

U.S. Department of Energy



Office of Science



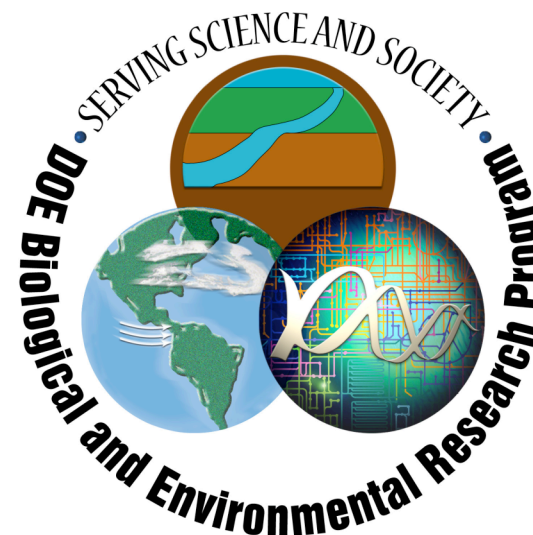
DOE User Facilities for Environmental Remediation Research

DOE Office of Science

Office of Biological & Environmental Research

Environmental Remediation Sciences Division

April 16, 2007

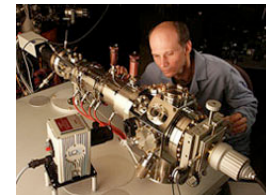




DOE User Facilities for Environmental Remediation Research

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

EMSL/MSCF

MPP2, HP Linux Itanium 2, 11.5 TFlops
HPCS-3, 100+ TFlops planned for FY08

LCF-ORNL

Jaguar, Cray XT (XT3 + XT4) w/ 11,508 dual core
compute CPUs, 119 TFlops

Phoenix, Cray X1E, w/ 1024 multi-streaming
vector processors, 18 GF

LCF-ANL:

IBM, Blue Gene/L, 5.7 TFlops

IBM Blue Gene/P, 100 TFlops planned for FY08

LCF Access:

80% of resources allocated through INCITE solicitation - mid May

<http://hpc.science.doe.gov>

NERSC-LBNL: Seaborg, IBM RS/6000 SP, 10 TFlops

Franklin, Cray XT4 w/ 9,672 dual core compute CPUs, 100+ TFlops
planned for FY08



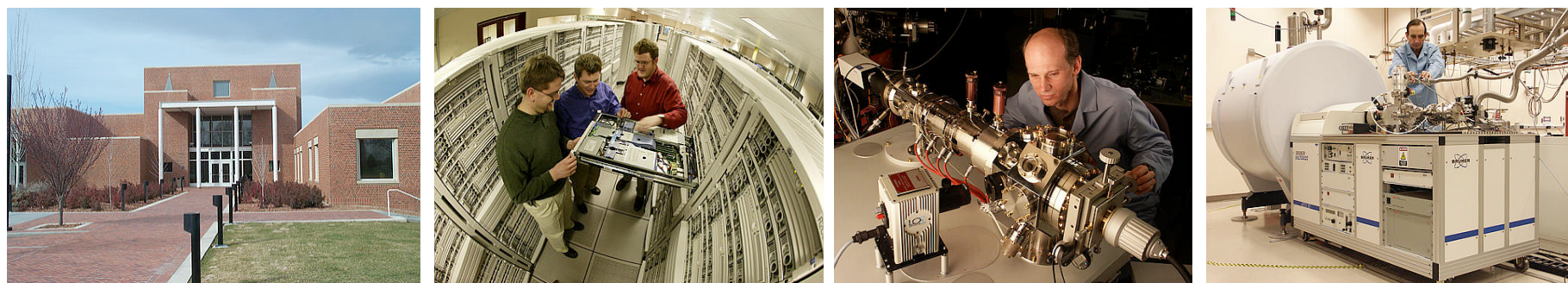
U.S. Department of Energy



Office of Science

Environmental Molecular Sciences Laboratory (EMSL)

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



William R. Wiley

EMSL

Environmental Molecular Sciences Laboratory

- 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.



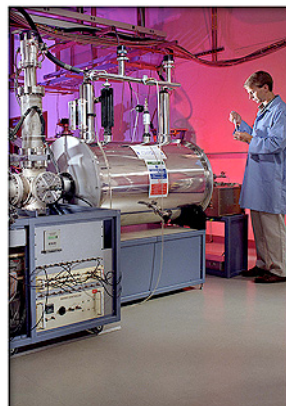
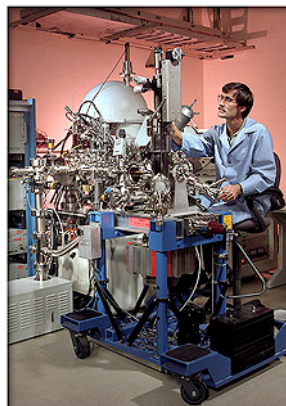
EMSL Facilities



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)



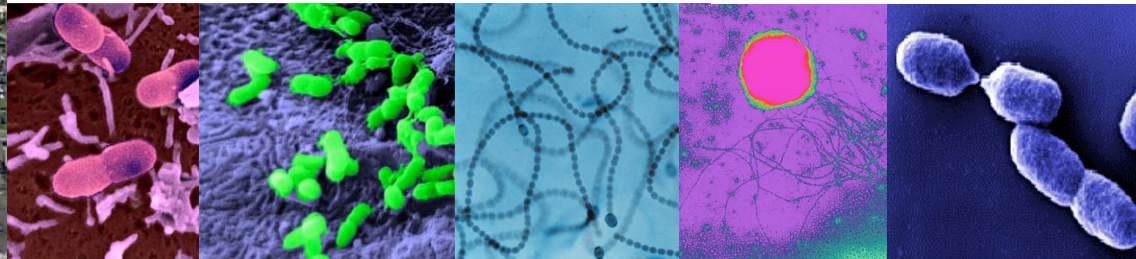
Office of
Science

U.S. DEPARTMENT OF ENERGY



DOE GENOMICS:GTL
SYSTEMS BIOLOGY
FOR ENERGY AND
ENVIRONMENT

OFFICE OF SCIENCE
U.S. DEPARTMENT OF ENERGY



- **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

Facility	SC POC	Lab POC
EMSL	P. Bayer/M. Kuperberg	A. Campbell/A. Felmy
JGI	D. Drell/D. Thomassen	D. Bruce
ALS	R. Hirsch/N. Woodward	S. Hubbard/P. Nico
APS	R. Hirsch /N. Woodward	K. Kemner/B. Ravel
NSLS	R. Hirsch /N. Woodward	J. Fitts/P. Northrup
SSRL	R. Hirsch /N. Woodward	J. Bargar/S. Webb
LCF-ANL	B. Helland/D. Hitchcock	R. Bair
LCF-ORNL	B. Helland/D. Hitchcock	D. Kothe
NERSC	B. Helland/D. Hitchcock	B. Kramer