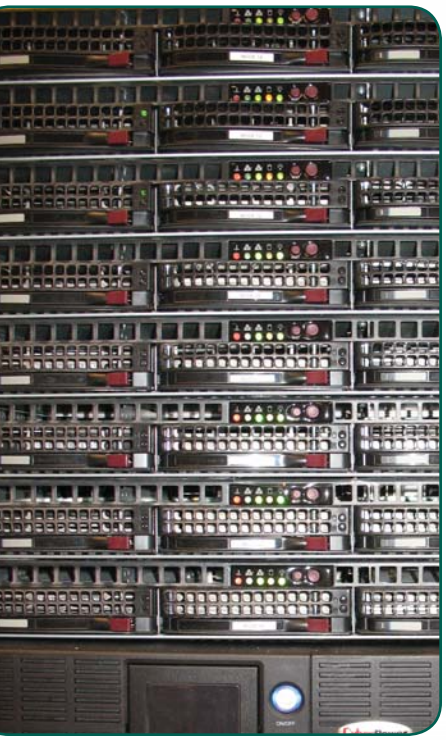
CASE STUDY

Nor-Tech HPC Clusters™

Bioinformatics Cluster is a powerful weapon in the fight against neurological disorders



In addition to GigE, Nor-Tech's Bioinformatics cluster uses InfiniBand to flow data between its nodes. InfiniBand offers significantly higher throughput low latency as compared to GigE.

The Bioinformatics Cluster uses a Qlogic InifiBand switch and Mellanox InfiniBand HCA's

The Challenge

Computational biology is an interdisciplinary field that combines computer science, applied math and statistics to address biological problems. One particular branch of this field, bioinformatics concerns the application of information technology to the field of molecular biology. By employing bioinformatics, researchers can increase our understanding of biological processes at a molecular level, investigating events which are too small and happen too quickly to be observed.

Alzheimer's disease, the most common human neurodegenerative disorder, is characterized by loss of neurons and synapses in the cerebral cortex and subcortical regions. Research suggests that a certain amyloid species may be to blame. It is believed that the neurotoxicity of the as yet unidentified species disrupts the neuron membrane, leading to neuron death. Research targeting the identification the species is complicated by the fact that they can be smaller than a nanometer and very unstable, with lifespans of only a few seconds.

The Solution

Biophysicists use molecular dynamics simulations to investigate molecular architecture and model nanoscale cellular events that occur in very short time intervals.

Nor-Tech developed a Rocks/Linux-based system with integrated InfiniBand and installed the necessary applications, including the NAMD simulation package.

NAMD (Nanoscale Molecular Dynamics) is an open source parallel molecular dynamics simulation package based on Charm++. Designed to conduct high-performance simulation of large biomolecular systems, NAMD scales to a multitude of processors on each cluster. NAMD can simulate the movement of proteins with millions of atoms, making it the world's fastest parallel molecular dynamics program.

Nor-Tech also installed CHARMM, a versatile molecular simulation program, Charm++, PBS, Torque and debugged the job scripts.

CHARMM allows generation and analysis of a wide range of molecular simulations. The program includes a large suite of computational tools that encompass numerous confrontational and path sampling methods, free energy estimates, molecular minimization, dynamics and analysis techniques ,and model-building capabilities.

The cluster is tied together with InfiniBand, a point-to-point low latency bi-directional serial link which is notable for its quality of service, failover, and high-speed interconnect. InfiniBand's performance and scalability make it particularly desirable for ever-expanding networks, such as those found in bioinformatics research environments. InfiniBand's performance boost to the cluster can be a huge advantage in the highly competitive molecular biology research.

Prior to deployment, Nor-Tech's cluster experts helped the customer get started with testing their input files. After the toxic species has been identified, scientists can begin to develop inhibitors to prevent its formation, which will go a long way toward understanding, and ultimately curing brain diseases such as Alzheimer's and Parkinson's.

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