William R. Wiley
EMSL
Environmental Molecular Sciences Laboratory

EMSL Monthly Report

May/June 2003

The W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research. At one location, EMSL offers a comprehensive array of leading-edge resources in six research facilities.

Access to the capabilities and instrumentation in EMSL facilities is obtained on a peer-reviewed proposal basis. Users are participants on accepted proposals. Staff members work with users to expedite access to the facilities and scientific expertise. The Monthly Report documents research and activities of EMSL staff and users.

Research Highlights

Progress Toward Structural Determination of a Complex Membrane Protein, Diacylglycerol Kinase

CR Sanders,[(a)] K Oxenoid,[(a)] and FD Sönnichsen[(a)]
(a) Case Western Reserve University, Cleveland, Ohio

Prokaryotic diacylglycerol kinase (DAGK) is a homotrimeric integral membrane protein composed of 13-kDa subunits, with each subunit having three transmembrane helices (Figure 1). Until recently, membrane proteins have proven largely refractory to structural determination by classical nuclear magnetic resonance (NMR) and crystallographic methods. DAGK represents a target for NMR structural analysis that is more difficult than other membrane protein structures solved by NMR techniques because of its much larger size (40 kDa homotrimer) and because it is a largely helical protein. The DAGK study demonstrates that NMR can also tackle structures of the important G protein-coupled receptors, which tend to have roughly the same molecular weight and number of transmembrane segments as the DAGK homotrimer. These proteins are the target of at least 1/3 of all known drugs.

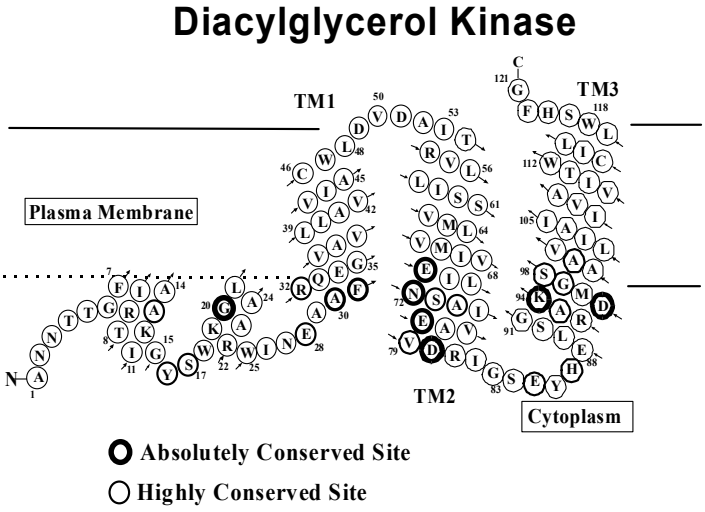

Figure 1. Topology of DAGK. DAGK functions as a homotrimer.

Based upon TROSY-based three-dimensional experiments at 800 MHz using perdeuterated DAGK, researchers were able to complete the assignment of about 80% of DAGK's 120 native backbone resonances. These data were initially collected by a member of the team onsite but were later collected by remote operation of the EMSL instrumentation. Oxenoid et al. 2002 presents a preliminary description of DAGK's secondary structure based on analysis of the ^{15}N and ^{13}C NMR chemical shifts measured for assigned residues. This paper acknowledged David Hoyt's contributions; lately, the team has also been consulting with Joseph Ford. Both Hoyt and Ford are staff members at EMSL's High-Field Magnetic Resonance Facility.

With assignments nearing completion, the DAGK NMR project is shifting towards the acquisition of restraints for structural determination (Nuclear Overhauser Effects and residual dipolar couplings). Requests for access to NMR spectrometers at EMSL, particularly the 900-MHz NMR, are anticipated to continue.

Citation

Oxenoid K, FD Sonnichsen, and CR Sanders. 2002. "Topology and Secondary Structure of the N-Terminal Domain of Diacylglycerol Kinase." *Biochemistry* 41(42):12876-12882.

Preliminary Proteomic Results from Three Strains of *Borrelia*

JM Jacobs[(a)] and X Yang[(b)]

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) State University New York, Stony Brook, New York

An initial proteomic survey of three *Borrelia* strains has provided insights into the field of Lyme disease analysis. A single tryptic digest of extracted *Borrelia* proteins from each strain was subjected to high-resolution, reversed phase capillary liquid chromatography coupled with MS/MS analysis for peptide identification. The *Borrelia burgdorferi* strain B31 protein database was used as the identification template for all three strains, even though sequence differences exist between the B31, N40, and JD1 strains.

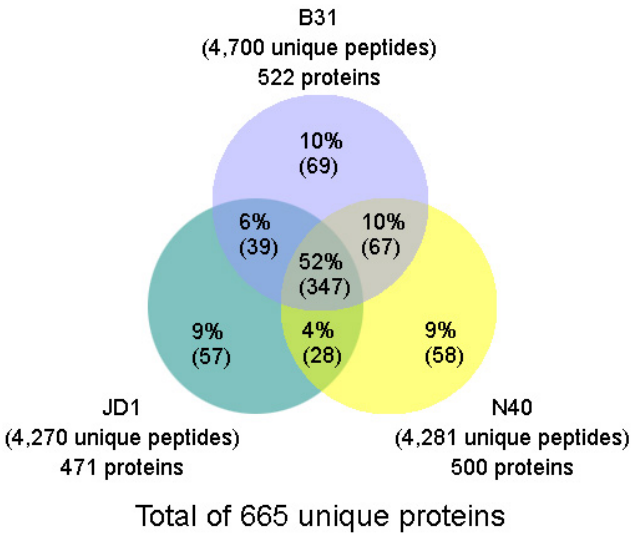

Figure 2. SCX *B. burgdorferi* strain comparison.

To increase the proteome coverage of the B31, JD1, and N40 strains, strong cation exchange (SCX) fractionation was employed for improved peptide separation and tandem mass spectrometry detection. Twenty-five SCX fractions were collected and analyzed for each strain. A summary of the SEQUEST results are displayed in Figure 2. For strain B31, 522 unique proteins were detected and a large protein overlap was observed (82 to 83%) when compared to the proteins detected for strains JD1 and N40. Many of the proteins found to be unique to strains JD1 and N40 have multiple identifying peptides, suggesting that the expressed proteome in strains JD1 and N40 differs from that of strain B31 under the batch culture conditions in which the strains were grown. Detection of proteins unique to strain B31 suggests that perhaps those proteins represent sequence variants of the similar proteins in strains JD1 and N40. Table 1 provides the subproteome distribution of the proteins unique to N40 and JD1. Of interest are five membrane proteins that may represent potentially important clinical markers for future genomic studies. A combined total of 665 unique proteins were detected among all three strains. Even with limited culture conditions and no fractionation at the cellular level, approximately 38% of the *Borrelia* strain B31 annotated database was observed in this preliminary work.

These proteomic results demonstrate a powerful analytical approach for comparing different strains of *Borrelia.* The results clearly demonstrate that significant differences can be observed among the proteomes of the invasive B31 strain and the non-invasive JD1 and N40 strains. The results also demonstrate the benefit of increased proteome coverage, as shown with the initial SCX fractionations of the tryptic digests of strains N40, JD1, and B31. A more comprehensive fractionation of all three strains (membrane isolation and preparation; more extensive SCX fractionation of tryptic peptides; peptide enrichment methodologies to reduce complexity) has the capability to greatly expand the overall coverage of the proteome.

Table 1. Proteins unique to strains JD1 and N40 as compared to strain B31.

Strain	Unique Proteins to Strain	Hypothetical	Membrane	Heat shock	DNA, RNA	Putative	Other Functions
JD1	85	38/85 (45%)	5/85 (6%)		9/85 (11%)	3/85 (4%)	30/85 (35%)
N40	86	33/84 (39%)	5/86 (6%)	1/86 (1%)	10/86 (12%)	7/86 (8%)	30/86 (35%)

High-Resolution Infrared Studies of Sulfur Trioxide

J Barber,[(a)] T Masiello,[(a)] ETH Chrysostom,[(a)] JW Nibler,[(a)] A Maki,[(a)] A Weber,[(b,c)] TA Blake,[(d)] and RL Sams[(e)]

(a) Oregon State University, Corvallis, Oregon
(b) National Science Foundation, Arlington, Virginia
(c) National Institute of Standards and Technology, Gaithersburg, Maryland
(d) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington
(e) Pacific Northwest National Laboratory, Richland, Washington

Sulfur trioxide (SO_3) is a molecule of importance both industrially and environmentally. The high-resolution spectrum of SO_3 has proved to be challenging because of extensive mixing of some of the vibrational levels attributed to Fermi resonance and Coriolis interactions. Thom Blake, EMSL, and Bob Sams, PNNL, working in collaboration with researchers from Oregon State University and the National Science Foundation/National Institute of Standards and Technology, published back-to-back papers (Barber et al. 2003a, Barber et al. 2003b) describing in great detail the high-resolution infrared spectrum of SO_3. The laboratory measurement of the spectroscopic properties of SO_3 and other atmospheric gases such as ozone, methane, and carbon dioxide have been used by researchers in a variety of disciplines as reference standards (such as www.hitran.com). For example, these data are used to support atmospheric modeling and remote sensing applications.

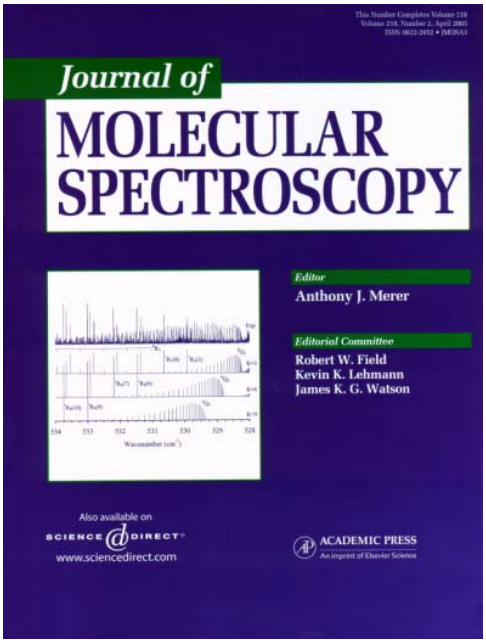

Figure 3. The cover of the April 2003 issue of the *Journal of Molecular Spectroscopy,* featuring the high-resolution infrared spectrum of SO_3.

A high-resolution spectrum from this research was featured on the cover of the April 2003 issue of the *Journal of Molecular Spectroscopy* (Barber et al. 2003a) (Figure 3). Related work performed in this laboratory was also featured on the cover of the October 2002 issue of the *Journal of Molecular Spectroscopy* (Brown et al. 2002).

Citations

Barber J, T Masiello, E Chrysostom, JW Nibler, A Maki, A Weber, TA Blake, and RL Sams. 2003a. "High Resolution Infrared Studies of the ν_2,ν_4 Bands of $^{34}S^{16}O_3$, Including Both Intensity and Wavenumber Perturbations." *Journal of Molecular Spectroscopy* 218(2):197-203.

Barber J, ETH Chrysostom, T Masiello, JW Nibler, A Maki, A Weber, TA Blake, and RL Sams. 2003b. "Analysis of the ν_2, ν_4 Infrared Hot Bands and ν_1 CARS Spectrum of $^{34}S^{16}O_3$." *Journal of Molecular Spectroscopy* 218(2):204-212.

Brown LR, RL Sams, I Kleiner, C Cottaz, and L Sagui. 2002. "Line Intensities of the Phosphine Dyad at 10 μm." *Journal of Molecular Spectroscopy* 215(2):178-203.

Estimation of Hanford SX Tank Waste Compositions from Historically Derived Inventories

PC Lichtner[(a)] and AR Felmy[(b)]

(a) Los Alamos National Laboratory, Los Alamos, New Mexico

(b) Pacific Northwest National Laboratory, Richland, Washington

Migration of radionuclides under the SX tank farm at the Hanford nuclear waste complex involves interaction of sediments with concentrated $NaOH–NaNO_3–NaNO_2$ solutions that have leaked from the tanks. This study uses a reaction path calculation to estimate tank supernatant compositions from historical tank inventory data. The Pitzer activity coefficient algorithm based on the computer code GMIN is combined with the reactive transport code FLOTRAN to carry out the simulations. An extended version of the GMIN database is used that includes aluminum and silicon species. In order for the reaction path calculations to converge, a pseudo-kinetic approach employing a rate limiter for precipitation kinetics is introduced. The rate limiter enables calculations to be carried out with the reaction path approach that previously could only be accomplished using a Gibbs free-energy minimization technique. Because the final equilibrium state is independent of the reaction path, the value used for the rate limiter does not affect the calculation for the tank supernatant composition. Three different tanks are considered: SX-108, SX-109, and SX-115, with supernatant compositions ranging from extremely to moderately concentrated. Results of the simulations indicate that sodium concentrations much higher than previously expected are possible for the SX-108 tank. This result has important implications for the migration of cesium released from the tank within the vadose zone. The mineral cancrinite was predicted to form in all three tanks consistent with recent experiments. The calculated supernatant pH ranged from 14 to 12.8 for the tanks considered and Eh was mildly reducing determined by the redox couple $NO_3–NO_2$.

Citation

Lichtner PC and AR Felmy. 2003. "Estimation of Hanford SX Tank Waste Compositions from Historically Derived Inventories." *Computers & Geosciences* 29(3):371-383.

Reactions at Interfaces as a Source of Sulfate Formation in Sea Salt Particles

A Laskin,[(a)] DJ Gaspar,[(a)] W Wang,[(b)] SW Hunt,[(b)] JP Cowin,[(c)] SD Colson,[(c)] and BJ Finlayson-Pitts[(b)]

(a) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington
(b) University of California, Irvine, California
(c) Pacific Northwest National Laboratory, Richland, Washington

Understanding the formation of sulfate particles in the troposphere is critical because of their health effects and direct and indirect effects on radiative forcing, hence on climate. Laboratory studies of the chemical and physical changes in NaCl, the major component of sea salt particles, show that NaOH is generated upon reaction of deliquesced NaCl particles with gas phase OH. The increase in alkalinity will lead to an increase in the uptake and oxidation of SO_2 to sulfate in sea salt particles. This chemistry is missing from current models, but is consistent with a number of previously unexplained field-study observations. Atmospheric models typically overestimate the amount of sulfur dioxide and underestimate the amount of sulfate near the Earth's surface. The explanation for this discrepancy may lie in the chemistry of sea salt particles thrown into the atmosphere by wind and waves, according to a team of scientists led by Alexander Laskin at PNNL. Using particles of NaCl, the major component of sea salt, they demonstrate that the salt can react with atmospheric hydroxyl radicals (formed from the reaction of ozone, light, and water vapor) to produce NaOH, shown in Figure 4 coating a salt particle. The NaOH increases the pH of the salt particles, and the alkalinity in turn promotes the oxidation of sulfur dioxide by ozone to yield sulfate. "This chemistry is missing from current models," the authors write, but is consistent with a number of previously unexplained field observations.

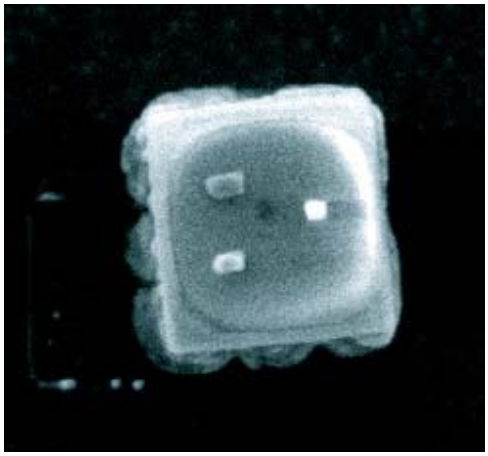

Figure 4. An image of NaOH coating an NaCl particle obtained using the environmental scanning electron microscope in EMSL's Chemistry and Physics of Complex Systems Facility. This image was recently published in *Science* (Laskin et al. 2003).

Citations

Laskin, A, DJ Gaspar, W Wang, SW Hunt, JP Cowin, SD Colson, and BJ Finlayson-Pitts. 2003. "Reactions at Interfaces as a Source of Sulfate Formation in Sea-Salt Particles." *Science* 301:340-344.

Receptor Tyrosine Kinases in Human Cell Lines

EF Strittmatter[(a)] and A Patwardhan[(b)]

(a) Pacific Northwest National Laboratory, Richland, Washington

(b) University of California, San Francisco, California

Deregulation of receptor tyrosine kinase (RTK) signaling is now recognized as an important event in the genesis and progression of human epithelial cancers, including breast cancer. This knowledge has stimulated the development of a broad range of RTK pathway inhibitors as anticancer agents. Analysis of the trypsin-digested membrane proteins purified from MCF7c18, MDA231, BT474, SKBR3, and EGFR human breast cancer cell lines was carried out using strong cation exchange fractionation combined with high-resolution reversed phase capillary LC-LCQ MS/MS (all cell lines combined together). These runs were analyzed using the PARALLAX program and mass tag database containing approximately 8,500 unique peptides from the human IPI protein database. Approximately half of the 70 RTK proteins contained in the multiplexed sample were identified including ERBB2, ERBB4, and the human epithelial growth factor RTKs. Expression of these proteins can now be systematically studied and compared against mRNA expression data to further understand the role of these proteins in cancer.

Awards and Recognition

Chemistry and Physics of Complex Systems Facility staff received top honors for a technical poster during an astrophysics conference held last month in Estes Park, Colorado. The poster, "Sticky Amorphous Ice Grains Aid Planet Formation," received best poster award in the Dust in Circumstellar Environments Origin and Evolution of Dust category. Congratulations to Hanfu Wang (post-doc); Richard Bell (post-doc); Greg Schenter and James Cowin, Chemical Sciences Division; and Martin Iedema, EMSL, as well as to Kai Wu and Thanos Teskouras, (previously post-docs at PNNL who have since left to assume positions outside the United States). The recognition for this research is significant because it demonstrates PNNL's ice physics capabilities in yet another scientific community. Current models of planet formation cannot explain how grains of dust in early solar systems could possibly stick together fast enough to grow planets. PNNL answered this question through measurements that show that low-temperature ice has surprising sticky tendencies due to its unique electrical and mechanical properties.

Sotiris Xantheas, a chief scientist at PNNL and an EMSL user, has been awarded the Friedrich Wilhelm Bessel Research Award from the Alexander von Humboldt Foundation in Bonn, Germany. From 2001 to 2003, the Foundation granted approximately 10 of these awards to outstanding young scientists already internationally recognized for significant contributions in their fields. His research interests lie in the application of high-level electronic structure calculations in order to elucidate the properties of hydrogen-bonded systems and the use of the quantum mechanical results in the development of empirical models to simulate their macroscopic properties.

Professional/Community Service

Pacific Northwest Microscopy Society Meeting

The annual meeting of the Pacific Northwest Microscopy Society (PNMS) was held at EMSL May 29-30, 2003 (Figure 5). PNNL's Alice Dohnalkova and EMSL's Jim Young organized this year's conference, which was attended by approximately 70 to 80 scientists and engineers from universities, medical centers, and industries within the northwest region.

Figure 5. Annual meeting of Pacific Northwest Microscopy Society (2003).

The Microscopy Society of America invited Lucile Giannuzzi from the University of Central

Florida, Orlando, Florida, to present the keynote speech regarding the current state-of-the-art in Focused Ion Beam (FIB) technology. The meeting included more than 20 contributed talks and 16 poster presentations. The conference focused on the current status of research in the applications of optical and electron microscopy in biological, environmental, and materials science. Platform sessions were held on the FIB technology, advances in analytical techniques for material science, flow cytometry, laser microscopies, three-dimensional cell reconstruction, and environmental applications. A short demonstration on flow cytometry received a positive response. Special emphasis was given to papers contributed by students. Cash prizes were awarded to the top three poster presentations. Stephen Reidel of PNNL's Applied Geology and Geochemistry group presented an interesting discussion on the geologic history of the Columbia River during the evening banquet at Gordon Brothers Winery in Pasco. Twelve vendors exhibited their recent product developments in optical and electron microscopy. In addition, several lab tours were organized for participants to learn more about the state-of-the-art electron and optical microscopy facilities at EMSL.

Nanoscience and Nanotechnology Course

Twenty students from as far away as Alaska and Florida attended the first of a series of intensive nanoscience and nanotechnology courses offered at PNNL on May 19-30, 2003 (Figure 6). The aims of the courses are to enhance education and research in nanotechnology and to speed undergraduate and graduate entry into the field. PNNL and the University of Washington (UW), Seattle, Washington, through their Joint Institute for Nanoscience, have a grant from the National Science Foundation to develop the curriculum for the series of courses. This effort includes significant contributions from Washington State University (WSU), Pullman, Washington, and the University of Idaho, Moscow, Idaho, and could be taken for UW or WSU credit.

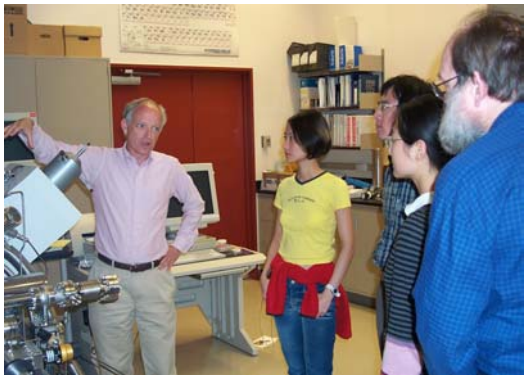

Figure 6. PNNL course coordinator, Don Baer, explains the utilization of one of the surface analytical systems in characterizing nanostructures to a group of students at EMSL.

The first course was coordinated by WSU Professor Lai-Sheng Wang and PNNL scientist Don Baer. The program included unmatched access to advanced scientific and technological tools in EMSL and provided an opportunity to meet and work with nationally recognized scientists. More information is available at http://www.nano.washington.edu/pnnl/overview.html.

The nanoscience course was highlighted in a May 26, 2003, *Tri-City Herald* newspaper article describing the enthusiastic opinions of students and instructors.

Environmental Management Science Program Workshop

The Environmental Management Science Program (EMSP) Workshop, held May 6-7, 2003, at EMSL, drew more than 225 attendees to the principal investigators meeting. PNNL's John Zachara and Sonia Enloe were the primary organizers of the event, which focused on subsurface science and high-level waste research and its application to the Hanford Site. They were assisted by Gary Josephson and Mark Freshley from PNNL. More than 70 of the attendees were EMSP principal investigators from the national laboratory and university community, as well as representatives from Hanford Site contractors, the DOE Richland Operations Office, the DOE Office of River Protection, and DOE Headquarters. Specific guests included Teresa Fryberger, Henry Shaw, and Roland Hirsch from the DOE Office of Biological and Environmental Research, as well as Mark Gilbertson, Caroline Purdy, and Chet Miller from the DOE Office of Environmental Management.

Other Activities

Tom Autrey and Nancy Foster-Mills chaired a session on "Properties for Chemical Process Design" at the 15th Symposium on Thermophysical Properties, June 22-27, 2003, University of Colorado, Boulder, Colorado.

Alice Dohnalkova gave a tour of the EMSL Electron Microscopy Laboratory to 12 local high school students participating in the "Young Women in Science" program sponsored by PNNL.

Theresa Windus was part of the organizational team for the Science Case for Large Scale Simulation workshop held in Washington, DC, June 24-25, 2003. More than 280 scientists, mathematicians, computer scientists and DOE program managers convened to establish large science cases associated with high-end computing and the requirements for accomplishing this science. A report based on the findings will be submitted to DOE program managers by July 30, 2003.

Major Facility Upgrades

All data from the scientific archive management (SAM) system was migrated into the new NWfs archive in May. Approximately 1.6 terabytes of files were successfully moved and reorganized over four days. The former SAM servers will be shut down and retired in June.

Version 4.5 of NWChem is now available for users to download and test. Major additions in this version include a port to the Phase I system (Itanium 2 with Quadrics interconnect); a time-dependent density functional module that also includes configuration-interaction singles capability; an electron transfer module; a projected augmented wave module; and a tensor contraction engine module that includes many high-level correlation methods created through an automated code generation package. Several other improvements and fixes to previous problems are also included in the 4.5 release. More information about the release is available at http://www.emsl.pnl.gov/docs/nwchem.

The beta release of the Extensible Computational Chemistry Environment version 3.1 is now available (see http://ecce.emsl.pnl.gov for complete information). Major new features in v3.1 include the following:

- Code registration user interfaces created with a Python wrapped graphic user interface toolkit, PyQt.
- Molecule Builder available "standalone" as a separate distribution (available for download later during the beta period).
- Export of POV-Ray format image files for publication-quality graphics.
- The ability to define chemical systems in Builder before creating calculations (alternate workflow).
- Full support for Suns again (download is no longer a special request).
- Greatly improved performance when working with large molecules in the Builder.
- Support for new NWChem Electrostatic Potential and Property run types.
- Calculation Viewer molecular orbital energy plots.
- Automatic creation of data server user accounts (can be disabled).
- Globus Toolkit (Argonne National Laboratory) v2.2 support.
- Numerous bug fixes.

News Coverage

The TOP500 list of the 500 most powerful commercially available computers was released in June 2003. The high-performance PNNL computer in EMSL's Molecular Science Computing Facility (Figure 7) was number eight on the list. When completed this year, the computer will have an expected total peak performance of over eleven teraflops (a teraflop is one trillion calculations per second). For the complete TOP500 list, see http://www.top500.org/list/2003/06/ as well as the TOP500 press release at http://www.top500.org/lists/2003/06/press-release.php.

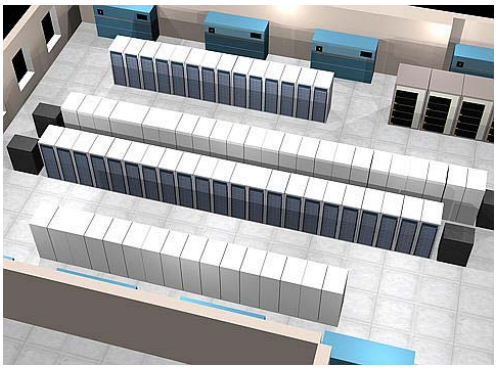

Figure 7. Computer rendering of the 11+ Teraflop cluster-based computer in EMSL.

The nanoscience course at EMSL, sponsored by the University of Washington, PNNL, and Washington State University, was featured in an article in the May 26, 2003, *Tri-City Herald* http://www.tricityherald.com/tch/local/story/3184906p-3209083c.html. The article, "Nanoscience Class One of Few," describes studies at the nano-level and some of EMSL's unique instruments for this type of research.

Nearly a dozen members of the *Tri-City Herald* editorial and news staff toured EMSL in June to learn more about the laboratory and its capabilities.

Don Baer was interviewed for a story in the June 16, 2003, issue of *The Scientist*., highlighting "dream labs" (http://www.the-scientist.com/yr2003/jun/lcprofile_030616.html).

Visitors and Users

Environmental Spectroscopy and Biogeochemistry Facility

- Paul Bagus (see Figure 8), Texas A&M University, College Station, Texas, in collaboration with Eugene Ilton, PNNL, Richland, Washington, compared *ab initio* models for the Cr3p spectra of an embedded CrO_6 cluster with the free ion model and experimental spectra for Cr_2O_3. They were able to demonstrate that the cluster model more closely modeled the experimental data. The primary reason was the influence of the crystal field, not charge transfer: the crystal field reduces the symmetry of the initial state of the Cr(3+) cation from 4F in the free cation to 4A2 in the crystal field. This is a new observation and will form the basis for a future paper.

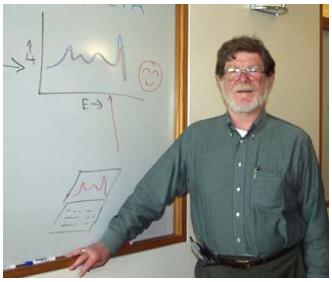

Figure 8. Paul Bagus from Texas A&M University.

- Thomas Borch, Montana State University's Center for Biofilms, Bozeman, Montana, in collaboration with Ravi Kukkadapu, EMSL, Richland, Washington used Mössbauer spectroscopy to characterize and understand the nature of biogenic iron phases in bioreduced ferrihydrite samples that were found active in trinitrotoluene (TNT) degradation.

- Hailiang Dong, Miami University, Oxford, Ohio, in collaboration with Ravi Kukkadapu, EMSL, Richland, Washington used Mössbauer spectroscopy to probe the bioreducibility of different Fe(III) sites in a "pure" reference illite clay from Illinois. This research will be useful in understanding the biotransformation of illite clays that are abundant in soils.

- Robin Gerlach (see Figure 9), Center for Biofilm Engineering at Montana State University, Bozeman, Montana, visited EMSL to use high-resolution transmission electron microscopy, scanning electron microscopy, and x-ray diffraction for analysis and imaging of biomineral formation induced by *Cellulomonas* species exposed to iron and chromium redox environments in a laboratory setup simulating natural soil conditions. He also gave a talk entitled "Direct and Indirect Cr(VI) Reduction by *Cellulomonas spp.* - Batch Kinetics and Meso-scale Tests."

Figure 9. Robin Gerlach from Montana State University.

- Andrew Stack, University of California, Davis, California, in collaboration with Jim Rustad, PNNL, Richland, Washington, worked on developing a molecular mechanics potential model of KH_2PO_4. The work involved computing potential surfaces and bulk crystal structures (KH_2PO_4, $KH_2PO_4.2H_2O$) with NWChem, and constructing potentials based on these calculations using Rustad's fitting codes. The findings will be used in simulations of KH_2PO_4 crystal growth in aqueous solutions.

- Chris Thompson, PNNL, Richland, Washington, measured Fourier Transform Ion Resonance (FTIR) spectra of supercritical carbon dioxide and xenon solutions containing selected chlorinated hydrocarbons. The measurements will be used to demonstrate the feasibility of applying FTIR spectroscopy for monitoring a novel sample-preparation process in which chlorinated hydrocarbons are incorporated into sediments using supercritical fluids.

High-Field Magnetic Resonance Facility

- Hanne Bertram, Danish Institute of Agricultural Sciences, Tjele, Denmark, recently used the 300-MHz spectrometer to work on the studies of "Post Mortem Energy Metabolism and Water Characteristics in Rabbit *M. longissimus* Studied by Dynamic Slow-Speed MAS NMR Spectroscopy and Relaxometry."

- Colin Fyfe, Darren Brouwer, and Celine Schneider, University of British Columbia, Vancouver, British Columbia, recently used the 800-MHz spectrometer for "Structural Investigations of Solid Materials by High Resolution Solid State NMR at Very High Field."

- Karl Mueller, Pennsylvania State University, University Park, Pennsylvania, recently sent Gary Crosson to work on the 800-MHz spectrometer for "High-field 1Q MAS and MQMAS Solid-State NMR Studies of the Dissolution of Montmorillonite Clays Under Alkaline Conditions."

- Gabriele Varani and graduate student Thomas Leeper, University of Washington, Seattle, Washington, recently worked remotely on the 600-MHz spectrometer for their studies of the "Structure of Telomerase RNA."

High-Performance Mass Spectrometry Facility

- David Gibb Camp II, PNNL, Richland, Washington, participated in "Preliminary Work on the Proteomes of Brains and Dissected Brains Obtained from Control Mice and Treated Mice Simulating Parkinson's Disease." Initial protein identifications from homogenized mouse brain samples were collected.

- Michael Daly, Uniformed Services University of Health Sciences, Bethesda, Maryland, sent samples that were analyzed on the 11.4-tesla Fourier Transform Ion Cyclotron Resonance (FTICR) mass spectrometer to gather data for a "Comparative Display of *D. radiodurans* Proteome After Exposure to Ionizing Radiation."

- Edward Dratz, Montana State University, Bozeman, Montana, examined the "Mechanism of Action of G Protein-coupled Receptors Studied by LC-FTICR Mass Spectrometry."

- Bing Gong, University of Buffalo, Buffalo, New York, worked on "Hollow Helices as Folding Nanotubes with Tunable Cavity Size." Preliminary data from the quadrupole time-of-flight mass spectrometer did not preserve the con-covalent interactions that were being investigated. Subsequent analysis on the 7-tesla FTICR was successful in showing specific binding for the nanotube helices as a mimic of biological systems.

- Mary Lipton, PNNL, Richland, Washington, analyzed samples from *Shewanella oneidensis* on the LCQ spectrometers (quadrupole ion-trap mass spectrometers equipped with a liquid chromatography system) to gather data to assess the effects of "Low Dose" radiation on the formation of complexes. Additional projects were carried out using new biotinylation reagents to identify proteins involved in the reduction of iron by *Geobacter*, and continuing studies of the proteome *Deinococcus radiodurans* under different stress conditions.

- Anil J. Patwardhan (see Figure 10), University of California, San Francisco, California, brought 6 mg of protein from MCF-7 and other breast cell cancer lines for analysis. Nearly 70 runs of the strong cation exchange fractionated samples were completed on the LCQ. Presently, these runs are being analyzed for the presence of receptor tyrosine kinase proteins and data analysis is continuing but incomplete. The information will be used in the paper "Identification and Relative Expression of Membrane Proteins in Breast Cancer Cell Lines."

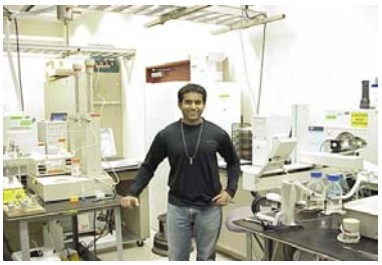

Figure 10. Anil Patwardah from the University of California, San Francisco.

- Linda Randall, University of Missouri, Columbia, Missouri, identified errors in the labeling of SecA proteins. New samples were prepared for "Identification of Covalent Modification of SecA."

- Amy K. Schmid, University of Washington, Seattle, Washington, sent samples that were analyzed on the LCQ spectrometers to gather data for the "Identification of Heat Shock Proteins in the Radioresistant Bacterium *Deinococcus radiodurans*."

- Wenzhong Xiao, Stanford University, Stanford, California, worked on "Functional Genomics and Proteomics of Mitochondria." Relative abundance data for mitochondria in yeast were collected and forwarded to the users.

Interfacial and Nanoscale Science Facility

- A number of scientists and engineers who attended the Pacific Northwest Microscopy Society Meeting visited the Interfacial and Nanoscale Science (I&NS) Facility and discussed ongoing and possible future collaborations with facility staff.

- The nanoscience course students who took part in the arranged tours of EMSL facilities interacted with several I&NS Facility staff and discussed possible future opportunities using the instrumentation for their research work.

- Soo Yin Chin, University of South Carolina, Columbia, South Carolina, attended the nanoscience course offered by PNNL and the University of Washington. Upon completion, she extended her stay to work on the characterization of noble metal catalysts for hydrogen production and purification in fuel cell applications in collaboration with Cathy Chin, PNNL, Richland, Washington, and Mark Engelhard and Chongmin Wang, EMSL, Richland, Washington.

- John Cliff, Oregon State University, Corvallis, Oregon, continued work on the investigations related to the use of carbon and nitrogen isotopes to trace soil chemical processes and biogeochemical nutrient cycling in collaboration with Dan Gaspar, EMSL, Richland, Washington.

- Charles Hibbitts, University of Washington, Seattle, Washington, worked with Shuttha Shutthanandan and Theva Thevuthasan, EMSL, Richland, Washington, at the accelerator facility on studies related to "MeV Ion Irradiation of Non-ice Solar System Analogue Materials."

- Richard Smith, Montana State University, Bozeman, Montana, worked with Shuttha Shutthanandan and Theva Thevuthasan, EMSL, Richland, Washington, developing low-cost and high-temperature corrosion- (oxidation-) resistant coatings for bipolar interconnect plates in solid oxide fuel cell stacks.

- Graham Tewksbury and Jack Keegan, Portland State University, Portland, Oregon, worked in collaboration with Jim Young, EMSL, Richland, Washington, to determine the size distribution of thermal spray powders and the tungsten carbide particles in coatings.

- Venugoplan Vaithyanathan and Lisa Edge, Pennsylvania State University, University Park, Pennsylvania, worked with Scott Chambers and Tim Droubay, PNNL, Richland, Washington, measuring the band offsets of epitaxially grown $LaAlO_3$ films on silicon substrates.

Molecular Science Computing Facility

- Don Archer and Bill Magro from Intel, Santa Clara, California, were onsite to discuss the future of high-performance technical computing.

- Dan Oscar Bonachea, University of California, Berkeley, California, worked on studies of "Developing High-Performance Parallel Languages on the SGI Altix."

- Styliani Constas, University of Western Ontario, London, Ontario, Canada, worked on studies of "Computer Simulations of Chemical Reactions in Confined Environments and Mesoscopic Clusters."

- Steven Dietz and Lawrence Snyder, University of Washington, Seattle, Washington, and Bradford Chamberlain from Cray Inc., Seattle, Washington, met to discuss possible collaboration regarding ZPL parallel array programming language for science and engineering computations. In particular, discussions were held concerning the use of aggregate remote memory copy interface in ZPL and the use of ZPL in Fock matrix building and Fast Fourier Transforms.

- Carl A. Fahlstrom, Eastern Oregon University, LaGrande, Oregon, began a three-month assignment working with Theresa Windus, EMSL, Richland, Washington, as his mentor in the Molecular Sciences Software group. Carl will be working on NWChem development as well as creating chemistry components using the common component architecture.

- Thomaso Frigato, Max Planck Institute of Biophysics, Frankfurt, Germany, visited the Molecular Sciences Software group and the Computational Biosciences group to collaborate on the implementation in the molecular dynamics module of NWChem of QHOP: a new method allowing the simulation of proton transfer events in biomolecular systems. Frigato is one of the original developers of this method. He also worked with TP Straatsma and Dayle Smith, PNNL, Richland, Washington, and Erich Vorpagel, EMSL, Richland, Washington, on electronic transfer calculations for the hemes of Flavocytochrome c3.

- Gary Geissler, SGI Vice President of Engineering; Steve Reinhardt, former Altix Project Manager, currently HPCS project manager; George Vandegrift, Gov. Business Developer, and Rick Scott, from SGI, Mountain View, California (location of corporate headquarters) were onsite to present details of their Department of Defense High Performance Computing Systems proposal and discuss possible interest in a joint DOE proposal for research.

- Scott M. Jackson, PNNL, Richland, Washington, worked on studies of "Gold - Accounting and Allocation Management."

- Sharon Joseph from Platform Computing, Markham, Ontario, Canada, presented an overview of local file system daemons and administration commands, along with specific training related to the configuration on the EMSL supercomputer.

- Werner Krotz-Vogel, Pallas, presented a tutorial workshop. Pallas Vampir is a visualization and performance analyzer tool for MPI programs. It will be available on Phase 2 of the supercomputer installation.

- Martinus Adrianus Nooijen, Princeton University, Princeton, New Jersey, worked on studies of "Benchmarking Localized Coupled Cluster Methods in the NWChem Package."

- Michael Charles Perkins, PNNL, Richland, Washington, worked on studies of "Holographic Imaging Radar Measurement System."

- Sanja Sekusak, PLIVA d.d., Zagred, Croatia, worked with TP Straatsma, PNNL, Richland, Washington, and Erich Vorpagel, EMSL, Richland, Washington, on molecular dynamics and quantum mechanics/molecular mechanics studies of macrolide molecules.

- Peter Thompson and Christopher Gottbrath, Etnus, Natick, Massachusetts, presented a tutorial workshop. Etnus TotalView is a parallel debugger that supports various types of parallel programming models (MPI, OpenMP, C/C++, and F90). It will be available on Phase 2 of the supercomputer installation.

- Wolfgang Tolle, University of Washington, Seattle, Washington, visited the facility. Tolle is the new special assistant for technology development at the University of Washington and visited PNNL to learn more about the work conducted here.

- Brian David Wood, Oregon State University, Corvallis, Oregon, worked on studies of "Modeling Complex Bacterial Cell Systems through Development of Segregated Models with Spatial Localization."

Molecular Sciences Software - New User Agreements with NWChem/Ecce:

- Angstrom Microsystems, Boston, Massachusetts
- BP Chemicals, Naperville, Illinois
- Bulgarian Academy of Sciences, Sofia, Bulgaria
- CDCC Center for Development of Adva, Montpellier, France
- CDCC Center for Development of Adva, Garneshkhind, India
- DSM Research BV, Limburg, the Netherlands
- Institute for Molecular Science, Okazaki, Japan
- Mogilev State Foodstuffs University, Mogilev, Russia
- North Carolina University, Raleigh, North Carolina
- Sandia National Laboratories, Livermore, California
- Universidad de Chile, Santiago, Chile
- Universidade de Sao Paulo, Sao Paulo, Brazil
- University of Alabama, Tuscaloosa, Alabama
- University of the Basque Country (EHU/UPV), Donostia-San Sebastian, Spain

New EMSL Staff

Christopher Oehmen and Douglas Baxter were hired as consultants in the Molecular Science Computing Facility Visualization and User Services group. Christopher Oehmen recently finished his doctorate in Biomedical Engineering through a joint program offered by the University of Memphis and University of Tennessee Health Sciences Center, Memphis, Tennessee. He will be heavily involved with the Genomes to Life computational biology effort. Douglas Baxter was hired for his expertise in parallel programming, with more than 20 years experience in software design and analysis for programs in high-performance computing on a wide variety of hardware platforms and software environments. Prior to coming to EMSL, his most recent work was as a private consultant for organizations such as Sun Microsystems, Inc. and the University of Phoenix, Tigard, Oregon campus.

Amy Selch joined the EMSL User Services and Outreach Staff as an Administrative Assistant.

Michael Froehlke joined the High-Field Magnetic Resonance Facility as a senior techician.

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