

William R. Wiley

EMSL In Brief

Environmental Molecular Sciences Laboratory

Contract Awarded to HP for New EMSL Supercomputer

HP has been selected to deliver to the Environmental Molecular Sciences Laboratory (EMSL) a new \$24-million supercomputer that will help users of the national scientific user facility advance molecular science in areas such as aerosol formation, bioremediation, catalysis, climate change, hydrogen storage, and subsurface science.

With this new system, EMSL users will be able to study more complex scientific problems with larger and more realistic models and get answers faster by scaling computational models to larger numbers of processors. The system will support a broad range of cutting-edge research, such as discovering safe and effective materials for producing and storing hydrogen; studying chemical processes in bacteria's behavior to address bioremediation and energy production issues; and developing computer simulation tools to aid in environmental cleanup.



HP has been selected to deliver EMSL's next-generation supercomputer that will replace the current system (shown above) in place since 2003.

The system will be delivered and tested in two phases starting in January 2008 and is expected to be fully operational in September 2008. It's architecture will run on HP ProLiant servers and will include an InfiniBand 4x DDR interconnect, 4,620 AMD Opteron™ processors, 37 terabytes of memory and aggregate disk bandwidth of about 950 gigabytes per second enabled by nearly 21,000 disk drives in HP enterprise virtual arrays. Consisting of 18,480 2.2 gigahertz AMD Opteron processor cores, the new HP supercomputer will have an expected total peak performance of about 163 teraflops.

"EMSL is a unique resource where users can access and conduct both theoretical and experimental molecular science," said EMSL Director Allison Campbell. "As its stewards, we recognize the importance of providing the right balance of science-driven computing integrated with interdisciplinary experimental resources.

"The HP system will allow us to acquire a greater level of detail than previously possible and therefore more complete answers to our scientific questions," she said. "This system's architecture is tailored to best serve the science and the scientists."

The Department of Energy's Office of Biological and Environmental Research funded the supercomputer's purchase. Scientists will be granted access to the new computer based on a competitive, externally peer-reviewed proposal process. For more information, contact Mary Ann Showalter (509-376-5751).

P.O. Box 999 Richland, WA 99352 • <http://www.emsl.pnl.gov> • 509-376-2553