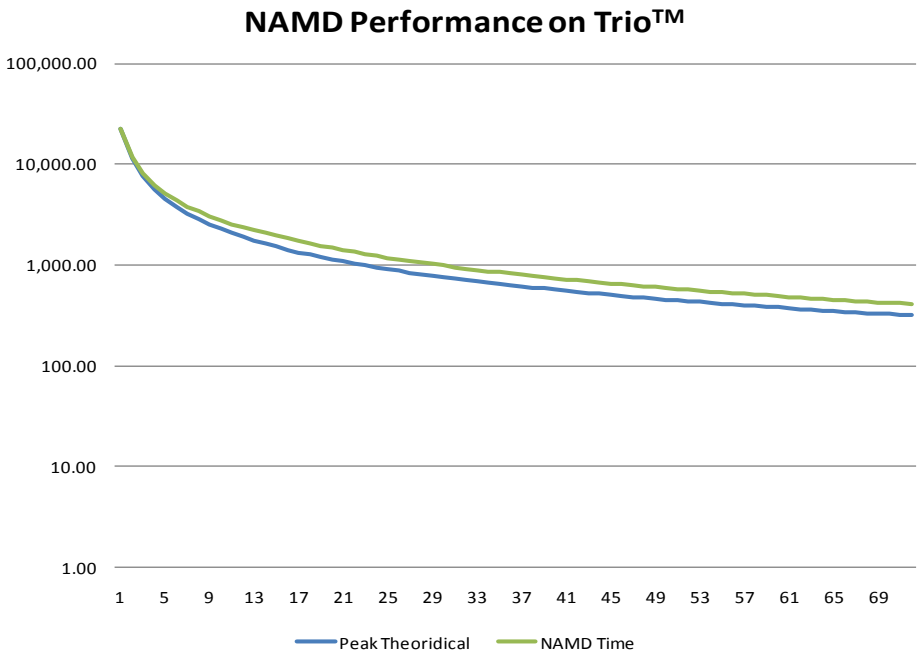
Trio™ Departmental SuperComputer

NAMD Performance





The molecular dynamics program NAMD was executed on a Trio™ Departmental Supercomputer. The run took 7 minutes and 30 seconds processing approximately 18,000 points per second with speed-up of 49 times with 64 cores and 55 times with 72 cores (77% efficiency). The following parameters were used:

- 317 amino acids
- 110,000 atoms
- The molecule was put in a solvent box of size 117x93x109 (803,439 points)

The NAMD results shown were optimized for energy minimization with a full atomic simulation. The protein and solvent were expressed explicitly with approximately 120 ions to generate a physiological concentration. The Particle-Mesh Ewald (PME) and Conjugate Gradient Minimization method were used in the calculation.

Trio™ Test System Configuration

Processors:	72 2.6 GHz AMD Opteron™ Cores
Memory:	384 GB 667 MHz DDR2 (8 GB DIMMs) (Global Shared Memory of 300 GB)
Node Interconnect:	40 Gbps InfiniBand

Trio™ Departmental Supercomputers are now available with 96 2.4 GHz AMD Opteron™ cores and 384 GB, 768 GB or 1.54 TB DDR3 memory.

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