CASE STUDY

Nor-Tech
HPC Clusters™

Nor-Tech provides computational advantage for molecular research giant

Nor-tech has built multiple HPC Bioinformatics clusters for MIT

The Challenge

MIT's Molecular Engineering Laboratory develops cutting edge molecular computational methods and applies them to address important industrial problems. Amongst their projects are applications for continuous pharmaceutical manufacturing, which could vastly increase the efficiency, flexibility, and quality of the way pharmaceutical products are made. Other applications include stabilization and formulation of biopharmaceuticals, and nucleation and crystallization.

Using sophisticated computational methods, researchers at the lab study complex chemical systems at the molecular level and engineer them for high-value chemical applications.

Researchers at the Molecular Engineering Laboratory at MIT are constantly developing new molecular computational approaches based on statistical mechanics and quantum mechanics.

This advanced level of bioinformatics requires highly specialized hardware and software working in congress to best process, manage and store the vast amount of information coming through the lab on a routine basis.

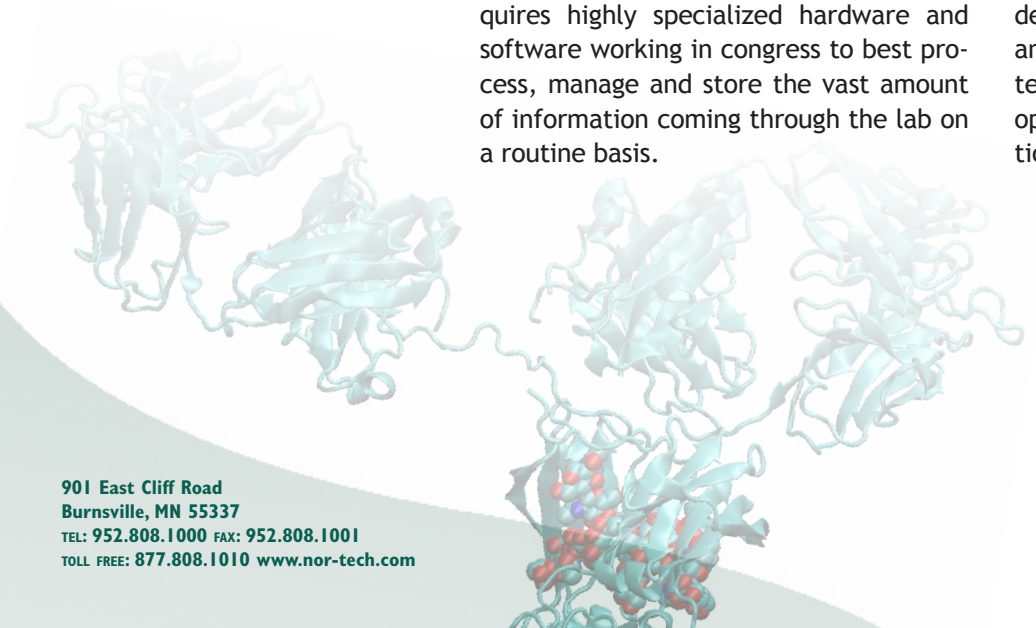
The Solution

Nor-Tech created an HPC cluster to be used for bioinformatics research by the Molecular Engineering Laboratory at MIT. The cluster uses Rocks® Cluster Suite and QDR Infiniband by Mellanox and is configured to automatically setup user storage in an XFS formatted DAS file system.

Nor-Tech's MIT Bioinformatic cluster flows data between its processors using InfiniBand, which offers significantly higher throughput and low latency as compared to GigE.

Additionally, Nor-Tech installed CHARMM, the versatile molecular simulation program, and NAMD, an open source parallel molecular dynamics simulation package based on Charm++, and setup example PBS/Torque scripts for running jobs.

The cluster shipped installed with cluster development tools and compilers. Intel® Cluster Toolkit Compiler Edition provides an extensive software package containing Intel C++ and Intel Fortran Compilers for developing applications targeted at IA-32 and Intel 64 architectures, plus all the Intel Cluster Tools to develop, analyze, and optimize performance of parallel applications on the Rocks cluster.



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