Supercomputing In Pennsylvania

WITH COMMONWEALTH OF PENNSYLVANIA SUPPORT, PSC PROVIDES EDUCATION, CONSULTING, ADVANCED NETWORK ACCESS AND COMPUTATIONAL RESOURCES TO SCIENTISTS AND ENGINEERS ACROSS THE STATE

ECONOMIC DEVELOPMENT

PSC’s high-performance computing and networking are world-class technology resources that officials and agencies can point to in promoting Pennsylvania as a location for business. During the past year, PSC provided Pennsylvania companies with over 15,000 hours of computing time. Among them, Pittsburgh-based PPG Industries uses LeMieux, PSC’s terascale system for computational modeling in several aspects of its product lines as a global supplier of coatings, glass, fiberglass and chemicals.

PSC’s networking group advises the Pennsylvania Department of Administration on how telecommunications can help attract new business to the state. Networking staff advised on developing a state-wide networking infrastructure, leading to a new agreement for K-20 organizations to participate in the Internet2 advanced network organization. They also consulted with the Center for Appalachian Network Access at Bedford Senior High School, a regional resource for deployment of internet access in rural communities.

From November 6-12, 2004, as a result of PSC’s global presence in computational science and technology, the annual Supercomputing conference — SC’04 — was held in Pittsburgh. More than 7,900 people from around the world gathered at the David Lawrence Convention Center. This annual conference, in Pittsburgh for the
second time in eight years, brings together scientists and engineers, hardware and software companies and many others to share ideas and assess new developments in the fields of high-performance computing, networking and storage. According to the Greater Pittsburgh Convention & Visitors Bureau, SC ’04 produced an economic gain for the southwest Pennsylvania region of $13 million.

OUTREACH & TRAINING
This year PSC presented the fourth in a series of annual technology-briefing days to staff from the Bechtel Bettis Atomic Power Laboratory in Pittsburgh. PSC consultants provided information on developing, managing and using a parallel distributed-computing environment.

PSC participates in a number of events each year to provide information on high-performance computing to companies and government agencies. In December 2004, PSC exhibited at the Annual Eastern Intergovernmental Technology Conference in Hershey, Pa. In August 2005, PSC exhibited at the TechTrends conference in Pittsburgh, an annual conference that highlights opportunities for government, academic and industrial collaboration in the four-state region of Pennsylvania, Delaware, Maryland and New Jersey.

RESEARCH IN PENNSYLVANIA
By supporting Pennsylvania university researchers, PSC resources help to attract research funds to the state. During the past year, more than 430 Pennsylvania researchers from 12 institutions used nearly 650,000 processor hours on PSC resources that are specifically targeted at Pennsylvania users. In addition, Pennsylvania researchers received allocations through the NSF process of nearly five million hours on LeMieux, PSC’s terascale system, along with 169,000 hours on PSC’s HP Marvel systems.

COOL DESIGN IN ELECTRONIC COMPONENTS
Cristina Amon is a specialist in cool design. Her research has pioneered the use of computational methods as a way to model the heat removed from micro-circuitry in portable electronic devices such as laptops and wearable computers. As director since 1999 of Carnegie Mellon’s Institute for Complex Engineered Systems, she has promoted research-industry collaboration in western Pennsylvania. In projects using resources at PSC, she has developed numerical methods to model the heat produced by and removed from microcircuitry. In the early 1990s, she applied her approach to the thermal design of VuMan, a first-generation wearable computer.

In more recent work, Amon collaborated with PSC scientist Marcela Madrid to develop an innovative method to calculate the thermal conduction in silicon “thin films”. The predominant material used to manufacture the “chips” of micro-electronics, silicon in some devices is deposited in very thin layers — from 10 to several hundred nanometers. In many applications, these silicon thin films are deposited on dielectric materials that conduct heat poorly, requiring that the heat produced must be removed by heat flow within the thin film itself. Thermal properties of silicon in these very thin layers differ from bulk silicon, and because of this, existing computational approaches have had limited usefulness.

Madrid’s specialty is an approach called “molecular dynamics,” which tracks the forces and interactions among atoms over time. In collaboration with Amon, she helped to develop a “potential” — a mathematical expression — to realistically represent thermal conductivity for applying molecular dynamics to silicon thin films. Applying this potential at the surface of the thin film overcomes inaccuracies introduced in prior computational approaches. This innovative approach allows effective use of molecular dynamics to model thermal conductivity of silicon thin films, and the results predicted for films ranging in thickness from two to 200 nanometers show good agreement with experimental data.