



Greenbook Workshop Focuses on Next Generation Supercomputing at EMSL

A computer with the capability to meet the most demanding computational challenges the science world has ever taken on is not something you can simply buy off the shelf. By the same token, identifying the science drivers and requirements for enhanced high-performance super computing is not something easily done by a single individual.

In that vein, EMSL used early December to host its “Greenbook” workshop on Scientific Computing as an opportunity to engage computational science leaders from around the country in a focused dialogue to identify the role that the next-generation Molecular Science Computing Facility (MSCF) will have in meeting the needs of the broader scientific community in chemistry, biology, subsurface transport, and regional hydrological climate models.

“The goal of the technical workshop was to demonstrate the role that a next-generation MSCF high-performance computing facility will play within three to five years across the scientific community,” said Theresa Windus, Chief Scientist and Technical Lead for the Molecular Science Software Group and the Visualization and User Services Group in EMSL.

Approximately 55 participants held in-depth conversations on future needs and are using the technical workshop results and previously solicited whitepapers to develop a visionary document that describes the science drivers and the associated requirements for enhanced high-performance computing, software and staff resources at EMSL in support of the DOE Office of Biological and Environmental Research. Following opening remarks by PNNL lab director Len Peters, Gordon Anderson gave an overview of EMSL within the DOE system, Dave Dixon of the University of Alabama gave a talk discussing computational sciences and their connection with DOE missions, and George Michaels, Associate Laboratory Director for the Computational and Information Sciences Directorate, provided insight on PNNL's computing strategy, and Theresa Windus updated the participants on the current state of the MSCF and shared the success stories and breadth of science that has been accomplished at the facility.

The Greenbook organizing committee, Bert (Wibe) de Jong, Steve Elbert, and Theresa Windus will produce a document to be made available in March of 2005.

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