



## *Celebrating 5 Years and Looking to the Future*

**EMSL opened its doors to researchers in October, 1997 and is celebrating five years of successful scientific discovery.**

On the occasion of the 5th anniversary of EMSL, Director Bill Rogers reflects on its history and what the future holds. “The first time I set foot in EMSL, I thought I was in a candy store for chemists. EMSL offers unique research opportunities and it is truly a beautiful concept by any standard.”

“In 1985, PNNL director William R. Wiley realized that the lab must build a strong science and technology base and envisioned a national user facility as the way to accomplish his vision. EMSL was a completely new concept and very different from what existed prior to 1990. It was a lab built from the ground up with new staff, and the vast majority of staff are young scientists.”

“Costing over \$230 million, EMSL was specifically designed so that the whole was greater than the sum of its parts. Research capabilities were selected and developed that would complement each other, enabling scientists to address important questions with not one but several different capabilities, ranging from high performance computers to optical spectroscopy.”

“The last 5 years represent a very spectacular growth stage. We’ve had 5500 users representing scientists from every state, 1100 technical publications, and more than 2000 user projects—6 percent from overseas. You’ve heard the saying “build it and they will come.” Here at

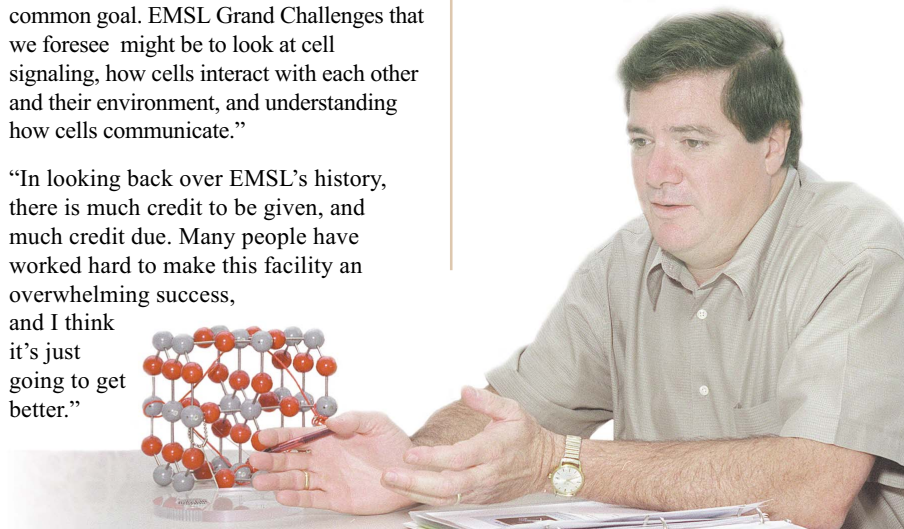
EMSL, we built it, invited users, and they came.”

“We are now developing an enhancement to our user program focussed on scientific grand challenges. The idea is to bring teams of users—the best scientists in the world—together to use the entire EMSL.” The initial focus will be on biology, subsurface science, catalysis and emissions science.”

“This is sort of an experiment in that sense, as this has not been done elsewhere. I think the closest thing you could point your finger to is the Human Genome project, which was very well defined—sequence every base pair in human DNA—and involved a diverse set of researchers working toward a common goal. EMSL Grand Challenges that we foresee might be to look at cell signaling, how cells interact with each other and their environment, and understanding how cells communicate.”

“In looking back over EMSL’s history, there is much credit to be given, and much credit due. Many people have worked hard to make this facility an overwhelming success, and I think it’s just going to get better.”

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“build it and they will come.”  
Here at EMSL, we built it,  
invited users, and they came.”*



J.W. (Bill) Rogers, Jr.  
Director, EMSL

## EMSL Users Collaborate on Air Chemistry

The minute you meet EMSL users Jim Pitts and Barbara Finlayson-Pitts, you can sense their love for science and fun – especially when both elements collide. The presence of the atmospheric chemistry experts has had a profound effect on their PNNL peers.

“I think I speak for all of us, the folks in our group and everybody they’ve worked with at the Lab, that it was wonderful to have them spend their sabbatical in the northwest,” said Carl Berkowitz, their friend and staff scientist/technical lead of the Atmospheric Chemistry Group. “Jim and Barbara are not only great scientists, but great people.”

Jim, however, quickly responded with a twinkle in his eye, “Barbara’s the brains of the operation. I just go along.”

The aforementioned sabbatical – four months collaborating at EMSL to address chemical aspects of air quality – began in September at the invitation of Steve Colson, Associate Director of EMSL’s Chemical Sciences Division. Barbara had previously collaborated with several PNNL and Battelle staff members, including Berkowitz and members of the Atmospheric Chemistry Group, and Battelle Columbus staff

member Chet Spicer, performing first measurements of molecular chlorine in the troposphere. Results of this work were published in *Nature* in 1998.

According to EMSL research scientist Dan Gaspar, with whom Barbara worked along with fellow EMSL scientist Alex Laskin on EMSL’s environmental scanning electron microscope and time-of-flight secondary ion mass spectrometer, “Barbara brings a real sense of background in atmospheric chemistry that allows us to focus on the appropriate questions. She has driven our experiments in a most useful direction.”

The appreciation is mutual – especially when it comes to their hosts at EMSL.

“I appreciate the brilliant scientists who were willing and anxious to collaborate,” says Barbara. “They were willing to go the extra mile and knocked themselves out on the experiments, even on nights and weekends.”

Jim cites the sense of humor among the scientists and excellent collaboration among the different groups. “The science is foremost, but we still had a lot of fun,” says Jim.

And how about picking up and leaving your home to live

temporarily in a state over a thousand miles away?

“The staff at EMSL and in Atmospheric Sciences at all levels were very helpful,” according to Barbara and Jim. “It was critical – they helped us with all of the aspects of the move, including after we took our ‘entrance exams’ here and joined the PNNL team.”

The couple returned at the end of December to the University of California – Irvine, where Barbara is a professor of chemistry and Jim is a research chemist. So far, they’ve penned two books together, the most recent – *Chemistry of the Upper and Lower Atmosphere: Theory, Experiments, and Applications* – published in 2000.

“Barbara is the senior author. It’s like ‘Sit! Stay! Write!’” says Jim, jokingly comparing the writing experience to their Golden Retriever’s stint in obedience school.

The Pitts expect to continue their collaborations with PNNL scientists, and to return to PNNL and EMSL periodically.

*Barbara Finlayson-Pitts worked with Alex Laskin (center) and Dan Gaspar to collect and interpret data using EMSL’s environmental scanning electron microscope and time-of-flight secondary ion mass spectrometer, allowing the researchers to understand the chemistry of aerosol sea salt particles.*



# Fond Farewell to IBM Computer

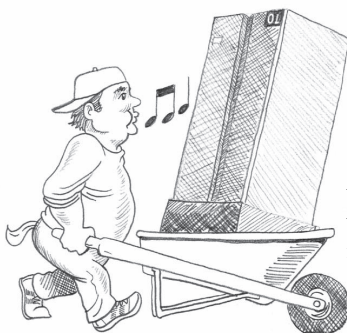
Given their experience here this fall, they have advice for the many new users who visit EMSL each year.

“Allow yourself lots of time, there is so much to see and do, so many people to talk to,” says Barbara, referring to how quickly their sabbatical passed.

“Know that everything is so close in the community. We overshot everything at first,” says Jim, referring to their initial trip to Costco. “Also, it’s a nice community to live in – the parents, kids, and the people you run across at the gas station or grocery store.”

As the interview ends, Jim and Barbara asked for copies of the photos taken with their peers during the interview session.

“I can hang the photos on my office wall and look at them while drinking my coffee and think ‘that’s where we were and what we did,’” says Jim, smiling at the memories. “Battelle is unique; there are very few places in the world that can do what they are doing here.”



On Sunday, December 15<sup>th</sup>, 2002, the IBM SP-based production computer in the Molecular Science Computing Facility was officially retired. Staff and users gathered to reminisce about the departing computer and to attend the first training session on utilizing the new production computer which, when installation is complete later this year, will be more than 45 times as powerful as the system it replaces.

PNNL was the first national laboratory to select IBM as the vendor for a production supercomputer. “Other labs were skeptical about this decision”

remarked Don Jones, MSCF Technical Leader of Visualization and User Services.

When delivered in 1996 and, at one-quarter of a Teraflop peak theoretical performance, the 512 node computer was the largest produced by IBM at that time and the 12<sup>th</sup> most powerful computer in the world.

Since its inception, the production computer has had over 800 users. The MSCF periodically issues calls for Grand Challenge proposals of research. Grand Challenge projects are multi-institution proposals of research to address important molecular science problems using computational techniques. Ten Grand Challenge projects have been completed and four are ongoing. Eighty other, smaller Pilot projects have been performed. However, after over six years of production, the facility reached the decision that the advanced computing required by EMSL users could no longer be satisfied by the existing system. A Request for Proposals was issued and, after a lengthy search, an award was granted to Hewlett-Packard to develop a Linux-based computer. Coincidentally, PNNL again led the way in being the first national laboratory to select Hewlett-Packard as the vendor for its primary production computer.

Delivery of the prototype HP system was made in May, 2002 and subsequently upgraded to the 1-Teraflop Phase I system. When installation is completed toward the latter part of 2003, the final system will have a peak theoretical performance of over 11 Teraflops, making it one of the fastest Linux clusters in the world.



*From left to right: Carl Berkowitz, Tom Jobson, and Jim Pitts next to the Proton Transfer Reaction Mass Spectrometer (PTR-MS). In an earlier study, the PTR-MS was deployed via airplane to research air quality issues from Seattle to Canada.*

## What's Happening at EMSL?

### MSCF Call for Proposals

The Molecular Science Computing Facility at EMSL issued a call for proposals in early March. Resources available for potential users include the new 11+ Teraflop Hewlett-Packard Itanium 2 Linux cluster. Proposals are due May 19, 2003 (pre-proposals are due May 2<sup>nd</sup>). Awards are on the order of 3 years for Grand Challenge projects and 1 year for Pilot projects. For details see <http://mscf.emsl.pnl.gov>.

### NMR Call for Proposals

The High Field Magnetic Resonance Facility at EMSL issues two proposal calls per year for research utilizing the equipment in this facility, including 12 NMR spectrometers and pulsed EPR instrumentation. Calls are issued with due dates of January 15 and July 16. This provides three months for proposal review with start dates on April 1 and October 1, respectively. For details, see <http://www.emsl.pnl.gov:2080/hfmr>.

### Visitors to EMSL

From October to January, visitors to the W.R. Wiley Environmental Molecular Sciences Laboratory included U.S. Senators Mike Hewitt and Pat Hale, Undersecretary of Energy Robert Card, Washington state Representatives Jerome Delvin and Shirley Hankins, Frank Chopp, and Bill Grant.



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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.