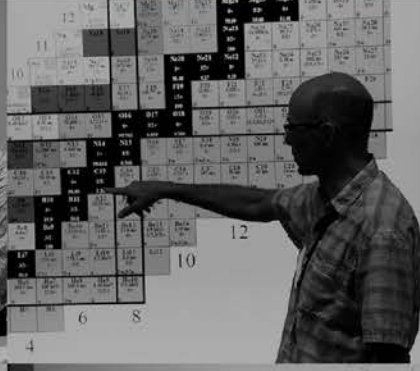
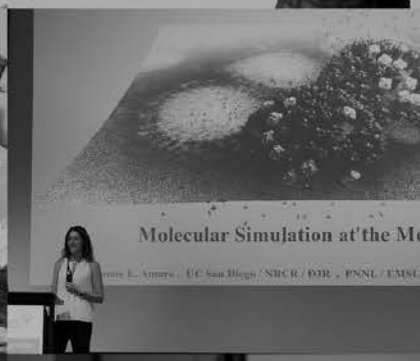


2018 Integration

Molecular Structure and Dynamics

in Biology and the Environment

August 6–8
Richland, Wash.

EMSL





Authors: N. Hess and J. Evans
Date: December 2018

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PNNL-28323

EMSL Integration 2018: Molecular Structure and Dynamics in Biology and the Environment Report on the Workshop Held August 6–8, 2018

Workshop Co-chairs: N. Hess and J. Evans,
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December 2018

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Pacific Northwest National Laboratory
Richland, Washington 99352

Executive Summary

Once a year, EMSL, the Environmental Molecular Sciences Laboratory, hosts a scientific meeting to engage key BER-relevant researchers as well as user communities. Almost 90 researchers attended EMSL Integration 2018: Molecular Structure and Dynamics in Biology and the Environment from August 6–8, 2018, at the Pacific Northwest National Laboratory in Richland, Washington. The attendees represented academia, national laboratories, federal agencies, and other institutions. Thermo Fisher Scientific helped sponsor the meeting.

For three days, the attendees explored the structure and dynamics of molecules important in biology and the environment using advanced techniques available at EMSL and other Department of Energy (DOE) user facilities.

Acting EMSL Director Harvey Bolton welcomed attendees at EMSL Integration 2018: Molecular Structure and Dynamics in Biology and the Environment

"The real takeaway from this meeting will be the realization that the caliber of science we all want to be doing now, and in the future, will require collaboration with multiple user facilities," said Acting EMSL Director Harvey Bolton in his opening remarks.

Representatives from several DOE user facilities attended the meeting and some delivered plenary and session presentations, gave user facility flash talks, and conducted tutorials. The other user facilities included Stanford Synchrotron Radiation Lightsource (SSRL), a user facility at SLAC National Accelerator Laboratory; National Synchrotron Light Source II (NSLS-II), a user facility at Brookhaven National Laboratory (BNL); Joint Genome Institute (JGI), a user facility at Lawrence Berkeley National Laboratory (Berkeley Lab); Advanced Light Source (ALS) at Berkeley Lab; Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL); and DOE Systems Biology Knowledgebase (KBase) open-source software and data platform.

"This meeting was unique in the way it brought together representatives from different user facilities all sharing their knowledge and ideas," said EMSL Deputy for Sciences Areas Nancy Hess. Hess and James Evans, Senior Research Scientist at EMSL, jointly organized the meeting and served as meeting co-chairs.

A tutorial during the final day of the meeting.

Following the plenary presentations and facility flash talks on August 6, the August 7 schedule included a morning of invited and contributed presentations on biological science while the afternoon focused on environmental science. Brief brainstorming sessions followed each series of talks. A facility tour of EMSL was also offered to all interested visitors.

The final day of the meeting occurred on August 8. The agenda comprised tutorials by staff from EMSL, SSRL, NSLS, and KBase. The tutorials were informational and showcased recent results, outlined new methods and capabilities, detailed how to access each facility, and included discussions of new types of insights that can be gained from integrating unique capabilities available across the various user facilities.

Acronyms and Abbreviations

3D	three dimensional
ALS	Advanced Light Source
ATP	adenosine triphosphate
BER	Biological and Environmental Research
Berkeley Lab	Lawrence Berkeley National Laboratory
BNL	Brookhaven National Laboratory
BSISB	Berkeley Synchrotron Infrared Structural Biology
CH_4	methane
CO_2	carbon dioxide
CRS	Coherent Raman Scattering
DOE	Department of Energy
DOM	dissolved organic matter
EMSL	Environmental Molecular Sciences Laboratory
JGI	Joint Genome Institute
KBase	DOE Systems Biology Knowledgebase
LCLS	Linac Coherent Light Source
M2	Matrix-2 protein
NSLS-II	National Synchrotron Light Source II
ORNL	Oak Ridge National Laboratory
SLAC	National Accelerator Laboratory
SNS	Spallation Neutron Source
SSRL	Stanford Synchrotron Radiation Lightsource

Contents

1.0 The Science

Importance of biological molecules in biology and environment

Molecules are the currency by which biological and environmental processes are conducted. The composition and structure of chemical constituents, and their spatial and temporal relationships between molecules and molecular complexes regulate all biological processes and provide the organizational framework for subcellular structure and larger-scale interactions. Gaining mechanistic insight into these processes is a necessary first step to manipulate the exchange and transformation of biomolecules among plants, microbial communities, and their environment that will result in sustainable production of bioenergy crops, as well as the development of predictive models of environmental response to perturbations.

Overcoming challenges associated with the development of sustainable and cost-competitive biofuels requires a detailed understanding of the following:

- How biomass is constructed and how to deconstruct it,
- How to optimize enzymatic pathways that produce desired molecules and biopolymers (bioproducts), and
- How these pathways are regulated in the context of cell metabolism.

Also needed is an understanding of how cellular and subcellular structures of individual organisms correlate with specific biochemical, molecular, genetic, and behavioral pathways. Similarly, environmental challenges need an understanding of how plant and microbial consortia communicate, allocate resources, and respond to changes in the environment. These diverse challenges require multidisciplinary teams using multimodal approaches to advance novel solutions. Recent advances in imaging and analytical approaches provide new opportunities for characterizing the structure, spatial location, and dynamics of biological molecules, complexes, and processes both at the molecular and cellular scales to infer function of these components.[(a)] User facilities already provide a wealth of such capabilities to a broad user base, but to date the cross-facility interactions have been minimal. Facilitating cooperation between the facilities, integrating data, and common-access mechanisms will provide an integral part of future research teams to accelerate DOE science.

The EMSL Integration meeting participants included a mix of science leaders in the areas of cellular ultrastructure and physiology, bioenergy and bioproducts, and environmental microbiology, as well as representatives from user facilities that provide capabilities that can address challenges in these research areas. The science landscape discussed at this meeting spanned vast spatial and temporal scales from the atomic to centimeters and from femtoseconds to days. The presentations represented only a fraction of the science possible across the facilities. In addition to fostering the transfer of knowledge and increasing networking between researchers and user facility staff, workshop brainstorming sessions also identified new ways that user facilities can work together to facilitate access to the multimodal capabilities needed to address the challenges associated with characterizing molecular and cellular systems relevant to bioenergy and environmental research.

Some meeting participants at EMSL Integration 2018.

[a] U.S. DOE. 2017. *Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment*, DOE/SC-0189, U.S. Department of Energy Office of Science. science.energy.gov/ber/community-resources/.

1.1 Monday, August 6, 2018, Plenary Talks

1.1.1 Soft x-ray tomography – Carolyn Larabell

Carolynn Larabell presented the cryogenic soft x-ray nanotomography capability available at ALS, which provides label-free, whole-cell three-dimensional (3D) reconstructions. This approach is ideal for carbon and nitrogen-rich compounds because they exhibit elevated contrast in the so-called "water window" where the instrument operates. The accurate segmentation and quantitation of the data are key for measuring distribution and abundance of subcellular components and for assessing the impact of genomic variability and response to treatments. The approach also allows tracking the evolution of disease states by comparing reconstructions from samples frozen at different time points. Carolyn pointed out that machine learning is becoming an important component to the segmentation process for more unbiased approaches to data interpretation.

Carolyn Larabell gave a plenary talk on soft x-ray tomography.

1.1.2 Molecular simulation at mesoscale – Rommie Amaro

Rommie Amaro presented her work on computational simulation of cellular organization and her software, CellPack. Computational simulation can enrich interpretation of data made possible by new imaging modalities and reveal complex interactions. Dynamic models can now incorporate everything from single molecules to molecular networks. "Improved algorithms, ever-more-powerful computing architectures and accelerating growth of rich data sets are driving advances in multiscale modelling methods capable of bridging chemical and biological complexity from the atom to the cell."[b] These computational simulations require inputs about cell and membrane composition, protein structure, protein abundance, and localization, as well as boundaries for subcellular structure to assemble the virtual cell. While enhancing the visualization of data, these models also inform future research directions and new hypotheses.

1.1.3 From roots to shoots to electrons – Britt Hedman

Britt Hedman presented an overview of work at SLAC using SSRL, Linac Coherent Light Source (LCLS), and cryo-EM. She highlighted synchrotron-based bioimaging approaches to probe biological systems across the tissue, cell, organelle, molecular, atomic, and electronic levels. These methods permit chemical tomographic imaging, capturing dynamics of biomolecules in solution, as well as probing biomass conversion, metal speciation, and microbial respiration.

1.1.4 Molecular to mesoscale biological processes using neutrons – Hugh O'Neill

Hugh O'Neill presented on the neutron spectroscopic and imaging modalities at SNS, which have exquisite sensitivity to hydrogen and deuterium and are penetrating, but non-destructive. These methods can analyze biomacromolecules and assemblies including protein complexes, DNA, lipids, viruses, and carbohydrates within large 3D crystals or in solution at lower resolution. He also highlighted recent work using neutrons to observe hierarchical structures for biomass structure and deconstruction.

1.1.5 Electron cryotomography – Grant Jensen

Grant Jensen presented past results and his future vision for cryo-electron tomography for imaging the structure of molecular machines as well as the organization of whole cells. He highlighted research combining super-resolution

[b] Amaro, R. E.; Mulholland, A. J., Multiscale Methods in Drug Design Bridge Chemical and Biological Complexity in the Search for Cures. *Nat. Rev. Chem.*, **2018**, *2*, 0148. https://www.nature.com/articles/s41570-018-0148

fluorescence microscopy with correlated cryo-EM to map the location of a labeled protein within the whole-cell ultrastructural context. His presentation highlighted how a picture is worth a thousand words as the direct images of intact cells can now show internal details and protein architecture in 3D with resolution and contrast that were once only dreamt about. He discussed the revolution occurring in cryo-EM that is helping redefine accessibility of structural biology for the general researcher by allowing direct analysis of proteins and cells without extensive sample preparation such as chemical fixation or growing 3D crystals.

1.1.6 Systems insights into C cycling at a leading edge of climate change – Virginia Rich

Virginia Rich discussed her research linking gene to ecosystems scales using molecular data and biogeochemical data to understand mechanisms (predominately microbial) that lead to the release of carbon (either as CO_2 or CH_4) in soil from permafrost regions to the atmosphere in a warming climate. She discussed collecting genomic and proteomic samples that provide community composition, metabolic potential, and protein expression levels, and linking that to dissolved organic matter (DOM) molecular chemistry under bog and fen biogeochemical conditions. These findings can be incorporated into metabolic models (BioCrunch) and upscaled to larger ecosystem models of nutrient cycling (Ecosys) as shown in Figure 1.

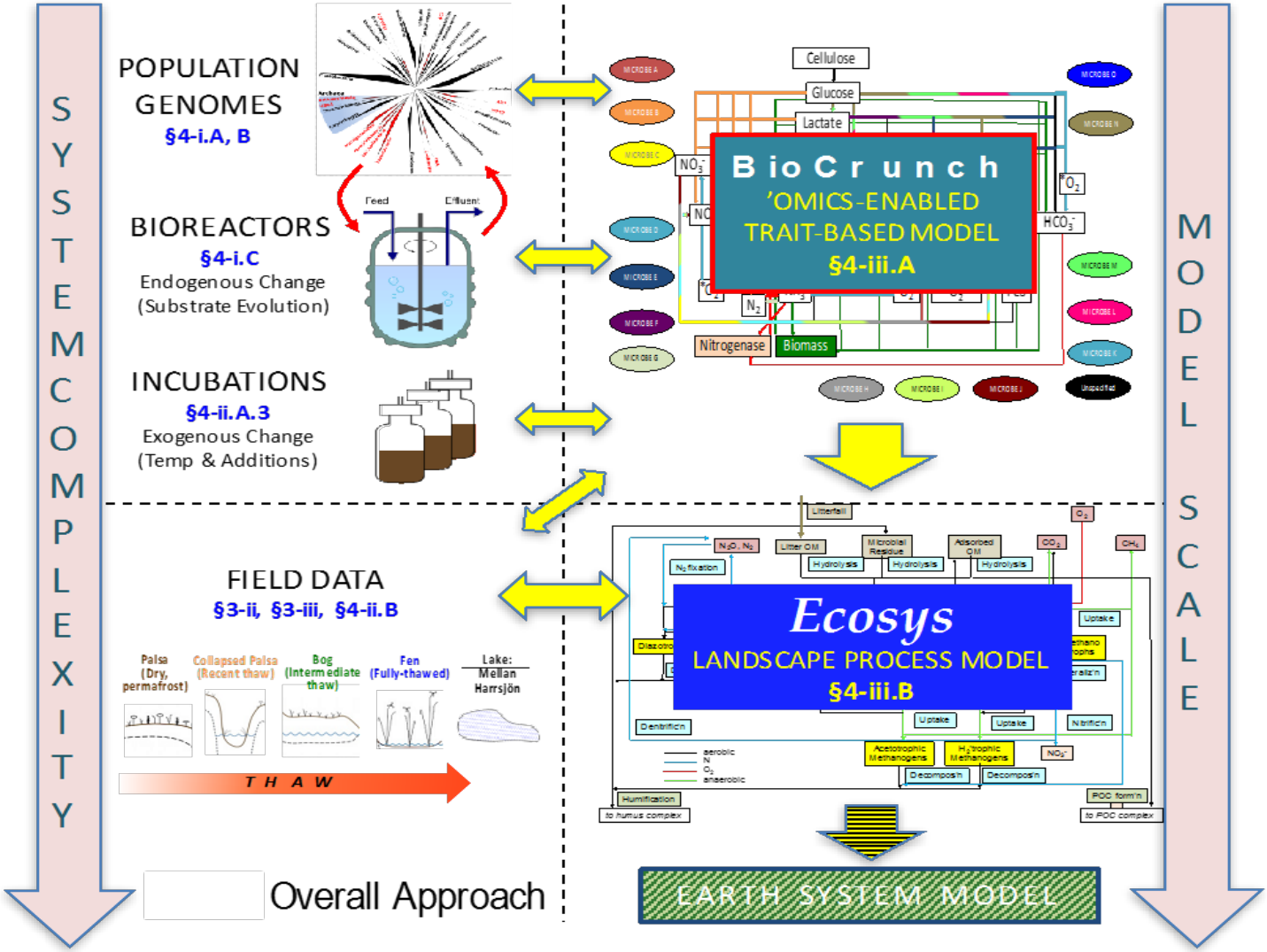

Figure 1

1.2 Tuesday – Biological Systems Invited Talks

1.2.1 Solvent dynamics in the influenza M2 proton channel – Jessica Thomaston

Jessica Thomaston presented her work using x-rays to probe the M2 proton channel complex that is necessary for viral replication. Some antivirals target blocking the M2 proton channel, but limited structural information existed about its structure and function which hindered a detailed understanding of its mechanism. Cryogenic synchrotron macromolecular crystallography revealed pH-driven confirmation changes within the channel and inferred the position of ordered water molecules that line the channel. However, room temperature measurements of the same samples showed less ordered solvent, which could have been an artifact from beam damage, or the order seen in the cryogenic sample could have resulted from a freezing artifact. To address this, Jessica and her team took measurements using LCLS (a DOE sponsored X-ray Free-Electron Laser) and showed that at low pH and room temperature the continuous network of ordered water molecules is present but is indeed less ordered than the cryogenic measurements. At higher pH there are fewer ordered water molecules suggesting proton conduction is likely inhibited.

1.2.2 Probing membrane protein structures in their native-like environment using cryo-EM – Po-Lin Chiu

Po-Lin Chiu presented his group's work using cryo-EM to determine the structure of various membrane proteins. While over 150,000 protein structures exist in the Protein Data Bank, structures of membrane proteins are vastly underrepresented. In nature, membrane proteins constitute about one third of all proteins, but less than five percent of the known protein structures relate to this class of proteins. Cryo-EM allows direct determination of protein structure from either single-particle, 2D crystal, or 3D crystal sample geometries. Single-particle analysis has proven very powerful in recent years allowing atomic resolution structures from purified proteins without requiring crystallization. Po-Lin highlighted the strengths of this approach by detailing the new insights provided by determining the atomic structure from a protein common across all domains of life—ATP synthase.

Seminar speaker, Xin Zhang, MT Thomas Postdoctoral Award winner.

1.2.3 Understanding plant cell wall structure by in-situ imaging – Shi-You Ding

Shi-You Ding presented an overview of new Coherent Raman Scattering (CRS) microscopy techniques that provide high-resolution spatial and chemical imaging of biomolecules in plant tissues. Using vibrational signatures, CRS can readily distinguish between lipids, cellulose, and lignin without requiring labels. It can also distinguish between saturated and unsaturated lipids classes. Shi-You then showed his work combining Atomic Force Microscopy and CRS to resolve changes in the structure of cellulose microfibrils and changes in the cellulose-to-lignin ratio in a series of poplar mutants.

1.2.4 Research in biogeochemical sciences at the Berkeley Synchrotron Infrared Structural Biology (BSISB) imaging program – Hoi-Ying Holman

Hoi-Ying Holman presented work on synchrotron-based Fourier-transform infrared spectroscopy for studying biological and biogeochemical samples non-destructively. The approach enables label-free spectroscopic analysis of cells using infrared light. It can detect cellular and chemical composition and, in combination with in-situ stages, can permit tracking dynamics over time. The resolution is largely diffraction-limited but is capable of interrogating bacterial communities and even plant-microbe interactions.

1.2.5 The transparent soil microcosm – Kriti Sharma

Kriti Sharma presented work on vibrational spectroscopy using isotopically labeled substrates as components of a multimodal approach for the investigation of extracellular enzymes that drive microbial decomposition as a collective activity. Use of transparent soils (nafion) and optical microscopy visualized the location of microbial cells, assembly of microbial clusters, and fungal-bacterial associations. Raman spectroscopy was used to quantify the microbial uptake of 13C labeled substrates through shifts in vibrational features, thereby revealing that when exoenzymes are freely available then planktonic microbes can uptake more substrate than individuals in microbial clusters due to increased competition.

1.3 Tuesday – Environmental Systems Invited Talks

1.3.1 Imaging trace elements in plants and soil with x-ray fluorescence microscopy – Ryan Tappero

Ryan Tappero presented research highlighting the x-ray imaging and microscopy beamlines available at NSLS-II and several applications relevant to environmental science. These included chemical and spectroscopic imaging of trichomes on leaves, comparative calcium distribution in leaves of wildtype and mutant cultivars, spectroscopic and diffraction evidence of arsenic uranium coprecipitation, and the geochemistry of arsenic mobility in coastal soils.

1.3.2 Impact of organic matter type on uranium complexation in anoxic contaminated sediments – Sharon Bone

Sharon Bone presented her research using multiple DOE user facilities to study the impact of organic matter on uranium biogeochemistry in Colorado plateau floodplain sediments. This work showed that uranium x-ray absorption spectroscopy at SSRL combined with nanoSIMS at EMSL and C NEXAFS at the Canadian Light Source reveals detailed chemical speciation information on the types of organic matter that can adsorb uranium at low concentrations and prevents precipitation in uranium solid phase. This insight provides a new conceptual framework for understanding uranium mobility in floodplain sediments.

1.3.3 A systems biology characterization of mercury-methylating organisms and synthetic model communities – Dwayne Elias

Dwayne Elias presented research demonstrating how a synthetic microbial community replicates the proposed Hg-methylation metabolic pathway that exists in contaminated sediments at DOE legacy sites. Cultured strains with >99% similarity to prevalent species in the Hg-methylating communities were created based on 16S, hgcAB, and metagenomic sequence data. The selected strains represent different anaerobic functional groups (iron and sulfate reduction, fermentation, syntrophy, methanogenesis) to simulate complete anaerobic carbon degradation. Strains are grown under steady state conditions in increasingly complex cultures with measurements of cell counts, Hg methylation rates, electron donors and acceptors, organic acids, H_2 and CO_2 concentrations, carbon balancing, and expression levels. This suite of analyses will allow us to directly characterize the phenotypic effects of multi-species interactions on Hg-methylation and cellular metabolism in these field-informed synthetic communities.

1.3.4 A molecular view into DOM-metal interactions – Rene Boiteau

Rene Boiteau presented recent results demonstrating the use of LC-ICPMS-ESIMS mass spectrometry to identify chemical structure of organic-metal complexes in soil that are used by plants, fungi, and bacteria to solubilize micronutrients such as Fe, Ni, Cu, and Zn.

1.3.5 Exometabolomic analysis of plant-microbe interactions in the rhizosphere of grasses – Kateryina Zhalnina

Kateryina Zhalnina presented her research on the analysis of rhizosphere metabolites and metagenomes released in grasses microcosms. Exudate profiles of grasses were largely represented by organic acids and amino acids at early developmental stages, while the abundance of quaternary amines and nucleosides increased at later stages of plant growth. bacteria that were stimulated by root growth and bacteria with traits related to potential relief of nitrogen stress were observed to preferentially consume aromatic organic acids. These aromatic acids were substantially exuded by roots during periods of active plant development and under nitrogen limited conditions suggesting that substrate specialization of rhizosphere bacteria, together with changing composition of root exudates, provides a mechanistic basis for plant development and response to environmental stress. This work used JGI and the techniques are now available to the broader science community through user proposals to JGI or FICUS.

1.3.6 Spies and bloggers: New synthetic biology tools for environmental science – Caroline Masiello

Caroline Masiello presented her research using synthetic biology to engineer microbes to report and record on their biologic activity by emitting easily detected rare gases. These activities include horizontal gene transfer, the production of extracellular enzymes to respire C substrates, and the production and/or consumption of N_2O and CH_4 which are hard to measure at the spatial scale that microbes respond to their environment.

There were many networking opportunities to catch up with colleagues.

1.3.7 Phylogenetically diversified multi-chassis engineering enables rapid activation of biosynthetic gene clusters – Yasuo Yoshikuni

Yasuo Yoshikuni presented his research using synthetic biology to activate gene clusters in bacteria that have enabled the large-scale identification of candidate secondary metabolite biosynthesis pathways routine. Successful activation of 6 biosynthetic gene clusters from 11 different proteobacteria genera identified 21 products, including several with likely roles in host-microbe interactions. This demonstrates how the regulatory and physiological diversity naturally present across bacteria can be harnessed for the exploration of novel bioproducts and provide a sizable panel of domesticated chassis strains to enable this strategy. This work used JGI and the techniques are now available to the broader science community through user proposals to JGI.

2.0 The Future

2.1 Recommendations from the brainstorming sessions

Meeting participants were asked to break into small groups and discuss new avenues for user facilities to increase outreach and accelerate scientific impact for the general user community. Several great ideas arose from the sessions.

- Joint website: One of the most prominent ideas was the possibility of a single, joint webpage that could feature various user facilities and the science possible at each facility, as well as direct links to the capabilities available to users and information about deadlines and procedures to apply for access. This joint page could be hosted on the DOE website and serve as a general portal for users to more easily become familiar with the diverse set of capabilities and expertise offered at each facility. It could also highlight publications for which users have accessed multiple facilities to empower an integrated multimodal framework to reveal new biological or environmental insights not possible at a single institution.

- Compatible technologies cross-walk: Another idea that arose from the brainstorming sessions was a simplified table to communicate the various capabilities and the scales they address in a format that is easy to understand. During his presentation and a later breakout session, Hugh O'Neill helped refine a table mapping the complementary techniques across the various BER user facilities, which is included below (Table 1). This table should be treated as a living document and expanded upon or updated continuously by the various facilities. It could also be incorporated in the joint webpage mentioned in the previous paragraph.

Table 1. Capabilities Available at BER User Facilities

	Neutron Technique	Complementary Technique	BER Facility
Molecular Systems			
• Macromolecules and complexes • Flexible/disordered systems • Membranes • Membrane proteins • Biopolymers	• D-labeling • Neutron diffraction • SANS (static/TR) • Dynamics–CNCS, QENS, NSE • Reflectivity	• DNA synthesis • XRD • SAXS (static/TR) • GI SAXS • Cryo-EM: • AFM • HP Computation	• JGI • Synchrotron X-rays • EMSL
• Cells • Organisms (e.g., plants) • Structure/dynamics of macromolecules in vivo • Biomass • Biomimetic systems	• D-labeling • SANS • Dynamics- CNCS, QENS, NSE • Reflectivity • Imaging	• NMR • Electron microscopy: SEM, ESEM, TEM, Cryo • AFM • Live cell single cell Fluorescence microscopy • Nano-SIMS • Scanning probe imaging • X-ray tomography	• EMSL • Synchrotron X-rays

- Design of universal to flexible sample holders to ease the analysis of samples by multiple techniques at different user facilities.

- Common or translatable sample naming schemes, metadata formats and data structures so that data from different facilities is more readily "findable, searchable and integrated" across experimental platforms.

Appendix A

Workshop Agenda

EMSL

www.emsl.pnl.gov

Environmental Molecular Sciences Laboratory
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EMSL Integration 2018
Molecular Biological and Environmental Science
August 6-8, 2018

AGENDA

Monday, August 6, 2018				Location
7:45am	Registration and Badging			Discovery Hall
8:20am	Welcome	Harvey Bolton, Acting EMSL Director	EMSL	Horizon
8:30am	Plenary #1	Carolyn Larabell- CT scans of cells and organisms in the native state	UCSF	Horizon
9:10am	Plenary #2	Rommie Amaro-Molecular simulation at the mesoscale	UC San Diego	Horizon
9:50am	Facility flash talks		NSLS & SSRL	Horizon
10:00am	Networking			Discovery Hall Lobby
10:30am	Plenary #3	Britt Hedman- From roots and shoots to electrons – "imaging" with synchrotron x-rays	SSRL	Horizon
11:10am	Plenary #4	John Eiler- The isotopic structures of molecules: The fundamental science and applications of an 'omics' of (nearly) everything	Caltech	Horizon
11:50am	Facility flash talks		EMSL & SNS	Horizon
12:00pm	Working Lunch - EMSL Capability Presentation			Horizon
1:00pm	Plenary #5	Hugh O'Neill - Opportunities for characterizing molecular to mesoscale biological processes using neutrons	SNS/ORNL	Horizon
1:40pm	Plenary #6	Grant Jensen- Advances in electron cryotomography	CalTech	Horizon
2:20pm	Facility Flash talks – JGI & KBASE		JGI & KBASE	Horizon

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2:30pm	Networking			Discovery Hall Lobby
3:00pm	Plenary #7	Virginia Rich - Systems insights into carbon cycling at a leading edge of climate change	Ohio State University	Horizon
3:40pm	Seminar	MT Thomas Post-doc award winner, Xin Zhang-Understanding the non-classical crystallization pathways enabled by advanced microscopy techniques	PNNL	Horizon
4:20pm	Facility Poster Session and Reception			Discovery Hall Lobby
6:20pm	Leave for dinner on your own			
Tuesday, August 7, 2018 – Morning Sessions – Biological Science				**Location**
8:00am	Talk #1	Jessica Thomaston – Solvent dynamics in the influenza M2 proton channel: a song of ice and fire	UCSF	Horizon
8:20am	Talk #2 (Contributed)	Norman Lewis - Dirigent protein family: Discovery, structure and function	WSU	Horizon
8:30am	Talk #3 (Contributed)	Garry Buchko - Solution protein NMR spectroscopy: structure determination just the tip of the iceberg	PNNL	Horizon
8:40am	Talk #4 (Contributed)	Mowei Zhou – Native mass spectrometry and electron microscopy decipher manganese biomineralization by a unique marine bacterial enzyme	EMSL	Horizon
8:50am	Talk #5	Po-Lin Chiu – Probing membrane protein structures in their native-like environment using cryo-EM	ASU	Horizon
9:10am	Talk #6 (Contributed)	Irina Novikova - Multi-scale protein production in a test-tube for versatile applications	EMSL	Horizon
9:20am	Talk #7 (Contributed)	Daniel Perea - Atom probe tomographic analysis of biological materials enabled by advanced specimen preparation approaches	EMSL	Horizon
9:30am	Break			

9:40am	Talk #8	Shi-You Ding – Stimulated Raman - Understanding plant cell wall structure by in situ imaging	MSU	Horizon
10:00am	Talk #9	Hoi-Ying Holman - Research in biogeochemical sciences at the Berkeley Synchrotron Infrared Structural Biology (BSISB) Imaging Program	LBNL	Horizon
10:20am	Talk #10	Kriti Sharma - Transparent soil microcosms: a window into soil microbial activity and decomposition at the microscale	UNC	Horizon
10:40am	Talk #11 (Contributed)	Ying Zhu - Single cell proteome mapping of tissue heterogeneity using nanoPOTS and ultrasensitive LC-MS	EMSL	Horizon
10:50am	Brainstorm		EMSL	Horizon
12:00pm	Working Lunch, Presentation, and EMSL Tour		EMSL	Discovery Hall/Lobby
Tuesday, August 7, 2018 – Afternoon Session – Environmental Science				**Location**
1:00pm	Talk #1	Ryan Tappero - Imaging trace elements in plants and soil with x-ray fluorescence microscopy	NSLSII	Horizon
1:20pm	Talk #2	Sharon Bone - Impact of organic matter type on uranium complexation in anoxic contaminated sediments: a combined NanoSIMS and x-ray spectromicroscopy study	SLAC	Horizon
1:40pm	Talk #3	Dwayne Elias - A systems biology characterization of mercury-methylating organisms and synthetic model communities	ORNL	Horizon
2:00pm	Talk #4	Rene Boiteau - A molecular view into DOM-metal interactions	EMSL	Horizon
2:20pm	Talk #5	Kateryina Zhalnina - Exometabolomic analysis of plant-microbe interactions in the rhizosphere of grasses	JGI	Horizon
2:40pm	Break			

2:50pm	Talk #6	Caroline Masiello - Spies and bloggers: New synthetic biology tools for environmental science	Rice University	Horizon
3:10pm	Talk #7	Yasuo Yoshikuni - Phylogenetically diversified multi-chassis engineering enables rapid activation of biosynthetic gene clusters	JGI	Horizon
3:30pm	Talk #8 (Contributed)	Susannah Tringe - Methane cycling in restored and unrestored industrial salt ponds	JGI	Horizon
3:50pm	Brainstorm			Horizon
5:00pm	Leave for dinner on your own			
Wednesday, August 8, 2018 – Tutorials				**Location**
9:00am – 4:00pm (working lunch at 12:00pm in Discovery Hall Lobby)				
A	SSRL + NSLS – all day			Discovery Hall Frontier
B	KBASE – all day			Discovery Hall Vista
9:00am - 12:00pm				
C	EMSL – Introduction to NWChem			Discovery Hall Horizon E
D	EMSL – Interactive visualization tools for EMSL users			Discovery Hall Horizon B
E	EMSL – NMR for biomolecular structure and dynamics			Discovery Hall Horizon A
F	EMSL – Super resolution and confocal microscopy. Closed-toe shoes required.			EMSL Labs 1102
G	EMSL – XPS and ToF SIMS Closed-toe shoes required.			EMSL Lab 1210
12:00pm	Working Lunch – Virtual EMSL tour – Nancy Washton, Vendor Show, Networking		PNNL	Horizon / Discovery Hall Lobby
1:00 - 4:00pm				

H	EMSL – Introduction to NWChem		Discovery Hall Horizon E
I	EMSL – R programing tools for FTICR analysis and visualization		Discovery Hall Horizon B
J	EMSL – Super resolution and confocal microscopy Closed-toe shoes required.		EMSL Labs 1102
K	EMSL – NMR for biomolecular structure and dynamics		Discovery Hall Horizon A
L	EMSL – XPS and ToF SIMS Closed-toe shoes required.		EMSL Lab 1210

Appendix B

Presentations

Appendix B – Presentations

This version of the report does not include presentations for easier and faster printing. The version of the report that does include presentations is also available on the EMSL website here.

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