DOE User Facilities for Environmental Remediation Research

DOE Office of Science
Office of Biological & Environmental Research
Environmental Remediation Sciences Division

April 16, 2007
Operations Funding Provided by the DOE Office of Science (SC)

- Basic Energy Sciences (BES) funds several types of relevant user facilities
  - Synchrotron Radiation Light Sources (ALS, APS, NSLS, SSRL)
  - Nanoscience Centers (ANL, BNL, LBNL, ORNL, SNL/LANL)
  - Neutron Sources (SNS at ORNL, Others)

- Advanced Scientific Computing Research (ASCR) funds several high performance computing centers
  - Leadership Computing Facility (LCF) at ORNL and at ANL
  - National Energy Research Scientific Computing Center (NERSC) at LBNL

- Biological and Environmental Research (BER) funds two relevant user facilities
  - Environmental Molecular Sciences Laboratory (EMSL), PNNL
  - Joint Genome Institute (JGI), Walnut Creek, CA
Synchrotron Light Source Resources for Environmental Remediation Research

Techniques

Infrared Spectroscopy
X-ray Absorption Spectroscopy - XAS, XAFS, EXAFS, XANES, XRF
X-ray Scattering - Diffraction, Small angle scattering
X-ray Microscopy - STXM, XRF mapping, microdiffraction, microspectroscopy
X-ray Tomography

Locations

Argonne’s Advanced Photon Source (APS)
Microprobe, MicroXAS, Spectroscopy

Brookhaven’s National Synchrotron Light Source (NSLS)
Diffraction, Microprobe, Spectromicroscopy (STXM), Spectroscopy

Berkeley’s Advanced Light Source (ALS)
FTIR, Microprobe, Microtomography, Spectroscopy

SLAC’s Stanford Synchrotron Radiation Laboratory (SSRL)
Diffraction, Spectroscopy, Small angle scattering
### High Performance Computing (HPC) Resources in SC

<table>
<thead>
<tr>
<th>Location</th>
<th>System Details</th>
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<tr>
<td><strong>EMSL/MSCF</strong></td>
<td>MPP2, HP Linux Itanium 2, 11.5 TFlops&lt;br&gt;HPCS-3, 100+ TFlops planned for FY08</td>
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<td><strong>LCF-ORNL</strong></td>
<td>Jaguar, Cray XT (XT3 + XT4) w/ 11,508 dual core compute CPUs, 119 TFlops&lt;br&gt;Phoenix, Cray X1E, w/ 1024 multi-streaming vector processors, 18 GF</td>
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<td><strong>LCF-ANL</strong></td>
<td>IBM, Blue Gene/L, 5.7 TFlops&lt;br&gt;IBM Blue Gene/P, 100 TFlops planned for FY08</td>
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<td><strong>LCF Access</strong></td>
<td>80% of resources allocated through INCITE solicitation - mid May&lt;br&gt;<a href="http://hpc.science.doe.gov">http://hpc.science.doe.gov</a></td>
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<td><strong>NERSC-LBNL</strong></td>
<td>Seaborg, IBM RS/6000 SP, 10 TFlops&lt;br&gt;Franklin, Cray XT4 w/ 9,672 dual core compute CPUs, 100+ TFlops planned for FY08</td>
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Environmental Molecular Sciences Laboratory (EMSL)

A national scientific user facility integrating experimental and computational resources for discovery and technological innovation

- Electronic user proposal submission
- **Non-Proprietary (Open) Research** - results are published and shared broadly within the scientific community. Typically **no charge**
- **Proprietary Research** - may be conducted in EMSL under a proprietary sales contract. Users engaged in proprietary research pay the full-cost recovery rate for use of the facility
- Integrated Problem-Solving Environment – coupling experimental and computational resources to solve scientific problems.
EMSL Facilities

Environmental Spectroscopy & Biogeochemistry

Chemistry & Physics of Complex Systems

High Field Magnetic Resonance

High Performance Mass Spectrometry

Interfacial & Nanoscale Science

Molecular Science Computing

Planned capabilities: TOF SIMS, Operando TEM, Microfluidics capability
EMSL’s Four Science Themes and Two Grand Challenges

**EMSL Science Themes** - four environmental molecular science themes that will help define and develop key collections of user projects

- Geochemistry/Biogeochemistry and Subsurface Science
- Biological Interactions and Dynamics
- Science of Interfacial Phenomena
- Atmospheric Aerosol Chemistry

**EMSL Grand Challenges** - complex, large-scale scientific and engineering problems with broad scientific and environmental or economic impacts whose solution can be advanced by applying high-performance scientific techniques and resources

- Biogeochemistry – understanding electron transfer at the microbial/mineral interface (Led by John Zachara & Jim Fredrickson from PNNL)
- Membrane Biology – using a systems biology approach to determine the underlying network that governs photosynthetic processes in cyanobacteria (Led by Himadri Pakrasi from Washington University)
Biogeochemistry Research at EMSL

- **Determining Chemical Forms in Sediments and Solutions**
  - Analysis of Fe compounds by Mossbauer, determination of chemical forms of Sr and Tc by NMR (900 MHz & rad NMR) and U by laser fluorescence

- **Characterizing Biological Systems**
  - Determination of cytochromes in outer membranes by AFM, imaging hydrated cells and cell/mineral interactions by cryo-TEM, protein identification by mass spectrometry, and understanding molecular mechanisms of radionuclide/cell binding by simulation

- **Mineral Surface Chemistry**
  - Determination of the mineral surface coating morphology, coverage and chemical composition and the form of Fe in the coating material by combining AFM, SIMS and XPS

- **Subsurface Flow and Transport**
  - Examining the impact of microbial growth on groundwater chemistry in intermediate scale flow cells and simulation of multifluid flow and multicomponent biogeochemical reactive transport in complex subsurface systems
Joint Genome Institute (JGI)

- **Community Sequencing Program**
  - Provides the scientific community at large with access to high-throughput sequencing at JGI for projects of relevance to DOE missions

- **Laboratory Science Program (LSP)**
  - Provides the DOE national laboratories with broad access to high-throughput nucleic acid sequencing in support of their DOE-relevant biology programs. LSP allocates approximately ten billion bases (i.e., ten gigabases) of raw sequence per year

- **Information for Collaborators**
  - http://www.jgi.doe.gov/sequencing/collaborators/index.html
## User Facility Contact Information

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<tr>
<th>Facility</th>
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<th>Lab POC</th>
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<tr>
<td>EMSL</td>
<td>P. Bayer/M. Kuperberg</td>
<td>A. Campbell/A. Felmy</td>
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<td>JGI</td>
<td>D. Drell/D. Thomassen</td>
<td>D. Bruce</td>
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<td>ALS</td>
<td>R. Hirsch/N. Woodward</td>
<td>S. Hubbard/P. Nico</td>
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<td>APS</td>
<td>R. Hirsch/N. Woodward</td>
<td>K. Kemner/B. Ravel</td>
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<td>NSLS</td>
<td>R. Hirsch/N. Woodward</td>
<td>J. Fitts/P. Northrup</td>
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<td>J. Bargar/S. Webb</td>
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<td>LCF-ANL</td>
<td>B. Helland/D. Hitchcock</td>
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