



PathScale Expands the Horizons of Biomedical Research at the University of Utah

**Center
for High-
Performance
Computing**
@ the University of Utah

Organization:
University of Utah, Center for High-Performance Computing

Industry:
Academic, Biomedical Research

Location:
Salt Lake City, UT

Applications:
DLPOLY, Amber (Molecular Dynamics), CPMD, VASP (Quantum Chemistry)

Solution Set:
1,000-CPU Linux Cluster built on AMD Opteron™ processor-based Titan64 Superblades from Angstrom Microsystems

PathScale Products Used:
PathScale EKO Compiler Suite™



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-- Martin Cuma, Scientific Applications Programmer, University of Utah

BUSINESS CHALLENGE: Researchers at the University of Utah with support from the National Institutes of Health and the National Science Foundation are working to solve some of the world’s greatest medical challenges by performing in-depth biomedical analyses and advanced simulations to better understand complex biological processes.

“In order to study these large bio-molecular systems on an atomic level using molecular dynamics methods, we started provisioning one of the fastest supercomputer clusters in the world during the latter part of 2003,” said Martin Cuma, scientific applications programmer at the University’s High-Performance Computing Center. “The system we are now using is a 1,000-CPU AMD Opteron-based Linux cluster from Angstrom Microsystems optimized by the PathScale EKO Compiler Suite. We are continuing to accelerate the throughput of this very powerful system by leveraging the advanced compiler technology and superior engineering support that we receive from PathScale.”

WHY PATHSCALE? The University of Utah is already pushing the envelope on the capabilities of their new cluster system, and securing funds for additional computing power is always difficult. Rather than adding more nodes to the cluster, the High-Performance Computing Center has adopted the PathScale EKO compiler suite to achieve more performance from their current system resources.

“The Opteron systems from Angstrom were the best price/performance option and the PathScale compiler is now a key component in making our 1,000-CPU cluster perform as well as it does.”

“This has been absolutely the best way for us to go,” Cuma said.

The combined power of the Opteron-based Titan64 Superblades from Angstrom Microsystems along with the PathScale EKO Compiler Suite enable University of Utah researchers to run applications two to three times faster than was possible with their previous supercomputer system.

“We run molecular dynamics applications that analyze hundreds of thousands of atoms, allowing us to see how atoms actually move in nature and analyze the reactions that occur. This helps researchers design new drugs and solve urgent global health problems,” Cuma explained. “Researchers who are focused on performance are now routinely using PathScale compilers. For my research, I have totally migrated to PathScale.”

PURSuing NEW FRONTIERS: Researchers can now complete a complex biomedical analysis in two months that previously would have required six months, resulting in three times more research being done in the same period of time.

“Another advantage with PathScale and Opteron is that when you have a faster system, researchers become more ambitious in what they attempt to do because they can study more extensive biological problems at a more detailed level to achieve a better understanding of what’s happening. Some of the new scientific and medical technologies emerging here today wouldn’t be possible without this kind of extra power,” Cuma added.