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Environmental Molecular Sciences Laboratory

William R. Wiley EMSL Environmental Molecular Sciences Laboratory

EMSL Team Develops Flexible, Lower-Cost Ion Trap Control System

Easily Built System Promises Benefit to Smaller Institutions

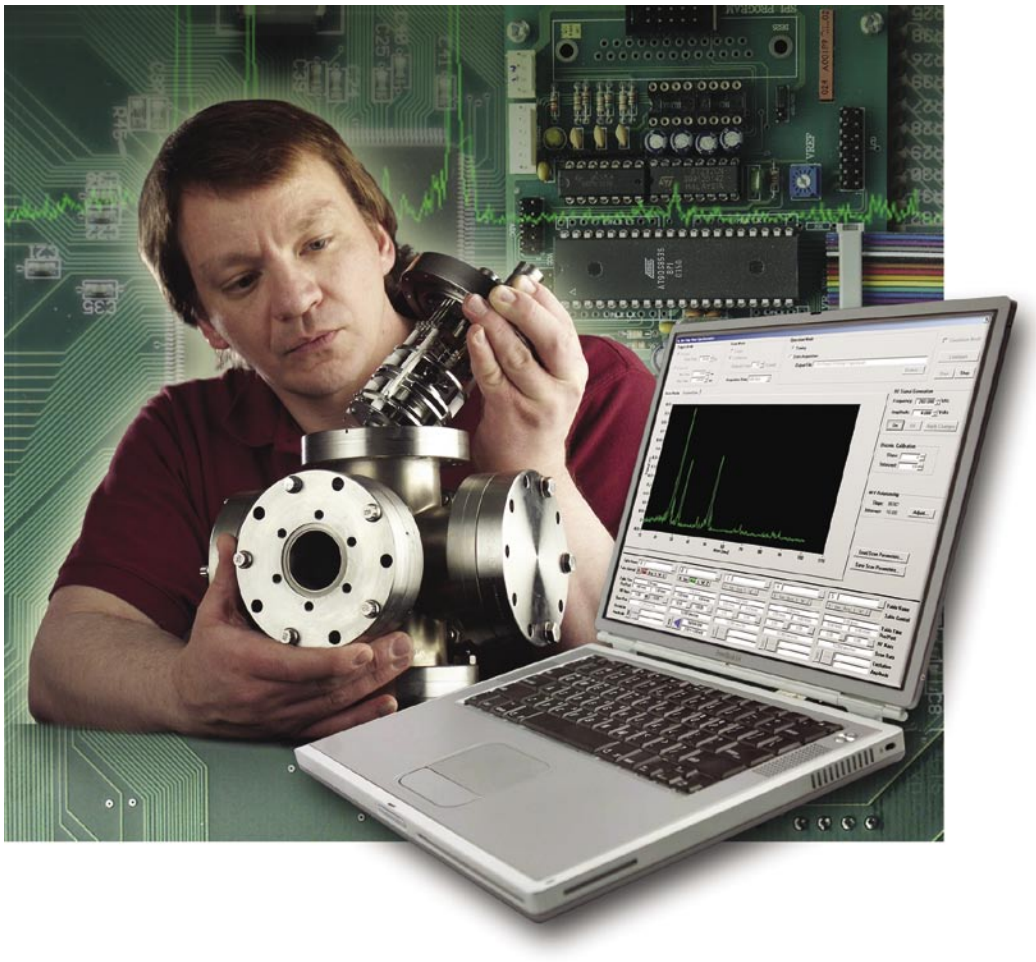
EMSL researchers Ken Swanson, Derek Hopkins, and Mike Buschbach, and EMSL user and Pacific Northwest National Laboratory scientist Mike Alexander, have developed a "blueprint" for an inexpensive and flexible control system for ion trap mass spectrometers that they believe will be of great benefit to researchers, particularly those at smaller institutions—where limited budgets can sometimes prevent the most brilliant minds from obtaining the equipment needed to conduct research. Lack of instrument versatility is also often an issue—a piece of commercial equipment in most cases cannot be easily modified and is dedicated to only one specific research application.

However, thanks to the team's research, a lower-cost and more flexible control system is now available that allows a single ion trap mass spectrometer to be adapted to a variety of research areas—such as chemical ionization techniques that address the need for highly sensitive and specific measurements, and analytical needs dictated by research areas such as atmospheric chemistry, catalysis, materials science, biology, and inhalation toxicology.

"The problem with commercial ion trap mass spectrometers is you can only buy systems that are more or less dedicated to a single application," says Alexander. "And for people at smaller universities, these instruments may be out of their price range." Not to mention that the instruments—much like computers—become "out of date" within five years and are often not supported after this time.

The team's control system is comprised of a marriage of key components such as commercial computer hardware (commercial boards, data acquisition boards, and control boards) and software written by team members that allows the researcher to "tune" the mass

(see ***Ion Trap***, page 4)



EMSL researcher Ken Swanson pictured here with the ion trap control system he helped develop.

National Science Foundation and EMSL Create Formal Affiliation with Grant Program

Thanks to a supplemental grant program implemented in March, university students, faculty, and post-doctoral users of EMSL's state-of-the-art resources and instrumentation can apply to receive up to $20,000 annually from the National Science Foundation (NSF) for travel and lodging expenses. The grants are awarded to those scientists whose research is supported by NSF programs in Biological Sciences; Computer and Information Science and Engineering; Engineering; Geosciences; Mathematical and Physical Sciences; and the Office of Polar Programs.

"Before these grants were made available, scientists who wished to work at EMSL had to pay out of their own or their program's pocket for travel and hotel or rent fees," says Allison Campbell, EMSL Associate Director for Scientific Experimental Resources. "This program will provide individuals—especially students—who otherwise don't have large research grants with some funding to be able to perform their science at EMSL for an extended period of time."

Applying for an NSF supplemental grant is a two-pronged process. First, the applicant must submit a user proposal electronically via EMSL's website at *http://www.emsl.pnl.gov/*, indicating that their proposal is associated with an NSF supplemental funding request. Then, if approved for use of EMSL capabilities, the applicant will receive a letter of approval from the EMSL Director that they must attach to their NSF supplemental grant application (submitted using the NSF FastLane Award and Reporting Module at *https://www.fastlane.nsf.gov/fastlane.jsp*). Final grant approval is determined by the NSF following the supplemental grant application process.

According to Len Spicer, Chair of EMSL's User Advisory Committee, the NSF is the first—but hopefully not the last—EMSL scientific funding entity to provide this type of grant.

"The User Advisory Committee has long recognized the importance of travel support for students, post-docs, and university scientists who visit EMSL to pursue their scientific objectives," says Spicer. "This grant program is an important response to that need, and I hope it will serve as a model for similar support from other funding sources."

Users such as Washington University Biology Professor Himadri Pakrasi—one of the first recipients of the NSF supplemental grants—are excited that these grants will make the cutting-edge resources of EMSL more available to the university researcher.

"These grants will allow younger scientists, such as graduate students from my lab, to visit EMSL and receive first-hand large-scale proteomics experience," says Pakrasi.

Proposals for the supplemental grants may be submitted at any time and are reviewed by the NSF as they are received. Up to 20 supplemental grants are expected to be awarded annually, depending on availability of NSF funds and EMSL resources, and the quality of grant request submissions. While the users are the primary and targeted beneficiaries, EMSL and the scientific community are not without reward.

"This program will jump start the Pacific Northwest National Laboratory's strategic thrust to increase the impact of EMSL's user program, broaden its user base, and foster partnerships with research universities throughout the nation," says Jean Futrell, Senior Battelle Fellow who championed the supplemental grant effort.

More information about the NSF supplemental grant program is located at *http://www.nsf.gov/pubs/2004/nsf04025/nsf04025.htm*, and an NSF grant proposal guide is available at *http://www.nsf.gov/pubsys/ods/getpub.cfm?gpg*.

Representative Nethercutt Visits PNNL

During his recent visit to the Pacific Northwest National Laboratory, U.S. Representative George Nethercutt, 5th District, visited EMSL's Molecular Science Computing Facility and was briefed on the collaboration with industrial partner Isothermal Systems Research on a "smart cooling" design for EMSL's 11.8-teraflop supercomputer. The smart cooling design is targeted toward aggressively cooling the microprocessor, rather than over-cooling the entire computer room. The final design has the potential to save EMSL a large fraction of the electrical bill for cooling the 750-KVA computer room. Representative Nethercutt was instrumental in obtaining some of the funding for the project.

Pictured left to right: George Michaels, PNNL Associate Laboratory Director, Computational & Information Sciences Directorate; Scott Studham, PNNL Associate Director for Advanced Computing, Computational Sciences, and Mathematics; Representative George Nethercutt; PNNL Director Len Peters; and Mike Schwenk, PNNL Economic Development and Communications Directorate.

Third EMSL User Meeting a Success

On June 14 – 16, researchers from around the nation attended ***EMSL2004***, a meeting that united existing and potential users for stimulating discussions and presentations about current leading scientific topics. This year's meeting, "Bridging Technologies in Structural Biology," highlighted EMSL's cutting-edge capabilities in nuclear magnetic resonance (NMR) spectroscopy.

EMSL2004 featured several speakers nationally renowned for their areas of research, including University of Washington biochemist Rachel Klevit, who outlined her studies of BRCA1-BARD1 Ubiquitin ligase complex related to breast cancer, and Colin Fyfe, professor of chemistry and pathology at the University of British Columbia, who discussed high-field solid-state NMR studies of inorganic materials performed at the Pacific Northwest National Laboratory (PNNL).

"We are serious about collaborating; we recognize that it is an important part of the future of this laboratory."

– Dr. Len Peters
PNNL Director

In his welcome speech to the attendees, PNNL Director Len Peters pointed to EMSL's future.

"We really want to make sure that as we move forward, EMSL has leading-edge technologies. We want to bring scientists together so as a group they can jointly solve problems," says Peters. "We are serious about collaborating; we recognize that it is an important part of the future of this laboratory."

EMSL Director Bill Rogers also addressed the audience by discussing recent changes, including development of a Science Advisory Committee and the facility's October 2002 reorganization that transferred the programmatic function from EMSL while retaining staff and the six technical user facilities and three support groups needed to sustain a user program that has grown by 25 percent per year since EMSL opened its doors in 1997.

Rogers also discussed many of EMSL's newest cutting-edge capabilities, including one of EMSL's newest acquisitions, the 900-MHz NMR spectrometer. This instrument became operational in November 2003 for characterization of structure function relationships for large molecular complexes.

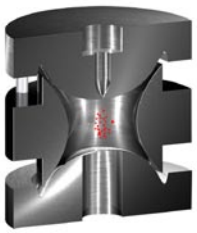
"The hole we had to dig for the NMR cradle was actually the first piece of ground that was broken for EMSL—so this instrument really dictated the footprint of EMSL as it now sits on this plot of land," says Rogers, of the long-anticipated NMR spectrometer. "This instrument is the only one in existence at this time."

EMSL2004 concluded on June 16, with a joint meeting with the American Vacuum Society.

Ion Trap (continued from page 1)

spectrometer to their needs. These components, interfaced with off-the-shelf vacuum and ion trap hardware, result in an ion trap mass spectrometry platform that can be custom-tailored to the researcher's applications.

"We came up with a design of a control system that could be put together for $10,000 to $20,000—fairly low cost," says Swanson. This compares with commercial ion mass spectrometers ranging from $60,000 to $200,000. "Now, anyone may replicate our control system. Here are the commercial boards, the model numbers and the company where you buy these boards, the wiring to put them together, the software, and the design for the ion trap hardware—and you've got your own instrument."



"With these components, we can make an ion trap mass spectrometry platform of any size," adds Alexander, who began thinking about the concept two years ago. "For example, in protein research we want mass range that goes up to a couple thousand amu—so you're going to have a bigger instrument. With atmospheric chemistry you only need 150 amu, so you need a more lightweight instrument that you can throw on an airplane."

Individuals who wish to use the team's control system can visit EMSL to learn how to construct it.

"It's a different idea of how a user facility such as EMSL would be used," says Alexander. "They're not just coming here to use an instrument, they're coming here to learn how to construct it—and then we're actually establishing collaborations with them."

Adds Swanson, who sees the control system as an excellent pathway for collaboration, "This is the way I view the philosophy of the Lab: You make something useful and then get it into peoples' hands," he says.

In the future, the team proposes a possible internet-based control system so that the researcher can control an ion trap mass spectrometer remotely from their home institution without having to travel to EMSL. According to Swanson, use of the control system can potentially evolve into many atmospheric chemistry and national security applications—such as internet-based use for remote sensor deployment in multiple locations.

"I'm really hoping that we can take this forward and realize a lot of different kinds of applications and capabilities using this control system," says Swanson. "There are several hardware, software, and data analysis opportunities, and there's a lot of online use for this technology, both as a teaching tool and for remote access."

A paper about the team's control system and details about each of the components was featured on the cover of the April 2004 issue of *Scientific Computing and Instrumentation* (http://www.scimag.com).

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The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a Department of Energy national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research.

For additional details about the capabilities and research being performed at EMSL, please visit our web site at http://www.emsl.pnl.gov or call us at 509-376-2553.