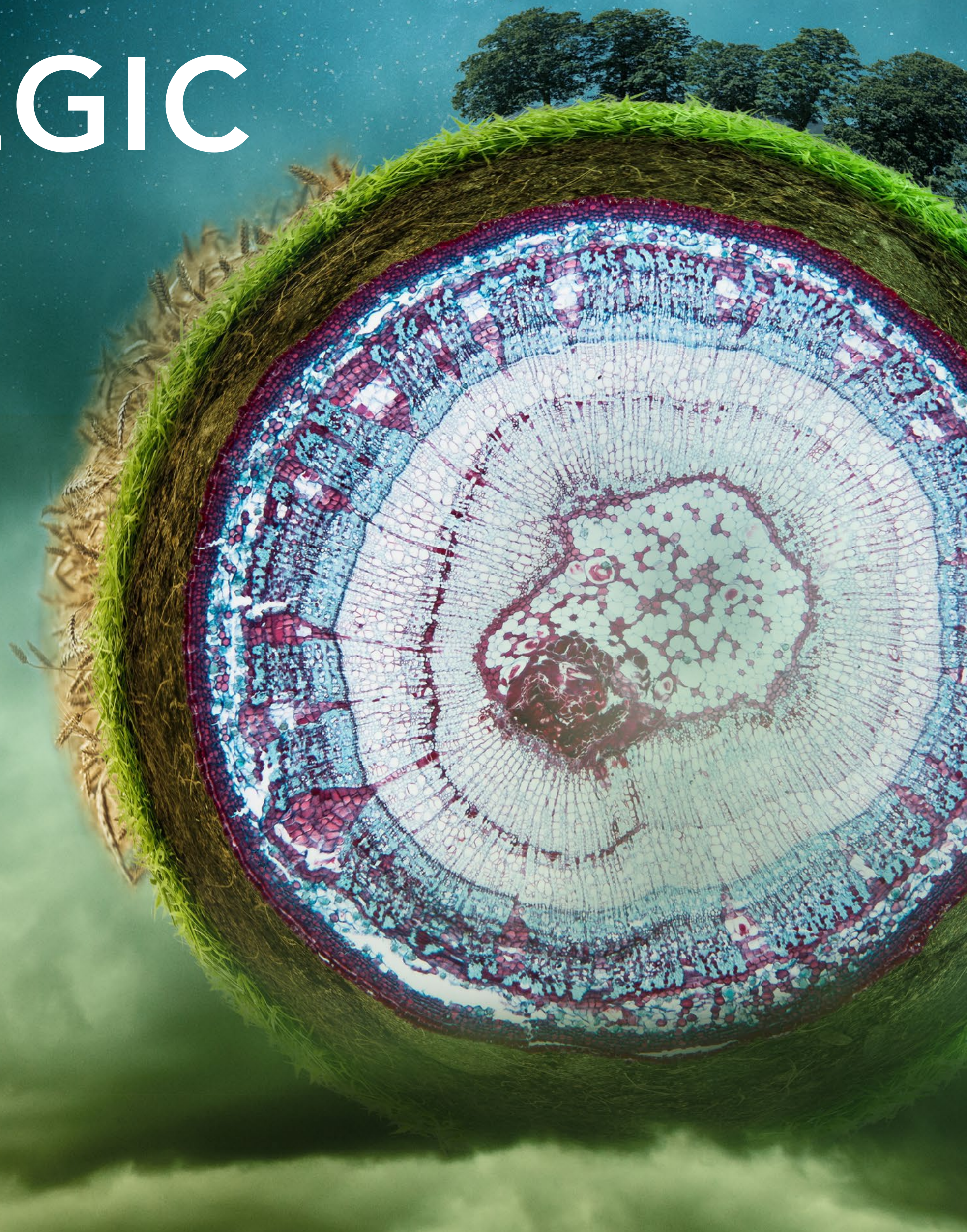
EMSL

2018

STRATEGIC PLAN



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EMSL 2018 Strategic Plan

April 2019

Prepared for the U.S. Department of Energy's
Office of Biological and Environmental Research
under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Our Mission

EMSL accelerates scientific discovery and pioneers new capabilities to understand biological and environmental processes across temporal and spatial scales.

Our Vision

EMSL partners with diverse scientific communities to develop predictive understanding of complex biological and environmental systems to enable sustainable solutions to the nation's energy and environmental challenges.

Acronyms and Abbreviations

AFM	atomic force microscopy
APT	atom probe tomography
ARM	Atmospheric Radiation Measurement
ASR	Atmospheric System Research
BER	U.S. Department of Energy Office of Biological and Environmental Research
BERAC	Biological and Environmental Research Advisory Committee
BRC	bioenergy research center
BSA	Biological Sciences Area
BS&T	Breakthrough Science and Technology
CyTOF	cytometry by time of flight
DART	days away restricted or transferred
DOE	U.S. Department of Energy
DTEM	dynamic transmission electron microscope
EBSD	Earth and Biological Sciences Directorate
EMSL	Environmental Molecular Sciences Laboratory
EPR	electron paramagnetic resonance
ERT	electrical resistivity tomography
ESA	Environmental Sciences Area
FICUS	Facilities Integrating Collaborations for User Science
FISH	fluorescence in situ hybridization
HIM	helium ion microscopy
HMM	Hidden Markov Model
IOPS	integrated operating system
JGI	Joint Genome Institute
LBNL	Lawrence Berkeley National Laboratory
MD	molecular dynamics
MS	mass spectrometry
NanoSIMS	nanoscale secondary ion mass spectrometry
NMR	nuclear magnetic resonance
NSF	National Science Foundation
NSLS-II	National Synchrotron Light Source II
ORNL	Oak Ridge National Laboratory
PI	principal investigator
PMAS	pressurized magic angle spinning
PNNL	Pacific Northwest National Laboratory

ROOTS	Rhizosphere Observations Optimizing Terrestrial Sequestration
SBR	Subsurface Biogeochemical Research
SC	Office of Science
SFA	Scientific Focus Area
SIMS	secondary ion mass spectrometry
SIP	stable isotope probes
SLAC	Stanford Linear Accelerator Center
SNS	Spallation Neutron Source
SOM	soil organic matter
SPIN	subambient pressure ionization with nanoelectrospray
TAMD	temperature accelerated molecular dynamics
TDDFT	time-dependent density functional theory
TRC	total recordable cases
UEC	User Executive Committee
XCT	X-ray tomography
XPS	X-ray photoelectron spectroscopy
XRD	X-ray powder diffraction

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1.0 Introduction

EMSL, the Environmental Molecular Sciences Laboratory, is a world-class U.S. Department of Energy (DOE) Office of Science (SC) User Facility located on the campus of Pacific Northwest National Laboratory (PNNL) in Richland, Washington. Stewarded by the DOE Office of Biological and Environmental Research (BER), EMSL's vision is to partner with diverse scientific communities to develop predictive understanding of complex biological and environmental systems to enable sustainable solutions to the nation's energy and environmental challenges. To accomplish this, EMSL strategically pursues its mission to accelerate scientific discovery and pioneer new capabilities to understand biological and environmental processes across temporal and spatial scales.

EMSL's strategy builds upon the recognition that next generation science often demands the integration of theory, experiment, and modeling by creative multidisciplinary teams to make progress. EMSL embraces an approach that lets science drive technology development and computational capabilities, provides access to multiple facilities, and supports open data sharing with the scientific community. Because of the rapid and accelerating pace of scientific and technological developments, this 5–year strategic plan will be updated regularly, allowing us to support the most impactful science by adapting to the rapidly changing research landscape.

We are excited to present this plan outlining EMSL's strategic approach. It is designed to align with DOE and BER research goals and to chart innovative directions for increasing collaboration across the broader complex of DOE user facilities to amplify the impact and productivity of user research. We are investing strategically in staff, instruments, and the facility to pursue breakthrough science and create new opportunities for our users and throughout the BER research community. We anticipate these approaches being of particular impact to our users:

- Increasing collaborations across the DOE-SC user facility complex, streamlining access to diverse capabilities;
- Developing robust, searchable data sharing between DOE facilities and the broader scientific community through MyEMSL; and
- Restructuring EMSL's capabilities into themed Integrated Research Platforms (IRPs) that facilitate the user proposal process and focus users' research efforts.

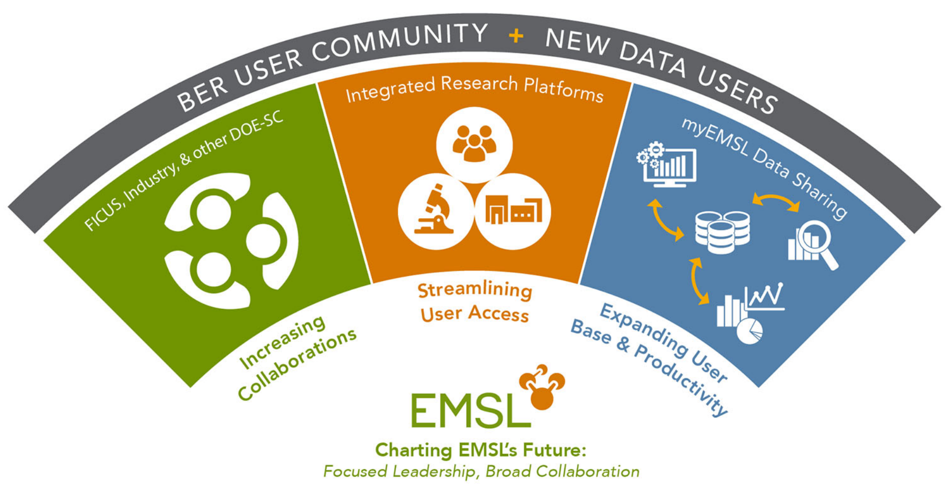

Figure 1. We are excited to grow our scientific leadership over the next five years by making strategic investments in synergistic partnerships and collaborations, improving access to EMSL capabilities, and establishing robust data sharing that will grow our user base and amplify our scientific impact across BER and the larger scientific community.

EMSL's 2018 Strategic Plan builds on our twenty years of service to the DOE-SC user community and charts new directions. Implementing this plan will sharpen EMSL's focus and impact, positioning us to deliver on our core ***strategic objectives***:

1. Address critical science and technology gaps to advance BER scientific goals.
2. Foster an engaged and productive user community through sustained excellence in outreach, data services, and operations and management.
3. Strengthen user resources by advancing EMSL's world-class expertise and state-of-the-art capabilities, and increase their utilization to enable scientific discoveries and breakthroughs.

EMSL's vision reflects deep commitment to BER's mission to support fundamental research that addresses critical challenges facing DOE and our nation. We are gaining an unprecedented view of how genomic information is translated into biological functions (BSSD 2015 Strategic Plan[1]) and how those functions drive environmental processes (CESD 2018 Strategic Plan[2]), due in part to the rapid pace of scientific discovery driven by powerful new technologies.[3] Expanding the Facilities Integrating Collaborations for User Science (FICUS) program, which encourages the scientific community to propose novel ways for user facilities to work together, will be a key component to the implementation of EMSL's vision. By combining the strengths of our users, staff, instrumentation, and facilities—and by collaborating with DOE's other scientific user facilities—EMSL's user community is poised to make significant scientific advances that meet BER mission goals.

In developing this strategic plan, we identified the broad scientific goals posed by government agency reports and strategy plans, and through consultation with advisory committees, leaders of the Joint Genome Institute (JGI) and the Bioenergy Research Centers and BER program managers, we identified the key technical challenges that impede progress. Capabilities and resources needed to fill critical gaps were then identified through BER and EMSL workshop reports,[4-6] in consultation with other scientists (e.g., EMSL users, visiting scientists) and through the literature. This resulting Strategic Plan will both address BER-aligned research objectives, provide effective mechanisms to achieve them, and maximize EMSL's overall scientific impact.

2.0 EMSL's User Science

EMSL's User Science focuses on BER mission and related priorities to understand and provide sustainable solutions to the world's growing need for energy and resources. Energy production and resource use can impact the environment, creating a need for more sustainable energy sources and more resilient ecosystems. Research programs supported by BER and other funding agencies with synergistic goals have a long history of measuring and predicting the biological and environmental impacts of energy production and its use, and of developing novel, biology-based solutions for creating sustainable fuels.[1]

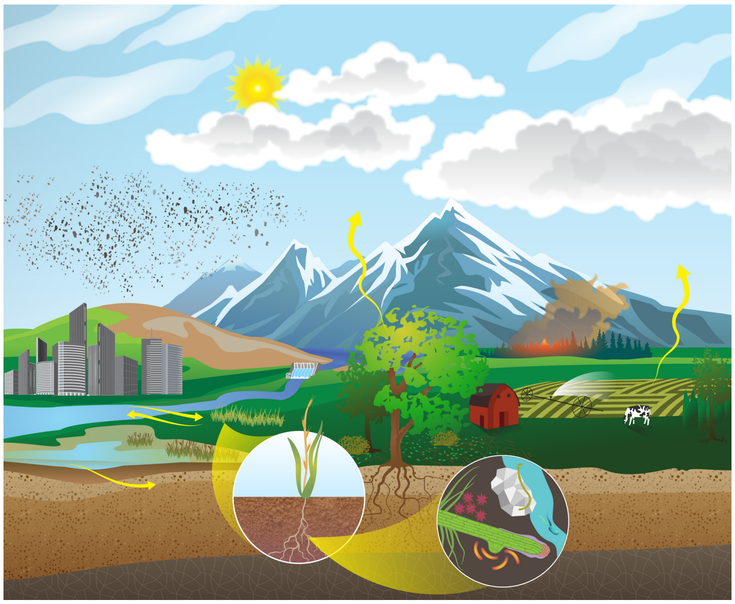

Figure 2. EMSL elucidates biological and environmental processes across scales to gain predictive understanding. Our critical science discoveries support BER's mission to provide sustainable solutions to the world's growing need for energy and resources.

The advanced capabilities at EMSL and other DOE-sponsored user facilities benefit and help to drive BER and other DOE research. In that spirit, EMSL will apply its molecular science strengths to advance the understanding of mechanisms and dynamics that underpin the structure and function of biological and environmental systems and phenomena of interest to BER and DOE (**Figure 2**).[7] Specifically, to support BER priorities, EMSL will focus resources to support BER priorities to (1) understand, predict, manipulate, and design biological processes that underpin innovations for bioenergy and bioproduct production; and (2) advance fundamental understanding of coupled biogeochemical processes in complex terrestrial and subsurface environments, and advance understanding of the dynamics of atmospheric aerosols through integrative theory, modeling, and experiment to enable systems-level environmental predictions.

EMSL's User Science consists of the **Biological Sciences Area** (BSA) and **Environmental Sciences Area** (ESA). The BSA and ESA roughly correspond to BER's two divisions, recognizing that there is extensive overlap between their scientific goals.[1-2,7] The BSA and ESA are described below, together with the specific BER research goals that corresponding user research will address over the next five years.

2.1 Biological Sciences Area

The BSA focuses on molecular "machines" and processes in and among microbes (archaea, bacteria, and algae), fungi, and plants. Research supported by this area will focus on improving mechanistic understanding of how genetic information is translated into processes across spatial and organizational scales by molecules, organisms, consortia, multispecies communities, and ecosystems. This will advance the accurate metabolic reconstructions and predictive cellular and process models needed to understand nutrient flux in the environment and will improve strategies for designing plants, microbes (including fungi), and integrated plant-microbe-soil systems for the production of biofuels and bio-based products. Collaboration with JGI and other DOE-SC user facilities via the FICUS program—as well as integration with BER investments in data science such as KBase and ESS-Dive—will further amplify the impact of user research in this area. The BSA is organized around three broad scientific topics: (1) biology of biofuel and bioproduct synthesis, (2) genome-enabled science for biodesign, and (3) biological control of material flux.

2.1.1 Biology of Biofuel and Bioproduct Synthesis

BER Goal: Provide a basic understanding of plant and microbial biology to underpin the production of biofuels and bioproducts from sustainable plant biomass resources.[1]

This requires identification and understanding of the enzymatic mechanisms and processes by which organisms generate and use energy-rich storage compounds, together with understanding of plant processes that affect their ability to produce biomass under diverse environmental conditions. Specifically, there is a need for the following:

- Identifying and modeling the central metabolic pathways whose intermediates provide building blocks for biosynthesis of biofuels and bioproducts;
- Characterizing cellular and molecular energy metabolism and storage processes, including their underlying molecular pathways, subcellular localization, and transport mechanisms;
- Enhancing models of the enzymatic systems that microbes use in biomass deconstruction based on a structural and mechanistic understanding of these systems; and
- Developing predictive models of plant growth, performance, and composition as a function of genotype and environment.

Understanding the structure of lignocellulose and the enzymes that can break it down will lead to new approaches for biomass deconstruction. Understanding of the structure and functions of the enzymes required for biomass biosynthesis/deconstruction will be facilitated by EMSL's IRPs. Collaboration with BER's four bioenergy research centers[8-11] will be particularly useful in advancing this research. Outreach efforts will encourage submission of research projects from these centers.

2.1.2 Genome-enabled Science for Biodesign

BER Goal: Develop the fundamental understanding of genome biology needed to design, modify, and optimize plants, microbes, and biomass for beneficial purposes.[1]

This requires understanding of how genetic information is translated into functional characteristics and traits. Work to identify the function of unknown genes is particularly needed, as are studies to understand gene and metabolic regulatory networks. Details include the assembly and regulation of intracellular compartments and the spatial-temporal regulation of metabolic processes. Specifically, there is a need for the following:

- Annotating genes of unknown function, expanding the "parts list" that can be used to engineer organisms

- Elucidating post-transcriptional and post-translational processes and modifications influencing and regulating metabolic pathways, energy storage, biomass accumulation, and abiotic stress tolerance;
- Defining/identifying the key (limiting) molecules, metabolites, and processes necessary to model and understand biological systems;
- Linking plant genomic information to phenotypic expression across scales, from molecule to plant-microbe-soil system
- Modeling, simulation, and visualization of metabolic pathways to support synthetic biology, coupled with data-driven validation;
- Understanding the dynamics of assembly and spatial organization of eukaryotic organelles and bacterial communities that impact the production and fate of biomolecules; and
- Integrating computational and structural biology studies to understand enzyme active site chemistry, protein-protein interactions, and molecular processes.

Synthetic biology research that combines computational and experimental methods to redesign enzymes and other proteins will improve functionality, production of commodity chemicals, and biofuels in plants, fungi, and microbes. We envision users pursuing genome editing and phenotyping projects that access JGI DNA synthesis capabilities in combination with EMSL molecular biology and microfluidic high-throughput multiomic and microscopy-based phenotyping. EMSL will actively seek partnerships with DOE-SC user facilities to provide imaging capabilities that complement EMSL's IRPs.

2.1.3 Biological Control of Material Flux

BER Goal: Gain predictive understanding of biological processes controlling the flux of materials (e.g., carbon, nutrients, and contaminants) in the environment and how these processes impact ecosystem function.[1]

This will require investigations of mechanisms and processes in natural systems such as how the structure and function of microbial communities are impacted by environmental variables. In addition, it will be necessary to understand how complex substrates are generated and/or degraded and how these processes are influenced by interactions between organisms including plants, fungi, and microbes, including knowledge of the molecular and transport processes occurring at cellular and subcellular interfaces. Specifically, there is a need to:

- Understand organic substrate transformation by cells, including spatial relationships between organisms and their substrates;
- Identify key components, reaction processes, and feedbacks that result in observed ecosystem variations and improve models of ecosystem function;
- Understand the regulation of nutrient (C, N, P, and S) flux through flux through plant-microbe-soil systems; and
- Model, simulate, and visualize multicellular systems (e.g., microbial consortia, microbiomes, plants, plant-microbe associations) to enable predictive understanding of carbon flux.

Elucidating the spatiotemporal structure and function of the plant-microbe-soil system and the mechanisms of intercellular communications (*e.g.,* quorum sensing) will enhance biomass crops, soil sustainability and ecosystem functions. The knowledge gained will facilitate engineering of microbial traits important to plant communities. This research will be facilitated by EMSL's large-scale imaging and multimodal measurement capabilities in EMSL's IRPs, as well as the capabilities for modeling carbon assimilation and utilization under development within EMSL's strategic science efforts (Section 4.2.1). We envision new partnerships with DOE light sources and neutron sources will provide highly resolved chemical measurements of microbe-plant-soil interactions in the rhizosphere and other hotspots of nutrient cycling in terrestrial and subsurface ecosystems.

2.2 Environmental Sciences Area

The ESA focuses on mechanistic and predictive understanding of fundamental processes in above- and below-ground terrestrial and subsurface ecosystems, the atmosphere, their interfaces, and their interactions from molecular to ecosystem scale. EMSL provides the experimental, data analytics, modeling, and simulation expertise to investigate the cycling, transformation, and transport of critical biogeochemical elements and contaminants, as well as the fundamental chemistry, physics, and molecular-scale dynamics of atmospheric aerosols. Coupled experimental and modeling approaches will accelerate understanding of the mechanisms and dynamics of processes and their interdependencies to inform models at larger scales and multi-decadal time scales.[2]

2.2.1 Mechanisms and Dynamics of Biogeochemical Reactions

BER Goal: Establish a mechanistic understanding of the molecular biogeochemical processes that govern nutrient and contaminant transformations and cycling in terrestrial and subsurface ecosystems.[12]

A focus on understanding discrete molecular mechanisms and their dynamics will provide data to understand how biogeochemical processes function, which can then be used to build integrated models at the larger scales as described above. Specifically, there is a need to:

- Understand the chemistry and molecular dynamics of mineral-organic matter interactions and how they influence microbial access to soil carbon;
- Understand mineral surface complexation/associations, redox reactions, nanoparticle and colloid formation, and their impact on the reactivity, fate, and transport of anthropogenic contaminants in terrestrial and subsurface ecosystems;
- Develop molecular-scale mechanistic understanding of the geochemical, biological, and hydrologic processes driving elemental (C, N, P, etc.) cycling dynamics and coupling in soils—especially rhizosphere root-microbe-fungi-soil interactions; and
- Identify molecular profiles and signatures indicative of specific ecosystem functions, responses to perturbations (e.g., nutrient limitation, hydrologic stress), and specific microbial metabolic pathways.

EMSL's strength in biogeochemical research on reactions that impact the subsurface fate and transport of contaminants has recently expanded to include investigation of natural organic matter in soil and groundwater. This is essential for mechanistic understanding of nutrient cycling in terrestrial ecosystems and developing quantitative models for predictive studies. This research is enabled by our mass spectrometry, in situ spatially resolved chemical imaging expertise, spectroscopic approaches, and molecular dynamics simulation expertise. Continued investment in these areas creates exciting opportunities to quantitatively understand the molecular chemistry of complex and multidimensional processes at diverse spatial and temporal scales.

To establish a mechanistic understanding of the molecular biogeochemical processes that govern nutrient and contaminant transformations, we will solicit proposals using our mass spectrometry, in situ chemical imaging expertise, and other spectroscopic approaches coupled with computational modeling and simulations. By employing multiple perspectives from biology to environmental disciplines, EMSL will bring together advances from research communities that infrequently interact, enabling transformational advances in understanding important rhizosphere processes.

2.2.2 Systems-Level Models of Biogeochemical Processes

BER Goal: Develop fundamental understanding of hydro-biogeochemical processes that drive nutrient and contaminant fate and transformation in surface and subsurface ecosystems, their interactions across scales, and response to perturbation.[12]

This will require integrating data from multiple disciplines (microbiology, geochemistry, hydrology, plant science) into a data analytics and modeling framework spanning multiple temporal and spatial scales. Specifically, there is a need to:

- Determine phenotypes or functional traits that impact ecosystem properties to improve models of ecosystem function;
- Understand the role of genetic and functional diversity in the resilience of plant and microbial communities and ecosystems to perturbation;
- Study the rhizosphere, emphasizing nutrients, metabolites, and regulatory compounds in the plant-microbe-soil-mineral-water-atmosphere system; and
- Investigate the role of hydrologic processes in creating biogeochemical gradients and microbial niches at pore- to core-scale in terrestrial and subsurface ecosystems.

Understanding the molecular mechanisms and dynamics of biogeochemical and microbial processes enables their representation in pore- to continuum-scale biogeochemical reactive transport models, which can be used to inform ecosystem scale models. This research relies on advanced capabilities to measure and quantify nutrient and contaminant fluxes and *in situ* tomographic imaging capabilities for studying intact root and nutrient allocation at the pore- to intermediate-scale, and a computational framework to support modeling across these scales. Research in this area represents a rapidly growing portion of the EMSL user portfolio, including ongoing FICUS projects with JGI focused on linking genomes to microbial processes and nutrient cycling in the environment. We are exploring expansion of our FICUS program to facilitate user access to the many SC lightsources (SSRL, APS, ALS, NSLSII) currently engaged in research in this area.

2.2.3 Formation and Characterization of Atmospheric Aerosols and Ice-Forming Nuclei

BER Goal: Improve the understanding of processes that determine the lifecycle and chemical, microphysical, and optical properties of atmospheric organic aerosols and ice nucleating particles.[2]

To understand the formation and growth of organic aerosols and how atmospheric processes and aging determine the chemical, physical, and cloud nucleating properties of organic aerosols and ice nucleating particles requires biological, chemical, morphological, and structural characterization of organic and ice nucleating particles. Specifically, there is a need to:

- Determine the physical and chemical attributes that make some nuclei better ice-forming nuclei than others;
- Understand the processes that result in the formation and growth of organic aerosols and aging processes that result in changes in their chemical, physical, and optical properties; and
- Investigate the role of primary biological particles as ice nuclei.

Understanding the fundamental chemistry, physics, and dynamic lifecycle of organic aerosols and ice-forming nuclei will improve their parameterization in large-scale earth system models (ESM), and also contribute to improved predictive understanding of the water cycle. Research into the chemical properties of organic aerosols requires mass spectrometry, spectroscopy, and chromatography characterization combined with computational simulations to calculate absorption spectra, the formation and reaction coordinates of small molecule clusters that lead to new particle formation, and thermodynamic analysis of these chemical reactions. Ice nucleation research will be enabled by EMSL's unique cryo-electron microscopy capabilities that allow visualization of this process and scanning electron microscopy to characterize the nature of the particles involved. ARM and ASR researchers have utilized EMSL previously for analysis of captured aerosol particles. Future FICUS efforts leverage ARM's upcoming unmanned aerial vehicle program to collect atmospheric aerosols and facilitate user access to EMSL capabilities for aerosol characterization.

2.3 User Engagement

2.3.1 Proposal Opportunities and Calls

EMSL provides access to its expertise, instruments, and facilities through various types of user proposals designed to ensure we are accelerating solutions for national energy and environmental challenges. Annually, calls for proposals identify topics of interest within each of EMSL's science areas. The topics announced in each open call— large-scale EMSL research and FICUS calls and the call for exploratory research (described below)—are developed in collaboration with BER program managers to focus user activities to accelerate results in emerging science areas of interest to EMSL, BER, and DOE.

The EMSL award cycles for open calls are scheduled approximately six months apart: (1) the large-scale EMSL research and FICUS calls provide at least two years of access, and both are focused on specific topics of interest, and (2) the call for exploratory research provides up to one year of access and is a targeted call, focused on increasing awareness and use by specific communities as determined by BER and EMSL management. Proposals to these open calls are externally peer reviewed and provide instrument time as well as EMSL-funded technical support.

Outside of the open calls, the additional opportunities for accessing EMSL resources are described on the EMSL web site.

2.3.2 Expanding the FICUS Program

The FICUS Program encourages the scientific community to propose novel ways for user facilities to work together. FICUS began as a joint call for proposals in 2013 between EMSL and the Joint Genome Institute, or JGI. It focused on DOE missions in bioenergy and the environment and combined EMSL's unique imaging, omics, and computational resources with cutting-edge genomics at JGI. To build on the success of the EMSL-JGI FICUS Program, EMSL plans to establish collaborations with other DOE user facilities within FICUS. The potential of these collaborations has been recognized by BER's Advisory Committee, and there are ongoing efforts to identify areas of synergy. As a preliminary step to realizing this potential, EMSL scientists have attended joint workshops at other user facilities, and several scientists form other DOE user facilities (e.g., NSLS-II, SLAC, SNS) participated in the 2018 EMSL Integration Meeting. A pilot FICUS program is planned with NSLS-II in the near future, and a similar effort with SLAC is also being planned.

3.0 Focus on the User Community

At EMSL, an engaged and productive research community has safe access to the resources needed to address critical science challenges relevant to BER.

To foster an *engaged* user community, EMSL promotes awareness with effective communications, by inviting user participation at conference sessions and workshops, and by building lasting partnerships through the FICUS Program and EMSL-initiated research. EMSL maximizes user *productivity* by seamlessly providing access to data collected from capabilities, providing open-source tools for analysis and interpretation, and advancing high-impact publications. EMSL creates a *safe* user research environment by reviewing planned experiments, assigning task-specific training, and assuring onsite guidance using PNNL's management and operations infrastructure (**Figure 3**). The User Executive Committee (UEC) is charged with providing objective, timely advice and recommendations to the EMSL Director and management team related to matters affecting the EMSL users and evaluating our effectiveness in serving the user community.

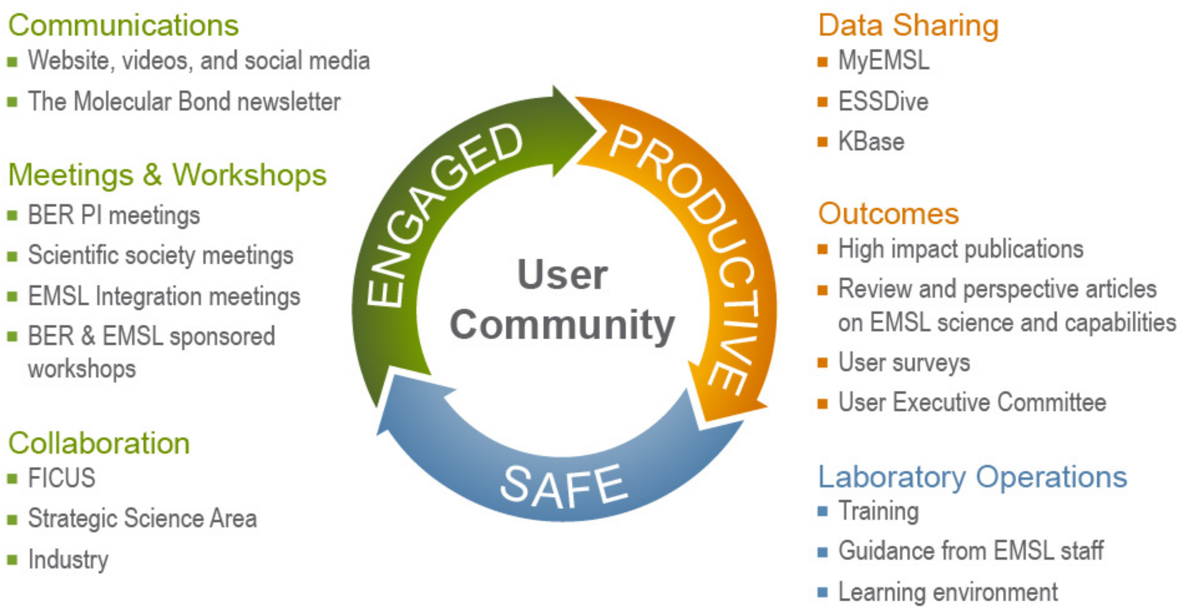

Figure 3. EMSL's strategy to foster an engaged, productive, and safe User Community.

3.1 Fostering an engaged user community

EMSL builds an engaged and enduring user community around important science questions relevant to BER missions by direct interaction with current and potential users, development of key partnerships, and by employing far-reaching communication methods.

EMSL staff present EMSL science and capabilities at the BER PI meetings and scientific society meetings. Promotion of EMSL capabilities and expertise at BER PI meetings maximizes EMSL's exposure to BER-funded PIs, early career staff, and graduate students. Staff are encouraged to propose and chair sessions, organize townhalls, or participate in panel discussions at national meetings, particularly those that are BER-relevant (e.g., American Geophysical Union [AGU], International Society for Microbial Ecology [ISME], American Chemical Society, Biophysical Society, Society for Industrial Microbiology and Biotechnology [SIMB], American Society for Plant Biology [ASPB], etc.).

The EMSL Integration Meeting is another platform that EMSL uses to highlight user science, invite early career and prominent researchers in the community as plenary speakers, and recruit new users to EMSL. These activities provide a venue for EMSL users to communicate the scientific impact of their research and the importance of EMSL as a national resource for state-of-the art capabilities and expertise.

EMSL-sponsored workshops are another opportunity to engage the research community. EMSL invites established and early career scientists to these workshops to assure alignment of new capabilities with BER science mission and research directions. EMSL supports fellowships for visiting professors and post-doctoral researchers to develop key collaborative partnerships. EMSL is also developing one- to two-week summer school programs to train the user community on the fundamental biological and environmental theory and practice of experimentation in selected topical areas. For example, one planned summer program will focus on the use of stable isotopes to understand the fate and transport of organic compounds. In addition to building collaborations, these workshops and summer schools attract potential users to EMSL by showcasing the areas of science, staff expertise, and capabilities housed within our IRPs.

The meetings, workshops, and summer programs are all mechanisms that EMSL is using to actively pursue collaborations with the DOE Bioenergy Research Centers (BRCs), the Next-Generation Ecosystem Experiments (NGEEs), and the National Laboratories Scientific Focus Area (SFA) projects to ensure that these important programs are aware of EMSL's capabilities to advance their science objectives. Past EMSL partnerships with industry have led to R&D 100 awards and patents and provide an opportunity to partner on SBIR/STTR funding. EMSL also seeks to increase the number of science partnerships with industry and expand the opportunities to translate the basic science knowledge to meet industrial needs by extending awareness of EMSL's staff expertise and state-of-the-art instrumentation to new industrial users.

EMSL employs effective communication mechanisms to *raise awareness* of EMSL within the scientific community, at BER and SC, and with key stakeholders. The EMSL external website is a primary communication mechanism for news and user proposal announcements with links to appropriate webpages for specific content. *The Molecular Bond* newsletter, distributed quarterly to subscribers, features scientific perspectives from EMSL scientists, staff, and users, as well as emerging areas relevant to BER. Additional communication approaches include posts on Twitter and Facebook about EMSL staff and user activities.

EMSL communicates the results and scientific impact of user projects through science highlights (typically two per month) that are sent to BER and posted on EMSL's web site. Peer-reviewed articles are selected for highlights based on scientific impact, relevance to BER and SC programs, and extent of EMSL usage. The highlights are written for a general audience suitable for the SC website, key stakeholders, and EMSL visitors. EMSL actively seeks feedback from the user community and BER to continuously improve its strategy and to assess the effectiveness of these communication mechanisms.

3.2 Maximizing the productivity of our user community

EMSL strives to ensure that users have the data, tools, and expert support necessary to be productive. Access to data combined with robust tools for analysis and interpretation of those data are central to establishing a productive EMSL user community. In the near-term, the greatest gains in user productivity will result from harnessing the power of open-access data streams available from EMSL and partner facilities. EMSL's data management and data portal systems facilitate near-real-time access to user data and open sharing of public data, combined with open-source analytical tools required to translate data into knowledge.

Our high-performance-computing-based advanced data analytics and visualization software facilitates integration of large amounts of multiomics data to effectively translate molecular measurements to biological understanding, for example allowing users to identify relationships between the experimental treatments and the measured values (e.g., omics features) in their samples.

EMSL's data repository, MyEMSL, ensures availability and usability of the data generated by EMSL staff, users, and the general scientific community. MyEMSL semi-automatically captures and stores user project data directly from an analytical instrument to a central repository. Currently, basic metadata associated with a user proposal and each instrument used are captured. EMSL plans to upgrade the MyEMSL system to capture all experiment metadata needed to comply with community-established standards and provide interoperability with other BER data facilities, including JGI, KBase, and ESSDrive. Bringing EMSL's metadata into compliance will allow the data to be seamlessly uploaded to community repositories and accessed by open-source software tools. EMSL also makes user data and metadata generally available through the EMSL User Portal. Users will be able to find and download their data sets as well as those from similar past EMSL projects. The portal will also provide access to standard operating protocols that specify how data were collected, as well as associated publications and presentations. The completion of EMSL's data repository during FY19 will thus enable public release of data and collaboration and dissemination of archived data. EMSL will also work vigorously to establish data-sharing and collaboration capabilities with FICUS partner user facilities. EMSL has plans to further partner with KBase to establish data standards and to expose the EMSL analytical tools within the KBase environment, and with ESS-DIVE to identify ways to coordinate data sharing and archiving. Measures of progress include the dissemination of information via our data portal as well as user feedback gained from user surveys.

3.3 Ensuring a safe operational environment

Ensuring the safety and welfare of EMSL users continues to be the highest operational priority.[13] To ensure a safe operational environment, EMSL leverages PNNL's worker safety and health and environmental sustainability programs to ensure that EMSL users fully understand their environmental, safety, and health responsibilities, which often differ and are more stringent from those at their home institution. PNNL's laboratory management program is currently under revision to provide increased oversight by focusing on the research activities of users. The new system, Lab Assist, replaces IOPS (Integrated Operations System) and will roll out in fiscal year 2019 and will continue to ensure that any hazards associated with the work activities are identified, mitigated, and communicated promptly and effectively. Training to incoming users will be based on both the lab space they will access and the specific research activities they will conduct. EMSL participates in PNNL's safety programs by having staff members become thoroughly familiar with laboratory hazards and research activities, and then interactively teaching safety and security expectations to users during the performance of lab activities. EMSL creates an active learning environment where users' concerns and questions are welcomed and respected.

4.0 Strengthening User Resources

As a DOE Office of Science User Facility, EMSL provides scientists with the capabilities necessary to conduct high-impact science in pursuit of BER's challenging science mission. The scientific community depends on EMSL for focused scientific expertise and premier instruments capable of measuring processes that span a broad range of spatial and temporal scales, along with EMSL's data analytics, modeling/simulation codes, and computer hardware that support the iteration between experimentation and simulation and enable the development of predictive models of biological and environmental processes.

4.1 Integrated Research Platforms

EMSL's IRPs encompass the sum of expert staff, state-of-the-art equipment, and mission-ready facilities, developed and deployed under these premises:

- *Science drives the capabilities* – Strategic goals and scientific needs drive our investment decisions for capability development.
- *The scientific community validates the needs* – We partner closely with the scientific community to develop and decide upon new capability needs and concepts.
- *The capabilities must facilitate leading-edge science* – Our capabilities are selected to provide a unique, integrated, and sought-after set of tools to advance science beyond what is currently possible.
- *Leverage capabilities at other user facilities* – Our capability investments are made to be synergistic with capabilities at our partner user facilities in order to bring the most value to the user community.
- *Lifecycle management* – We manage instruments from conception and design, through maximum utilization and enhancement, to cessation and disposal, with expert staff trained to operate and maintain state-of-the-art equipment.

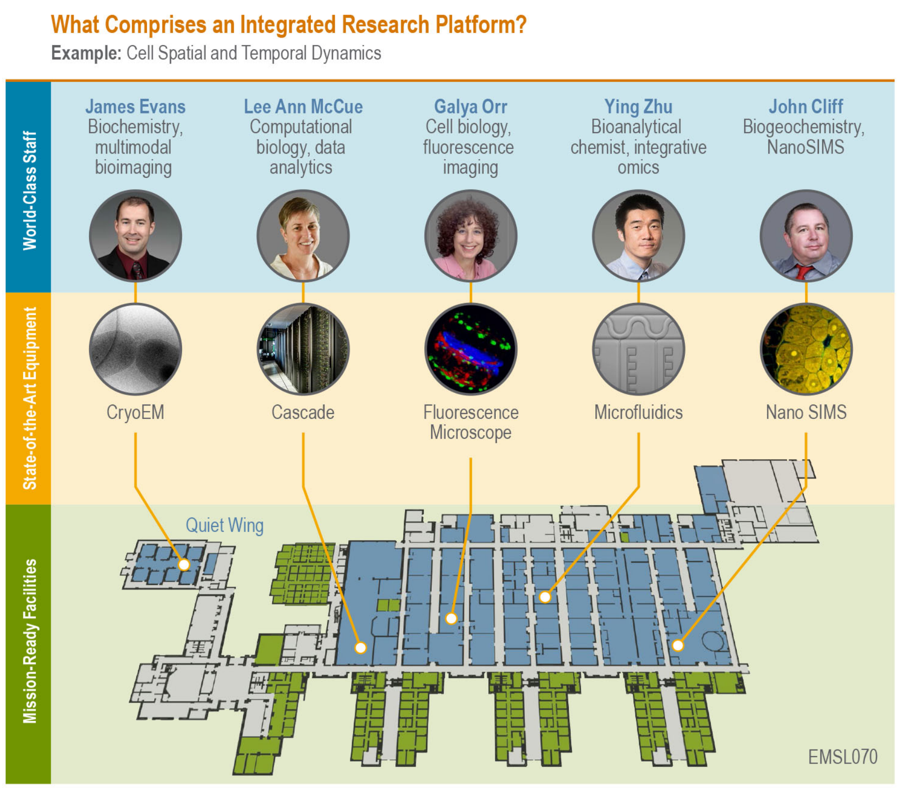

Figure 4. EMSL's integrated research platforms combine scientific expertise, premier instrumentation, and specialized laboratory space. For example, the Cell Spatial and Temporal Dynamics platform permits exploration of complex biological systems at molecular and single-cell levels by combining instrumentation and staff expertise in multimodal imaging, data analytics, fluorescence imaging, microfluidics, and nanoSIMS.

EMSL's IRPs provide the framework to address and solve key research questions through the integration of experimental, analytic, and modeling approaches. Each of our six platforms combines scientific expertise, premier instrumentation, and specialized laboratory space specifically designed to advance the science of the EMSL user community. EMSL's IRPs include the following:

- **Proteomics, Metabolomics, and Transcriptomic**s**:** provides molecular-level information governing biological and environmental processes in plants, fungi, and microbes that enable systems approaches to understand complex and interdependent processes.
- **Bioimaging and Structural Analysis:** provides structural and biochemical information about small molecules, proteins, and protein complexes, enabling dynamic observations at nanoscale spatial and temporal resolutions.
- **Cell Spatial and Temporal Dynamics:** provides molecular-scale understanding of the cell microenvironment and the functional consequence of expression patterns on the metabolic interplay between organisms in their native environment.
- **Isotope and Chemical Analysis:** elucidates dynamic processes through the use of stable isotope markers to track the transformation of labeled biomolecules in biological and environmental systems.
- **Plant, Soil and Subsurface Transport:** reveals the dynamic molecular- to meso-scale processes that occur in and among plants, microbes, soils/subsurface sediments and water, and enables phenotyping of holistic plant systems.
- **Theory and Simulation, Data Analytics, and Visualization:** facilitates multiscale modeling, simulation, and data integration, including advanced data analytics and visualization.

These integrated research platforms are designed to be ***interrelated and complementary*** to enable effective execution of comprehensive experimental and computational approaches in one building. Our current platforms and future directions are described below.

4.1.1 Proteomics, Metabolomics, and Transcriptomics (Multiomics)

EMSL has achieved decades-long expertise and leadership in multiomics by developing unique and integrated capabilities that combine advanced mass spectrometers, nuclear magnetic resonance (NMR) spectrometers, and next-generation sequencers that have identified critical metabolic processes for biofuel production and nutrient cycling. In particular, major technological advances in EMSL have greatly accelerated scientific discovery by speeding the rate, dynamic range, and resolution of the analysis of proteins and metabolites. Mass spectrometry imaging (MSI) capabilities have combined molecular characterization with spatial context to decipher biological complexity and heterogeneity.

The need for increased throughput and integration of genomics, transcriptomics, proteomics, and metabolomics has been recognized as critical to address the challenges in biological complexity and heterogeneity (BERAC Grand Challenges[12] 2.1–2.5) that will lead to more efficient biofuel production and robust prediction of nutrient cycling in the environment. We will continue to push the frontiers of MS- and NMR-based measurements by upgrading our instruments to state-of-the-art technology. This will enable the research community to probe genes/proteins/metabolites of unknown function and to quantify the functional components of complex systems.

We combine advanced mass spectrometers, NMR spectrometers, and next-generation sequencers to identify and quantify diverse molecular species in complex systems, including intact proteins in microbes and plants, and a wide variety of analytics from complex environmental mixtures. Major technological advances at EMSL have greatly accelerated scientific discovery by speeding the rate, sensitivity, and accuracy of the analysis of proteins and metabolites. For example, EMSL's 21T FTICR-MS provides unmatched ability to identify and quantify diverse molecular species in complex systems. We have also demonstrated that a combined approach using NMR spectroscopy and MS (liquid chromatography-MS, gas chromatography-MS, or ion mobility spectrometry-MS) yields greater metabolome coverage and more accurate metabolite identifications than any one technique alone [14], thereby improving our ability to identify the mechanisms of microbial communication and interaction. Mass spectrometry imaging (MSI) capabilities facilitate spatially-resolved metabolomics studies by combining qualitative and quantitative molecular information with spatial information. We use our high-performance-computing-based advanced data analytics and visualization software to *integrate* large amounts of multiomics data to more effectively translate these molecular measurements to biological understanding by mapping these data to prior knowledge (e.g., metabolic pathways).

We will continue to build our NMR and MS expertise in structurally and spatially resolved omics. We will continue to advance our standards-free approaches for metabolomics and proteomics data analysis and our microfluidic platforms for ultrasensitive analysis of biomolecules at or near single-cell resolution. Our multiomics approach will increase the coverage of microbial and plant biomolecules and will facilitate characterization of the mechanisms that inform higher scale processes. This will be facilitated by exploiting our high-performance-computing expertise and by developing multiscale modeling approaches and new software tools for integrating and visualizing multiomics data.

4.1.2 Bioimaging and Structural Analysis

EMSL is pushing the frontiers in bioimaging, structural analysis, dynamic imaging, and in situ measurements with our integrated microscopy, APT, protein expression, MS, and NMR capabilities. These imaging and structural data provide crucial insights into the assembly, structure, and function of protein complexes that are essential for biodesign and bioengineering efforts for advanced biofuels and bioproducts. In particular, EMSL has pioneered the application of high-spatial-resolution methods such as APT for biological samples and is developing novel multifunctional capabilities under the BER Bioimaging Technology program that will reveal detailed structures and mechanisms of macromolecular complexes (i.e., molecular machines) and protein interactions important to biofuel production or biogeochemical cycling. Visual proteomics is the next frontier that will enable EMSL users to characterize and quantitate macromolecular complexes in their native assembly to understand the protein interactions that underlie cellular functions.

The integration of high-resolution spatiotemporal imaging and structural data will address several measurement challenges identified in BER's 2017 Technologies Workshop,[3] including locating all proteins and complexes of known structure within three-dimensional tomographic reconstructions of whole cells. These capabilities also address the need to understand the complexity of plant and microbial metabolism and interfaces across scales (BERAC Grand Challenge[12] 2.1). We employ diverse technologies, including cryo-EM, native MS, EPR, NMR, NanoSIMS, scanning probe microscopy, atom probe microscopy, and expression/purification platforms to enable protein functional studies, elucidate protein structure, and examine proteins and protein complexes in their native states.

EMSL will continue to advance its bioimaging and structural analysis capabilities to offer a *visual proteomics* capability to visualize the spatiotemporal relationships between proteins and protein complexes as well as the *dynamics* of protein activity (DTEM) within cells. EMSL's recognized strengths in proteomics, imaging, and high-performance computing, combined with the structural biology capabilities at the synchrotron and neutron facilities (e.g., SSRL, APS, SNS), will provide unique and innovative capabilities to the research community. Combining this biomolecule structural information with computation and bioinformatics provides the ability to infer function, design new functions, and characterize proteins of unknown function[1] to provide the links between genotype and cellular phenotype.

4.1.3 Cell Spatial and Temporal Dynamics

EMSL's strengths in high-resolution live-cell microscopy coupled with expertise developing novel methods to tag single biomolecules (e.g., enzyme, protein, transcript) provides real-time dynamic imaging and quantitation of metabolic pathways and the transport of materials. These approaches are crucial to understand how the cell microenvironment modulates gene and protein expression patterns, the functional consequence of these patterns, and the impact on metabolic interplay between organisms in their native environment. For example, we combine fluorescent in situ hybridization and super-resolution fluorescence microscopy to accurately detect and quantify transcripts in single cells and provide dynamic imaging of extracellular interactions within a community. We utilize our HIM and SEM capabilities to image microbial communities and plant-microbe associations in the rhizosphere and to employ nanofluidic techniques to develop quantitative analysis of biomolecules in small numbers of individual cells. We have led the world in the development of "liquid" SIMS that probes the spatial location and chemical identity of biomolecules at native biological surfaces and interfaces.

The ability to quantitate metabolic interdependencies, exchanges, and feedbacks at the single-cell level will address several measurement challenges identified in BER's 2017 "Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment" workshop report.[3] These include detection and visualization of cellular dynamic processes—such as metabolic cycles, signaling and trafficking in plants, and interactions among microbial and fungal communities that are critical to understanding the biological complexity of plant and microbe metabolism and interfaces (BERAC Grand Challenge[12] in Biological Systems Science 2.1)—and provides the basis for biodesign and bioengineering efforts.

We will continue to advance our expertise in multimodal, high-resolution, live-cell imaging to probe the structure and function of cells and tissues. Our ability to quantify transcripts, proteins, and metabolites within *intact cells in their native communities*, and within small numbers of isolated cells will be advanced by leveraging our expertise in super-resolution fluorescence microscopy, microfluidics, and single-cell analysis. Specifically, we will enhance our technologies for quantitative single molecule detection and combine them with multiplexed approaches for simultaneous analysis of multiple biomolecules in single cells in their native environments and will develop new computational approaches to handle the complex, noisy data sets that arise from single-cell analysis techniques. We will pursue opportunities to coordinate efforts with the synchrotron and neutron facilities, for example the soft X-ray tomography and FTIR spectromicroscopy capabilities available at ALS.

4.1.4 Isotopic and Chemical Analysis

EMSL provides a unique multimodal approach that combines spectroscopic chemical analysis and imaging with mass spectrometry to characterize the exchange of labeled molecules between organisms and between organisms and the environment. EMSL also has recognized expertise characterizing the chemical, physical, and optical properties of aerosols, which is critical for understanding their growth, evolution, and subsequent effect on the Earth's energy budget and climate. These capabilities afford our users the ability to resolve fundamental mechanisms underlying metabolic pathways, nutrient cycling, and land-atmosphere interactions. These mechanisms inform the spatial and temporal predictive models of biological and biogeochemical processes necessary to predict, design, and control molecular processes.

Deciphering the complex interactions between biotic and abiotic components that control the flux of materials (e.g., carbon, nutrients, contaminants, and aerosols) in the environment and impact ecosystem function addresses four BERAC Grand Challenges[12] in Microbial to Earth Systems Pathways (4.1–4.4). Parameterization of atmospheric aerosols in Earth system models was identified as BERAC Grand Challenge[12] in Earth and Environmental System Science 3.3. Enabling EMSL user research in this broad area will require combining the ongoing expansion of our stable isotope probing capability with our surface science expertise and capabilities to understand the relationship between nutrient flux and the biochemistry of complex surfaces and interfaces in the environment.

We identify and spatially resolve biomolecules and mineral surfaces with multiple techniques including spectroscopy, tomography, mass spectrometry, and multimodal imaging. New developments in this platform will establish EMSL leadership in research focused on the flux of materials in a complex chemical environment by combining existing stable isotope analysis techniques with chemical imaging to achieve a robust spatiotemporal characterization of nutrient cycling through biological systems and the environment. We will leverage partnerships with projects supported by BER's Mesoscale Bioimaging Technology program to expand the capabilities available to the research community.

4.1.5 Plant, Soil, and Subsurface Transport

EMSL has an established history investigating subsurface processes, including developing and utilizing intermediate-scale flow facilities and microfluidic pore-scale micromodels for studies of subsurface flow and transport under controlled conditions. Tightly integrated with reactive transport codes developed at PNNL and elsewhere, this capability has successfully deployed against complex legacy contamination issues at DOE sites such as Hanford. Recently these capabilities and expertise have been extended to investigation of material flow both above-ground (e.g., gas exchange between plants and atmosphere) and below-ground (e.g., water and nutrients between soil, microorganisms, and plant tissues in the rhizosphere).

Determining the flux and transformation of materials and energy through the environment and how these change under environmental stress is an emergent area of EMSL's focus. This emerging area is aligned with the CESD strategic goal to understand and predict the cycling and transport of nutrients and contaminants in soils and subsurface. Research in this IRP will address BERAC's Grand Challenges[12] to understand the link between genotype and phenotype in organisms and communities of organisms (Grand Challenge 2.4), to characterize biogeochemical exchanges driven by plant-microbe interactions under changing environmental conditions (Grand Challenge 4.1) and to develop the infrastructure to study organisms in their natural habitats (Grand Challenge 7.6). Addressing these challenges will enable researchers to undertake multiperspective, holistic investigations of *intact* portions of ecosystem components across spatiotemporal regimes.

Nascent capabilities include phytotrons for plant growth under controlled conditions that allow simultaneous measurement of photosynthetic activity; rhizoboxes for temporally resolved measurements of exudates, porewater, etc.; and platforms for nondestructive, nonevasive measurement of root-system architecture. Existing surface sensitive spectroscopy and diffraction methods provide important information about interfacial processes and the structure of minerals from soil and the subsurface. The close integration of this platform with EMSL's other Integrated Research Platforms establishes a one-of-a-kind resource for sophisticated plant *molecular phenotyping* and nutrient cycling. To extend beyond existing "plant in a pot" systems that fail to capture the complexity and heterogeneity of native ecosystems, EMSL is developing conceptual plans for an Ecosystem Simulator (EcoSim) Facility that will enable investigation of several cubic yards of intact native ecosystem under tightly controlled and heavily instrumented above and below-ground conditions.

4.1.6 Theory and Simulation, Data Analytics, and Visualization

EMSL has extensive expertise developing and using in silico approaches to apply to challenging science questions. Notably, open-source computational chemistry code (*NWChem*) developed in EMSL has been adopted by thousands of users for ab initio quantum chemistry and electronic-structure calculations. Working in concert with experimentalists, computational scientists have developed multiscale modelling platforms and data visualization approaches (e.g., *Trelliscope*) for large and disparate data sets. These platforms and approaches have provided unparalleled insight into the physiochemical effects on environmental nutrient cycling, metabolic pathway interactions, and microbial community dynamics.

Critical to developing predictive understanding of biological and environmental systems is full integration of experimental and computational methods.[2] A cohesive approach will accelerate achieving mechanistic understanding of molecular soil-microbe-plant-atmosphere processes and a more thorough understanding of biological processes controlling the flux of materials (e.g., carbon, nutrients, and contaminants) in the environment. This is consistent with the BERAC Grand Challenges[12] to integrate large omics datasets with biochemical and biophysical measurements (Grand Challenge 2.3), develop suitable algorithms and programming models to effectively model complex coupled systems (Grand Challenge 6.3), and develop integrative and interpretive computational approaches that can handle large, disparate data types from multiple and heterogeneous sources (Grand Challenge 8.5). To further these objectives, EMSL will continue to develop methods to analyze and visualize data in spatial and temporal context in order to enhance pattern recognition and statistical validation and to contribute to scale-aware models of complex systems.

The large, complex data generated by EMSL's analytical instruments will continue to drive our development of approaches to *analyze and visualize* data and temporal sequences of data. These approaches will be complemented by expanding our predictive modeling capability to model across scales from *molecular structures and activity* to *cellular and community-scale processes* to understand microbial metabolism and nutrient cycling in the environment. We will pursue opportunities to engage with ASCR-supported programs including the SciDAC Institutes and IDEAS.

4.1.7 Linkages to EMSL's User Science Program

EMSL's IRPs strongly align with our science objectives (**Table 1**). New capability development will continue to make state-of-the-art instrumentation, expertise, and specialized laboratory space available for BER-goal-aligned user science.

Table 1. Correlation of integrated research platforms to research components of EMSL's User Science Program.

Science Objectives	Proteomics, Metabolomics, Transcriptomics	Bioimaging and Structural Analysis	Cell Spatial and Temporal Dynamics	Isotopic and Chemical Analysis	Plant, Aerosol, and Soil System	Theory and Simulation, Data Analytics, and Visualization
Biological Sciences Area						
Biology of biofuel and bioproduct synthesis	●, ○	●, ○	●	●		○
Genome-enabled science for biodesign	●, ○	●, ○	●		●, ○	
Biological control of material flux	●	○	○	●, ○	●, ○	
Environmental Sciences Area						
Systems-level understanding of biogeochemical processes	●		○	●,○	●, ○	●, ○
Molecular mechanisms of biogeochemical processes	●, ○	●	●, ○	○		●, ○
Formation and characterization of atmospheric aerosols and ice forming nuclei				●	○	●
● – uses existing capabilities; ○ – anticipates new or extended capabilities						

4.2 Growing EMSL Expertise and Capabilities

EMSL grows scientific expertise and develops new capabilities to fill critical scientific and technology gaps that inhibit the user community from achieving BER research goals and related scientific advances. These developments directly benefit the user community in two ways: (1) new technology or capabilities are deployed to support users' projects to support future user projects, and (2) new staff expertise advances users' projects. The primary metrics for success are significant scientific discoveries, utilization of new capabilities and methods, and high-impact publications.

4.2.1 EMSL Strategic Science Directions

During the next triennial period, EMSL will expand its scientific leadership, demonstrate our IRPs, and create new opportunities for user science in the BSA and ESA through focused investment in EMSL-initiated research. This research will center on ***understanding carbon***

transformations in plant-microbe-soil systems through the lens of molecular interactions. The overarching science goals for this research are three-fold: (1) to elucidate how environmental conditions and perturbations influence carbon uptake, transformation, and utilization; (2) to advance biological and environmental systems-scale science research from reliance on observations and correlative findings to mechanistic, dynamic, and predictive understanding of how biological units interact with their environment to produce system-level responses; and (3) to demonstrate the power of multi-modal approaches to the multi-dimensional complexity of nutrient flux, exchange, and transformation within the rhizosphere domain.

This research will leverage EMSL's science and technology strengths, address key science challenges that bridge the Biological Systems Science Division (BSSD) and Climate and Environmental Sciences Division (CESD) strategic goals, and fill critical technology gaps that impede progress toward achieving predictive understanding of complex biological, earth, and environmental systems. This research will demonstrate the power of using multiple capabilities to solve complex science problems and will provide new capabilities to users. As newly developed capabilities become available, planned "first-science" experiments will demonstrate their scientific impact to the user community. Making these new capabilities known to the broader research community will be accomplished by the many communications mechanisms detailed in Section 3.1, with the assistance of the UEC and other advisory committees. Success will be judged by the number of high-impact papers generated, the new capabilities and methodologies developed within EMSL, and subsequent user demand.

4.3 Next Steps

We will continue to advance and integrate our capabilities to provide both scientific and technical leadership to the scientific community. Evolution of our capabilities to meet important science challenges will continue to be based on information from BER and EMSL workshops, scientific advisory meetings, and other discussions and interactions with the science community. EMSL maintains an evolving recapitalization plan to refresh the instrumentation necessary to implement our strategic plan. The critical actions required implement EMSL's Strategic Plan over the next three to five years are described in Section 5.0.

5.0 Critical Actions

Section 1.0 described our overarching goals and the following three strategic objectives:

- Address critical science and technology gaps to advance BER scientific missions (Strategic Objective 1, Section 2.0).
- Foster an engaged and productive user community through sustained excellence in outreach, data services, and operations and management (Strategic Objective 2, Section 3.0).
- Strengthen user resources by advancing EMSL's world-class expertise and state-of-the-art capabilities and increase their utilization for breakthrough science (Strategic Objective 3, Section 4.0).

The following sections describe EMSL's plans for implementing critical actions that will be required to sustain and focus EMSL's efforts and resources over the next five years to ensure that these objectives are attained. In addition, the metrics to track progress are also defined.

5.1 Advance EMSL's Scientific Impact and Leadership

Demonstrating scientific leadership is essential to EMSL fulfilling its role as a premier user facility for the BER research program. That requires conducting high-impact science by assisting users and maintaining the recognition and engagement of the scientific community. To lead the scientific community in discovering molecular pathways that influence biological and environmental systems, we will (1) focus annual user calls for proposals on areas that fill important knowledge gaps in the scientific objectives described in Section 2.0, aligned with BER goals and priorities; (2) ensure a diverse and highly productive portfolio of outstanding user projects in the BSA and ESA, and (3) develop our strategic, EMSL-initiated research on molecular interactions in plant-microbe-soil systems (Section 4.2.1).

Because visible and recognized scientific leadership is critical to EMSL's success, the EMSL leadership team is committed to attracting, developing, and retaining a diverse, engaged, and productive workforce. EMSL's success ultimately relies on this scientific strategy, the leadership of EMSL's scientists and staff, and on EMSL management's ability to recruit, foster, and grow staff to the highest levels of scientific achievement. To do this, EMSL management plans a variety of approaches, including (1) targeted hiring, (2) mentoring early career staff, and (3) professional staff development through enrollment in PNNL University. Hiring priorities will be updated quarterly, and advertisements for open positions will be posted in social media, relevant journals, and professional societies.

Measures of our progress toward advancing our user program include the response to our annual user calls; the number of user publications in premier journals (*Science*, *Nature* and *Nature series*, *PNAS*); the number of citations soon after publication; and the number of BRC, SFA, and NGEE investigators and Early-Career-program-funded scientists attracted as users. Measures of progress toward advancing EMSL scientific leadership will be increased success in targeting new hires, publishing and being cited in premier journals, receiving DOE Early Career Awards, participating in external workshops to define future scientific directions, having fellows named in scientific societies, receiving national and international awards, and receiving promotions to Laboratory Fellow (PNNL's highest scientific rank).

5.2 Foster an Engaged, Productive and Safe User Community

A vibrant user community is critical to EMSL's success. Consequently, we have a proactive strategy to target established scientists and early career researchers and to establish sustained relationships with existing EMSL users, as described in Section 3.0. Proven mechanisms for attracting users are communication of EMSL's scientific impact and leadership, highlighting the unique capabilities and expertise that EMSL provides, and providing streamlined processes and opportunities to access EMSL. To accomplish these plans, EMSL will:

- Expand outreach strategies to attract new users through presentations at national meetings and publication of science highlights in electronic newsletters and social media.
- Encourage current users and scientists to acknowledge and promote EMSL through presentations at scientific meetings and conferences, journal publications, and discussions with colleagues.
- Conduct annual user meetings (i.e., the EMSL Integration Meeting) focused on science areas that increase awareness and build partnerships with new and existing users.
- Evolve EMSL's external website to support and expand development of an engaged and diverse user community.
- Benchmark performance against other user facilities and within the user community to identify best practices in order to continuously improve performance.

Metrics of success will be an increase in the number of new investigators submitting proposals, the number and quality of user publications, and the productivity of users conducting BER-funded and BER-aligned research.

Using innovative data tools that enable scientists from multiple and disparate locations to work together productively will accelerate science delivery. EMSL's data management and data portal systems will facilitate near-real-time access to user data, provide open access to public data, and seamless access to other BER user facility data archives. EMSL will also provide the analytical tools required to translate data into knowledge. To achieve this vision, EMSL will complete the MyEMSL repository and integration of its capabilities within the EMSL User Portal. Doing so will fully enable public release of data and collaboration and dissemination of archived data. EMSL will work vigorously to establish data-sharing and collaboration capabilities with partner user facilities.

The safety and welfare of our staff and users continue to be our highest operational priorities. PNNL's new laboratory management tool, Lab Assist, will ensure that any hazards associated with user activities are identified, mitigated, and communicated promptly and effectively. In addition, EMSL staff and management conduct regular assessments and walk-throughs of all EMSL laboratory spaces throughout the year to ensure safe operations.

Metrics of an engaged and productive user community include an increase in the number of new investigators submitting proposals, the number and quality of user publications, and productivity of users conducting BER-relevant research, the number of data downloads and data DOI minted, publications of EMSL generated data by primary and secondary users, and downloads of our data processing and analysis tools. EMSL's dashboard captures measures of our operational environment, including days away, off-normal events, and first aid cases, which are reported quarterly to BER.

5.3 Identify, Develop, and Rapidly Deploy Capabilities to the Scientific User Community

EMSL has one of the most comprehensive and unique suites of integrated scientific capabilities for addressing BER and BER-aligned research needs in the world and is poised to catalyze scientific advances in biological and environmental systems research. Section 4.0 describes our current capabilities in the context of IRPs. EMSL's regularly updated recapitalization plan[15] details the near- and long-term investments needed to maintain and strengthen our unique and state-of-the-art technical capabilities and expertise to solve complex systems science challenges.

EMSL engages the scientific community through workshops and sessions at scientific meetings to define the science needs and capability-development efforts needed to support the science. In part, these efforts guide and form the basis of EMSL's recapitalization plan. At the same time, EMSL identifies and works to deactivate and sunset instruments that are no longer aligned with biological and environmental systems research, or are underused by the scientific user community.[13] This ensures that existing financial and personnel resources will be available for new research directions.

As new instruments are deployed, EMSL will take the following actions to maximize their use and benefit to the scientific community and BER research priorities: (1) highlight new capabilities through the EMSL website and social media, and (2) emphasize the availability of new capabilities in the annual user call, particularly highlighting new major instruments (e.g., DTEM) to inform the scientific community and generate interest and sustained user demand.

Measures of progress will include the number of new and fully functional capabilities deployed in a timely manner each year, capabilities sunsetted each year, number of proposals requesting use of new capabilities each year, time from deployment to first publications highlighting new capabilities, number of high impact publications and citations over time, patents, and R&D 100 awards.

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