

**Laboratory Directed Research
and Development Program
FY 2016**

June 2017

**Report on
Ernest Orlando Lawrence
Berkeley National Laboratory**

**Laboratory Directed
Research and Development
Program**

FY 2016



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Berkeley, CA 94720

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Introduction

The Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab or LBNL) is a multi-program national research facility operated by the University of California for the Department of Energy (DOE). As an integral element of DOE's National Laboratory System, Berkeley Lab supports DOE's missions in fundamental science, energy resources, and environmental quality. Berkeley Lab programs advance four distinct goals for DOE and the nation:

- To perform leading multidisciplinary research in the computing sciences, physical sciences, energy sciences, biosciences, earth and environmental sciences, and energy technologies in a manner that ensures employee and public safety as well as protection of the environment.
- To develop and operate unique national experimental facilities for qualified investigators.
- To educate and train future generations of scientists and engineers to promote national science and education goals.
- To transfer knowledge and technological innovations and foster productive relationships among Berkeley Lab's research programs, universities and industry in order to promote national economic competitiveness.

Berkeley Lab's research and the Laboratory Directed Research and Development (LDRD) program supports DOE Strategic Themes that are codified in DOE's 2014 Strategic Plan, with a primary focus on the theme of Scientific Discovery and Innovation. For that, the Fiscal Year (FY) 2016 LDRD projects support Goal 1 through multiple strategic objectives described in the plan. In addition, LDRD efforts support the goals of Management, Performance and Nuclear Security (unclassified fundamental research that supports stockpile safety and nonproliferation programs). The LDRD program also supports Office of Science strategic plans, including the 20-year Scientific Facilities Plan and the Office of Science Strategic Plan. Berkeley Lab's LDRD research also supports the strategic directions periodically under consideration and review by the Office of Science Program Offices, such as LDRD projects germane to new research facility concepts and new fundamental science directions.

Berkeley Lab's LDRD program also plays an important role in leveraging DOE capabilities for national needs. The fundamental scientific research and development conducted in the program advances the skills and technologies of importance to our Strategic Partnership Projects (SPP) sponsors. Among many directions, these include a broad

range of health-related science and technology of interest to the National Institutes of Health, such as breast cancer, accelerator research supported by the Department of Defense, detector and engineering technologies useful to the Department of Homeland Security, and particle detection valuable to the Environmental Protection Agency.

The *Berkeley Lab Laboratory Directed Research and Development Program FY2016* report is compiled from annual reports submitted by principal investigators following the close of the fiscal year. This report describes the supported projects and summarizes their accomplishments. It constitutes a part of the LDRD program planning and documentation process that includes an annual planning cycle, project selection, implementation and review.

Berkeley Lab's LDRD program is a critical tool for directing the Laboratory's forefront scientific research capabilities toward vital and emerging scientific challenges. The program provides the resources for Berkeley Lab scientists to make rapid and significant contributions to critical national science and technology problems. The LDRD program also advances Berkeley Lab's core competencies, foundations and scientific capabilities, and permits exploration of exciting new opportunities. All projects represent work in forefront areas of science and technology. Areas eligible for support include:

- Advanced study of hypotheses, concepts or innovative approaches to scientific or technical problems;
- Experiments and analyses directed toward "proof of principle" or early determination of the utility of new scientific ideas, technical concepts or devices; and
- Conception and preliminary technical analyses of experimental facilities or devices.

The LDRD program supports Berkeley Lab's mission in many ways. First, because LDRD funds can be allocated within a relatively short time frame, Berkeley Lab researchers can support the mission of the Department of Energy (DOE) and serve the needs of the nation by quickly responding to forefront scientific problems. Second, LDRD enables Berkeley Lab to attract and retain highly qualified scientists, and to support their efforts to carry out world-leading research. In addition, the LDRD program also supports new projects that involve graduate students and postdoctoral fellows, thus contributing to the education mission of Berkeley Lab.

Berkeley Lab has a formal process for allocating funds for the LDRD program. The process relies on individual scientific investigators and the scientific leadership of

Berkeley Lab to identify opportunities that will contribute to scientific and institutional goals. The process is also designed to comply with DOE Orders, in particular DOE Order 413.2C (dated October 22, 2015). From year to year, the distribution of funds among the scientific program areas changes. This flexibility optimizes Berkeley Lab's ability to respond to opportunities.

Berkeley Lab's LDRD policy and program decisions are the responsibility of the Laboratory Director. The Director has assigned general programmatic oversight responsibility to the Deputy Laboratory Director, with administration and reporting on the LDRD program supported by that office. LDRD accounting procedures and financial management are consistent with the Laboratory's accounting principles and stipulations under the contract between the University of California and the Department of Energy, with accounting maintained through the Laboratory's Chief Financial Officer.

In FY2016, Berkeley Lab was authorized by DOE to establish a funding ceiling for the LDRD program of \$27M including General & Administrative (G&A) overhead, which equated to ~3.6% of Berkeley Lab's FY2016 projected operating and capital equipment budgets. This funding level was provided to develop new scientific ideas and opportunities, and to allow the Berkeley Lab Director an opportunity to initiate new directions. In all, about \$24.5M was expended for operating expenses.

In FY2016, scientists submitted 180 proposals, requesting about \$44.3M in funding prior to assessing laboratory overhead. Eighty-five projects were funded, with awards ranging from \$66K to \$834K.

Development of a compact laser-driven ion beam accelerator for Discovery Plasma Science

Principal Investigator: Qing Ji
 Co-PI(s): Sven Steinke and Stepan Bulanov

Project Description

The purpose of this project is to lay the foundation of an advanced laser-driven ion acceleration system using the PW laser at the Berkeley Lab Laser Accelerator (BELLA) center, with beam transport/handling capability to achieve ion beams at various beam energies and intensities as high as 10^{10} /shot. This technology can not only be used as an injector for conventional accelerators, but also has a variety of potential applications, such as radiography, biomedical research in cancer treatment, material science and warm dense matter research, and studies of fast ignition schemes etc.

We will carry out realistic 2D and 3D modeling of the interactions between PW laser pulses and materials to find the optimum scenario for the PW laser at BELLA to generate ions with kinetic high energies (> 250 MeV for protons, > 800 MeV for helium, > 1 GeV for carbon etc.). Concepts for high repetition-rate targetry, beamlines and detectors to use the full capabilities of BELLA (1 Hz) will be developed. With the ultra-high intensity ($> 10^{21}$ W/cm²) achieved by the unique PW laser in addition to short focal length optics, advanced nano-engineered targets, theory and simulation of ion generation, leading expertise in ion beam control and manipulation, we will develop a design for a new generation of high performance ion accelerators.

Accomplishments

We have laid out three phases of BELLA-i development: I) ion acceleration using the existing long focal length BELLA beamline; II) experiments in the existing BELLA cave with two laser beamlines (short- and long- focal length); and III) experiments in a new cave with improved shielding and ion beam transport system. Our most significant accomplishments have been the physics design of Phase I experiments for producing protons up to 15 MeV using the long focal length BELLA beamline, target design for acceleration mechanisms that can be achieved in Phase I, and engineering design of a Thomson Parabola Ion Spectrometer that can be used as beam diagnostic tool. We have engaged program managers at DOE Fusion Energy Sciences in their high energy density physics program and have submitted a proposal for follow up funding after the LDRD.

We have modeled the production of ion beams by PW laser pulses in Radiation Pressure Acceleration (RPA), Magnetic Vortex Acceleration (MVA), and Directed Coulomb Explosion (DCE) regimes in 2D (using REMP and WARP codes) for a wide range of initial parameters and have finished 2D simulation specifically using Phase I and II BELLA parameters. We are in the process of adapting the 3D Particle-in-cell code WARP for full simulation of the laser ion accelerator. We have also designed an ion beam transport system that consists of combined function magnetic quadrupole lens and dipoles using alternating-gradient canted cosine theta (AG-CCT) superconducting magnets. By varying the magnetic field, the system is flexible to select and transport of ions out of a large range of ion beam energies.

The results of simulation and design studies were presented at several international conferences and published in peer-reviewed journals.

High-Performance Advanced Particle Accelerator Simulator

Principal Investigator(s): Jean-Luc Vay, Rémi Lehe

Project Description

The goal of this project was to develop simulation tools that provide nearly real-time feedback (under one hour) to experiments on advanced plasma-based particle accelerators.

Laser-driven plasma-based electron accelerators (LPAs) have recently produced high-quality electron beams at several giga-electronvolts in cm-scale distances [LPA]. This demonstrates a critical path forward in the development of compact accelerators for a wide variety of new applications in fundamental research, industry, security and medicine. While computer modeling has been a key factor in the rapid progress in plasma-based (electron and ion) accelerators in the last decade, high-fidelity simulations often require weeks of computer-time on parallel supercomputers for standard experimental configurations.

Cutting the runtime to below one hour, and eventually to minutes, will enable much faster turnaround and feedback between simulations and experiments, and allow for critical parametric optimization. This will decrease significantly the time needed to interpret the experiments and to converge to optimized designs. This is necessary, in particular, for the accurate prediction of particle trapping in LPA experiments and tracking of ultra-low emittance beams over very long distances for the design of LPA-based colliders. Some of the developed tools will be relevant to other applications such as the modeling of laser-plasma interaction (LPI), free electron lasers, coherent synchrotron radiation, or laboratory and space plasmas.

Accomplishments

Our most significant accomplishment has been to develop (in partnership with colleagues from DESY in Germany) a novel approach for solving Maxwell's equations in a relativistic Particle-In-Cell (PIC) code, which is free of the so-called "numerical Cherenkov instability" (NCI) for a plasma streaming at relativistic velocity. The NCI, which was first exposed by Brendan Godfrey in a seminal paper in 1974, has been the bane of relativistic streaming plasma simulations for over forty years. Since the instability was exposed, many researchers, including our group in collaboration with Brendan Godfrey, have attempted to eliminate it, with great success in some cases, but never as successfully and elegantly as with the new method.

The cornerstone of the new approach (conceptually simple, yet mathematically sophisticated) is that Maxwell's equations (which describe the electromagnetic fields that act upon the plasma) are solved analytically using a Galilean comoving coordinate system. Instead of having the plasma move along a fixed coordinate system, as is the rule with the standard PIC technique, the coordinate system moves together with the plasma. Unlike previous methods, the method does not require a small timestep, and can be used with Cartesian or quasi-cylindrical coordinates. Detailed empirical and theoretical stability analyses have been conducted for a uniform flowing plasma, demonstrating the capabilities of this technique and showing that it indeed mitigates the NCI. Computer simulations of laser-plasma accelerators in an optimal Lorentz boosted frame demonstrated the effectiveness of the method for real applications, both in Cartesian coordinates using our code Warp, and in quasi-cylindrical coordinates with our code FBPIC.

Analytically integrable spectral Maxwell solvers, which we successfully implemented in the context of massively parallel computing environments in a previous LDRD, have been essential to implementing the new approach. The new approach is among the key methods that are to be implemented in the new WarpX code in development under our DOE-ECP Exascale project.

A New Concept for High Average Power Ultrafast Lasers

Principal Investigator: Russell Wilcox

Project Description

The purpose of this project is to develop scalable technologies for high energy, high repetition rate, ultrafast laser sources using fiber amplifiers. Fiber lasers have advantages in efficiency, beam quality and average power capability, but are limited in peak power due to nonlinear and damage effects. We therefore must develop methods of scaling energy output by combining the outputs of many lasers. This has been done for continuous wave (CW) lasers using beam combination based on a diffractive optic beamsplitter, although this method cannot be used with ultrashort ($\sim 100\text{fs}$) pulses due to angular dispersion and pulse front tilt.

We will develop a new, scalable method of beam combination using diffractive elements, which solves the problem of pulse front tilt. This is based on a scheme with two elements, acting like a grating pair for each beam. With two gratings, the residual dispersions will be temporal dispersion and spatial chirp, which can be rendered negligible by correct choice of parameters. Using only two elements and two-dimensional arrays of beams, many beams can be combined while maintaining high efficiency and power handling capability.

Accomplishments

We have demonstrated combination of four ultrafast pulses, in both numerical modeling and laboratory demonstrations. Using an optics modeling code which adds electric fields, we have shown that four pulses can be propagated through two diffractive optics (a grating and a splitter), and added in phase with a high efficiency. Our model also shows that the temporal dispersion is negligible on this time scale and that pulse front tilt is cancelled for the coherently added beam.

The laboratory experiment uses diffractive optics designed using the same modeling software we are using, so the model elements are identical with those used to manufacture the real elements. A 100fs, 1040nm modelocked fiber laser is the source, which is split into four beams using free space optics, and sent to the diffractive combiner pair. Each of the four beams is controlled in phase. As the light exits the diffractive combiner, the central beam should be maximized while adjacent satellite beams are minimized. These adjacent beams are measured by a photodiode, which is read by the computer and a stochastic algorithm used to minimize the uncombined beams. The efficiency of forming the combined beam from all diffracted beams is affected by several imperfections, notably pulse front tilt coming from the beam splitting array. We have measured the pulse width before and after the combiner, and it is unchanged, indicating that bandwidth is preserved and temporal dispersion is low. These promising results indicate that the concept is sound, and improvements to the optical scheme will result in increased efficiency.

We are currently adding a fiber amplifier to the source in order to increase available signal power, changing the way the four beams are formed, and working to extend the scheme to eight beams in a 2-dimensional array.

High-Pressure Soft X-ray Spectroscopy of Fluids

LDRD Postdoc: Ruimin Qiao; **ALS:** J.-H. Guo, A. MacDowell, M. Kunz, and C. Wang; **ESD:** B. Gilbert, J. Ajo-Franklin, and P. Nico; **MSD:** D. Prendergast, J. Schuck, and J. Urban

This LDRD is proposed to construct the high-pressure (HP) fluid flow cells for soft X-ray (SX) spectroscopy and scattering experiments. The HP-SX cells will enable multiple soft X-ray spectroscopy and scattering characterization tools at ALS for novel measurements with the focus on the molecular structure of fluids relevant to geological carbon sequestration (GCS) of CO₂ and with impact to the *in-situ* study of CO₂ storage in MOF materials and membrane technology in water-energy environment science. It has also potential applications of studying catalytic reactions in real-world industrial conditions.

The LDRD postdoc, Ruimin Qiao was hired in March 2016. The technical goals of the project are: 1) To create SX transparent windows stable beyond the critical point of CO₂ (75 bars; 31°C); and 2) To construct single-windowed HP flow cells for SX spectroscopy.

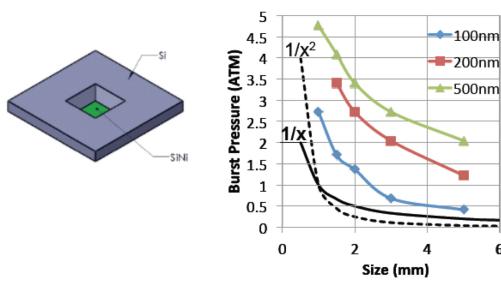


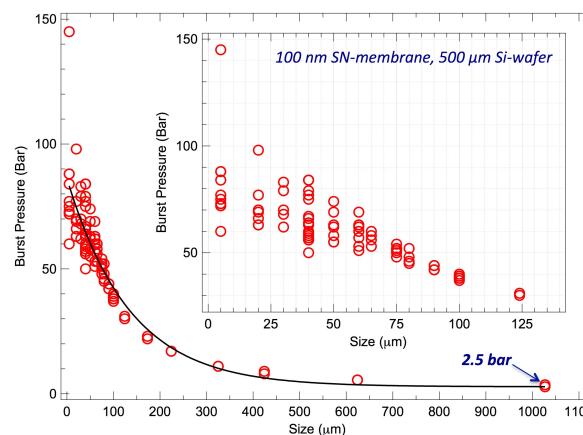
Figure 1. Theoretical prediction of the burst pressure for silicon nitride membrane windows.

Figure 1 shows the calculated burst pressure for the SN-membrane windows of different thickness and opening dimensions. The commonly used SN-membrane windows (100-nm thick membrane with 1 mm x 1 mm opening on the 200 μ m thick Si-wafer) shows a burst pressure at about 2.75 bar, and the

calculation shows that we could achieve 25 bar by using 200-nm thick SN-membrane window with 20 μ m x 20 μ m. We started the test on this kind of window and were able to achieve a pressure of 80 psi (close to 6 bar) in May 2016. The experiment indicate that the known theoretical specs may not to entirely correct, thus we are refining the theoretical modeling parameters and planning further experimental tests.

Figure 2. Experimental test of the burst pressure for the SN-membrane windows.

New membrane windows are fabricated with support from Weilun Chao, a CXRO scientist for achieving higher pressure. Figure 2 shows the experimental test of burst pressure for a collection of the SN-membrane windows. We can now retain the pressurized liquids under about 75 bar using a SN-membrane window of 100 nm thick with the opening less than 50 μ m x 50 μ m opening. Further experimental test ongoing. Meanwhile, the micro-fabrication microfluidics cells is processing for testing in a higher-pressure range of 10-100 bar.



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**Tender Resonant X-ray Scattering (TReXS): A Spatio-Chemical Probe for Materials,
Biology and Energy sciences**

Principal Investigator(s): Alexander Hexemer, Peter Zwart, Howard Padmore

Project Description

The purpose of this project is to develop a new scientific technique in the ALS. The plan is to develop Tender Resonant x-ray Scattering (TReXS) as a probe for soft and hard matter, utilizing the strong absorption edges primarily in the few keV energy range to elucidate the chemical structure of materials, from polymers and biological membranes to dynamical studies of energy storage materials. TReXS is the only research tool that allows characterization of multicomponent systems at the tender x-ray regime (i.e. 2 keV-5 keV), using fluorescence and scattering detectors simultaneously. K absorption edges including Phosphorus and Sulfur are the main targets for this technique, as both P and S are of great importance in the field of biological and material sciences.

TReXS can be further enhanced by exploiting the ultra-bright, high coherent, high flux beam from an optimized undulator as provided by the ALS-u. Expected improvements enabled by the ALS-u include the ability to significantly reduce the sample volumes needed, enhanced by the increased x-ray cross sections in the tender X-ray region. The high flux, small focal spot and high coherence of an ALS-u TReXS beamline will also allow one to routinely perform fluctuation scattering experiments and extract higher-order intensity correlations, leading to more detailed structural models of materials. This project also provides a very strong supporting case for the extension of the traditional core soft x-ray research program into the few keV energy range, vastly increasing the range of science that will be optimally carried out on ALS-u. The scientific community will greatly benefit from the availability of this technique at ALS; the Balsara and Gomez research groups have already expressed strong interest in TReXS user access.

Accomplishments

During the last year of LDRD project, we have developed the TReXS end-station at BL 5.3.1 at ALS. TReXS beamline have significantly improved by installing a new Pilatus 300K detector, as our order suppressor and a crystal monochromator developed further, allowing access to the extreme Bragg angles needed to access the tender energies (i.e. 4-2.1 keV). We have also installed additional slits before Helium sample chamber to obtain a better data resolution, and now it is possible to collect both fluorescence and scattering spectra simultaneously. At BL 5.3.1, we have collected very promising data for free stand sulfonated block-copolymer membranes. From the collected data, it is obvious that tender resonance at S K-edge is distinguishable, in excellent agreement with data collected at BESSY-II in Berlin/Germany. The absorption spectra have also been measured, demonstrating the mono accuracy of about 1 eV at Sulfur edge. We have also collected TReXS data for a variety of samples at 2.4-4 keV, including Li-S pouch battery cells. The significant improvements have been made at 5.3.1, will open new opportunities for ALS and ALS-u in the coming year. In 2016, several new collaborations with groups at UC Berkeley, Michigan University, and Penn State University have been established as well.

PROBING SPATIALLY-RESOLVED INTERMITTENT CHEMICAL KINETICS IN CONFINED SPACES USING X-RAY PHOTON CORRELATION SPECTROSCOPY

Principal Investigator(s): Sujoy Roy

Project Description

The project is aiming for a better understanding of the gas adsorption dynamics in a group of micro-porous sorbents, namely Metal-Organic Frameworks (MOFs), using X-ray photon correlation spectroscopy (XPCS). The time depended nanoscale structural fluctuation probed by the experiment can help reveal the nature of the gas-MOF interaction and possible intermittent state, thus lead to better fine tuning of MOF structure for energy efficient CO₂ removal from post combustion flue gas.

To achieve this target, a system with in-situ material activation and gas delivery ability under ultra-high vacuum environment needs to be developed. And this system must grant enough photon transparency to enable time-dependent analysis of the structure fluctuation, in the meantime, it has to be capable of standing the ultra-high vacuum environment to enable soft X-ray experiment. Once the system is ready, a series of high-performance MOF materials will be investigated to extract any useful structural information about the CO₂-MOF interaction. The result will be the first spatio-temporal correlation study of MOFs and the result will be fed back to our MOF-synthesis collaborator to help improve the next generation MOF sorbent.

Accomplishments

We have made significant progress so far. In the first ear we have successfully made cells and sample holders that can be operated in-situ in the x-ray beam. A miniature size in-situ environment cell (Figure 1) with material activation and gas flowing function has been developed. The cell consists of a Polyether ether ketone (PEEK) body, compress sealed gas input and output, two custom made silicon nitride membrane with heater and spacer and a metal cover. All the parts are carefully designed and machined to a total size of approximately 0.8 inch and is mounted on a custom made insert rod so that it can fit into the XPCS chamber at beamline 12 at the ALS. A set of gas flow and control system is also built near the beamline. MOF sample will be deposited and heated under vacuum on one of Silicon Nitride membranes, which has gold heater fabricated on the surface. This heating process will drive away all the pre-adsorbed solvent, gas or any other molecules which may affect the CO₂ adsorption.

Currently, the function and reliability is under examination. The vacuum tightness of the cell under UHV has been tested ex situ. Gas flow line and controller was also tested and proved functional. The test of the system under working condition will be conducted soon. We are working closely with Rebecca Siegelman from Prof. Jeff Long's group at the UCB Chemistry department for the MOF sample. A polydispersed Mg based MOF (dobdc) with an average crystallite size of 70 μm has been synthesized. A colloidal solution of the MOF was spin-coated onto a SiN membrane. Peak were obtained due to x-ray diffraction from the sample with the incident beam tuned to the K-edge of Mg. Measurements were done both in transmission as well as reflection geometries. We calculate that the real space periodicity that give rise to the diffraction peak is 19 Å. Since the pore-pore distance in the MOF is 20 Å this means the peak that we observed is from the pores. The scattering intensities were weak and we are optimizing the sample coverage to maximize the scattering efficiency.

High-dimensional ptychographic imaging for studying nanoscale dynamics, chemistry and morphology at the ALS and ALS-U
Principal Investigator: David Shapiro

Project Description

The Advanced Light Source (ALS) has established itself as the world leader in ptychographic imaging by achieving the highest resolution ever recorded and demonstrating spectro-microscopy with nanoscale resolution in the study of chemical phase transformations in battery electrode materials. We have developed a powerful capability which is unique in the world, however, new experimental and computational methods are needed in order to address the reality that soft x-rays have limited depth of field at high spatial resolution and thus cannot achieve high resolution when imaging three-dimensional structures using standard methods. The limited depth of field removes one of the key advantages of x-ray microscopy, long penetration depth. In order to take full advantage of optimized x-ray beamlines at the ALS and ALS-U we will develop experimental and analytical methods for ptychographic imaging of chemically heterogeneous and three-dimensional systems at high spatial resolution. These techniques will be particularly important for *in situ* microscopy of materials in an enclosed medium such as electrochemistry in functional batteries or hydration reactions. The ability to image complex structures at high resolution is an essential tool for materials science and this proposal will bring that tool to the energy sciences through the x-ray ptychographic microscopy program at the new COSMIC imaging beamline.

Accomplishments

Working with the ALS detector group we have optimized our data acquisition system for high-resolution coherent x-ray diffraction measurements. Currently, our prototype ptychographic microscope is commissioning at a low brightness x-ray bend magnet beamline but will be moved to the very high coherent flux COSMIC beamline in early 2017. At the current beamline, high-resolution measurements can be achieved with very long dwell times. Such measurements are therefore possible but practically challenging. Regardless, using various nano-material systems we have experimentally verified the presence of limited depth-of-field in our ptychographic reconstructions as resolution is increased. This effect presents itself as defocus artifacts when imaging extended objects and ultimately limits the reconstructed resolution in both two and three dimensions.

Utilizing multi-slice ptychographic reconstruction algorithms, which account for sample depth effects, we have shown the ability to computationally extend the depth of field of our images and enhance the resolution of reconstructed projections. This has been demonstrated before with both visible light and hard x-rays but our achieved resolution is more than a factor of 10 better than previous results because of the high performance of ALS beamlines. We have also generated a full tomographic dataset from a test sample with 5 nanometer features that will serve as a final test of our ability to improve the reconstructed resolution to the diffraction limit of our data. The dataset contains 320 projections spanning a full rotation of 160 degrees and has over 2 TeraBytes of diffraction data. Ptychographic analysis of such data is very time consuming so we have also begun the process of implementing GPU accelerated software for near real-time analysis.

Novel Accelerator Techniques for Diffraction Limited Light Sources

Principal Investigator: Christoph Steier

Project Description

Improvements in brightness and coherent flux of about two orders of magnitude are possible using multi bend achromat lattice designs. These improvements can be implemented as upgrades of existing facilities or as newly built green-field facilities. In the case of upgrades, much of the existing infrastructure can be reused, thereby reducing cost and time needed to reach full scientific productivity. Achieving the extremely small beam emittances in such lattices requires solving many challenges, both in engineering and in accelerator physics. An R&D program has been carried out to understand and where possible retire the highest technical risks associated with multi-bend achromat lattices, with a special emphasis on the challenges posed to reach the diffraction limit for soft x-rays.

Accomplishments

In the accelerator area, the R&D included development programs to demonstrate pulser and kicker technology for swap-out injection (particularly for bunch trains), vacuum technology to enable ultimate performance of polarized undulators, highly integrated and high-stability magnet and vacuum assemblies for beam stability, advanced radiation-production sources for the highest coherent flux, and optimization of algorithms and tools for fast commissioning. In the area of beamlines, R&D was carried out to study high-power mirror technology. Significant progress was made in all of these areas. Specific achievements include: Construction and testing of a full-prototype pulser suitable for swap-out injection; production and testing of very small NEG-coated, including initial tests of in-situ activation; study of collective effects at the required bunch-lengthening factors greater than four; development of lattices with improved momentum apertures and test of their robustness; initial analysis of coherence-preserving photon optics, including advanced cooling. Some successful results of accelerator technology R&D are illustrated in the figure below.

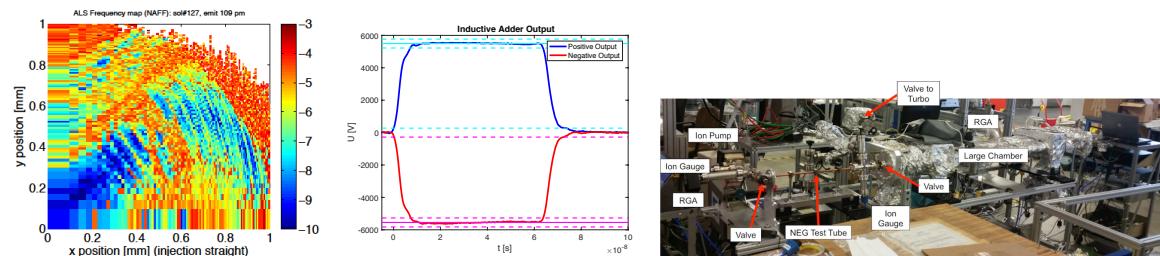


Figure: (Left) Dynamic aperture of optimized nine-bend achromat lattice, including the effects of errors; (Middle) Pulse waveform of LBNL inductive adder at full voltage, demonstrating required rise and fall times; (Right) vacuum test-stand to quantify pumping efficiency of small NEG chambers and test in situ-activation schemes.

URBan Integrated System (URBIS): A Data and Computing Platform for Urban Systems
 Principal Investigator(s): Tianzhen Hong, Michael Wetter

Project Description

More than two-thirds of people in the U.S. live in urban areas, where most buildings and infrastructures are aging. Cities are facing growing challenges of retrofit and expansion to increase operational efficiency to reduce resource use and GHG emissions, and to meet sustainability goals and improve resiliency to combat nature extreme events. We propose to design and develop a data and computing platform to support urban systems research and development. The platform enables city stakeholders to make holistic and quantitative decisions considering complexity and opportunity of urban systems.

We will build the foundation of data and workflow automation, and integrate existing urban data models, energy modeling and optimization tools into the platform using open standards, i.e., Modelica for district energy simulation, Functional Mockup Interface (FMI) for co-simulation and CityGML for 3D city models. We will also explore the concept of emergent behavior, how a group of buildings together can have potentially much lower energy use than the simple sum of individual building performance. We will demonstrate the usability of the URBIS platform through: (1) retrofit analysis of buildings in a city block that reduces their energy use by up to 40%, and (2) an optimal design and operation of low-exergy district energy systems that targets energy savings of up to 40%.

Accomplishments

Our most significant accomplishments have been: (1) to develop the City Building Energy Saver (CityBES) which builds upon CityGML and open city data that can model every building in cities and visualize their performance. CityBES is used for retrofit analysis of 540 commercial buildings in Downtown San Francisco that achieve 30-40% energy savings; (2) to develop Modelica tools to model advanced district energy systems, which is used to design and simulate the performance of bi-directional district heating and cooling systems that integrate heat recovery among buildings and heat exchange with bay water, achieving energy savings of 40%.

We explored a theoretical thermodynamic framework that can be used to evaluate and benchmark energy performance of district energy systems. Three campus-based district energy systems were studied and compared to improve understanding of their energy performance and potential improvements.

We also launched a journal club to read and discuss research articles on urban sciences. A direct follow-on funding has been achieved through the DOE exascale computing project, multiscale coupled urban systems (started in FY17 as a seed project).

Advanced Combustion Technology for Transportation Refrigeration Units

Principal Investigator(s): Peter Therkelsen, Vi Rapp, Tom Kirchstetter

Project Description

The FY16 funded LDRD, “Establishing LBNL Leadership in Small-Power Generation,” is aimed at expanding the new ETA Small-Scale Engine Research and Development Test Facility, develop a proof-of-concept technology, and build upon ongoing scientific research. This FY16 activity builds upon the success of FY15 LDRD research in which a 10hp engine test stand was established and engine pollutant and particulate matter emissions data were collected. With ETA ALD approval, a strategic change in scope of work for the FY16 activities was made due to the emergence of Co-Optima as a clear pathway to new US DOE EERE multi-year funding that will establish ETA leadership in biofuel suitability studies and classification

The DOE Fuel-Engine Co-Optimization (Co-Optima) initiative is focused on accelerating the introduction of affordable, scalable, and sustainable biofuels and high-efficiency, low-emission vehicle engines. Nine national laboratories have been funded in FY16 to begin working on Co-Optima. The simultaneous research and development of fuels and vehicle engines is designed to deliver maximum energy savings, emissions reduction, and on-road vehicle performance. The Co-Optima initiative is funded by EERE’s VTO and BETO with a multi-year research roadmap.

LDRD Strategic Change of Scope Deliverables for FY16

1. Establish a framework for a rapid, high throughput fuel property test protocol,
2. Commission existing equipment to measure laminar burning velocity, and
3. Produce initial fuel property results that demonstrate LBNL ability to meet Co-Optima needs and secure FY17 US DOE funding.

Accomplishments

The project has resulted in commissioning of equipment capable of measuring laminar burning velocity at LBNL. This experimental system has been validated and used to collect data in collaboration with the ABPDU. The system is incorporated in the LBNL Combustion Laboratory suite of tools that comprise the ability to rapidly test fuel properties in support of traditional and advanced liquid fuels. Conversations with private and public potential funders are scoping out use of the systems and future expansion.

The capability to measure laminar burning velocities has been reported to DOE and the other national lab members of the Co-Optima initiative. The new LBNL capability were drafted into early stage FY17 AOPs for funding.

The capabilities of the LBNL Combustion Laboratory continue to expand and the newly commissioned experimental system has gained addition interest for use from startup companies who are able to now produce ml volumes of biofuels.

In Situ Multi-modal Probing of Chemical Reactions via Windowless Micro-reactors

Selim Alayoglu, Stefan Minasian, Don Tilley, John Hartwig, Musahid Ahmed

Project Description-

Earth-abundant first-row transition metals have the potential to replace toxic and expensive precious metals in many energy-related applications for homogenous catalysis. For monitoring their chemical reactions in the liquid phase, we proposed deployment of micro-droplet reactors coupled to spectral methods using X-ray synchrotron radiation, mass spectrometry and optical-laser based spectroscopies. The novel windowless reactor design enables simultaneous application of mass spectrometry as well as IR, UV/Vis, and X-ray absorption spectroscopy (XAS). The entirely windowless configuration is particularly advantageous for detection of intermediates or other low concentration species using soft X-ray radiation, where use of windows could render spectroscopic detection difficult. This micro-droplet reactor scheme will be employed to probe low-Z elements at the K-edge as well as core level transitions of the first-row transition metals. By such a multi-modal probing of catalytic transformations in micro-reactor environments, a refined mechanistic picture of catalytic chemistry could be determined, and used for experimentally-led rational design of next generation catalysts and catalytic networks.

Accomplishments-

The synergistic effort has encompassed organic and inorganic synthesis, synchrotron instrumentation, and spectroscopy. We designed and built a microdroplet reactor which serves as an experimental chamber to generate flowing micro-droplets and to measure XAS spectra from liquid solutions. It operates under flowing He (< 1 atm), and is equipped with a photodiode for fluorescence yield detection (bulk-sensitive) and an electron collector for total electron yield detection (surface sensitive). Using this setup, we successfully generated ~500 μm droplets of many solvents including water, ethanol, and toluene. Preliminary results were obtained at O and Mg K absorption edges from aqueous solutions of $\text{Mg}(\text{NO}_3)_2$ using continuously flowing micro-droplets at the ALS demonstrating the promise of this micro-droplet reactors for use with soft-X-rays. For tender X-rays, Pd L₃, Cl K and Co K absorption edges were successfully monitored using our micro-droplet reactor and photodiode detection scheme. The micro-probe in beamline 10.3.2 will render possible mapping entire micro-droplets for mixing inhomogeneity on the surfaces and in the bulk, as well as complimenting the XAS results using soft X-rays, which penetrates into near surfaces and probe shallow core levels. We have also built a custom-design Raman spectrometer using a 532 nm CW laser excitation source and coupled to a fiber-optic cable for remote delivery. Performance of this spectrometer was tested on aqueous micro-droplets containing a rhodamine dye.

For the first phase of studies, we have synthesized and characterized an isostructural series of coordination compounds stabilized by a multidentate salen ligand with first-row transition metals including Cr, Mn, Fe, Co, and Ni. Initial studies have also focused on synthesizing a series of iron, ruthenium, and osmium silylene compounds with reactive silylene functionalities (M=Si double bonds) that have been implicated in hydrosilylation catalysis. Si K-edge XAS was used to characterize the silylene functionalities, which revealed a low energy Si 1s $\rightarrow \pi^*$ transition in the Si K-edge XAS that may be a signature of the M=Si bonds.

Design of Mesoscale Catalyst Networks

John F. Hartwig and Douglas S. Clark

Project Description. This research program aims to develop multi-step, multi-catalyst systems, termed “catalytic networks.” We conducted studies toward systems containing mutually incompatible catalysts that become compatible by confinement reacting with rates of individual steps that are regulated by feedback mechanisms as in biosynthetic pathways. To this end, we have surveyed several strategies to create confined catalysts and several strategies to create multi-step, multi-catalytic reactions. During FY2016, we continued to pursue artificial metalloenzymes that catalyze a set of reactions completely separate from those that are catalyzed by any natural enzyme and multi-catalytic systems for multistep reactions that benefit by maintaining a low concentration of an unstable intermediate. Our results on these two topics are described below.

Accomplishments. 1) Creation of artificial metalloenzymes as modules for multistep processes. The last year of our three-year LDRD proposal gave us the ability to bring our preliminary studies on creating artificial metalloenzymes to the point of three publications, one in *Nature*, one in *Science*, and one provisionally accepted to *JACS*. Our first paper disclosed the strategy of creating artificial metalloenzymes by formally exchanging the metal on myoglobin to a series of platinum-group metals and abiological first-row metals. We showed that these artificial enzymes would catalyze abiological transformations, such as the insertion of a carbene into a C-H bond. In the second paper, we conducted related studies to exchange the iron in P450 enzymes with a methyliridium fragment. We conducted the second set of studies on P450 enzymes because these enzymes contain a binding site for organic molecules, whereas the Myoglobin proteins we used initially bind oxygen and have a solvent-exposed active site. By using a P450, we were able to create an artificial metalloenzyme that reacts more than 1000 times faster than any prior artificial metalloenzyme and with kinetics that are similar to those of natural enzymes in biosynthetic pathways. Finally, in our third publication, we showed that the artificial P450 enzymes containing iridium catalyze chemoselective reactions of sulfonaryl azides to undergo intramolecular insertions of nitrenes into C-H bonds. P450 enzymes containing iron catalyze these reactions, but the selectivity for C-H amination versus reduction of the azide to a sulfonamide is unfavorable. In contrast to the roughly 1:1 ratio of these two products formed by P450 enzymes containing the natural metal iron, our artificial metallocenzymes form the product from amination in a 20:1 ratio versus that from reduction. Finally, this P450 system catalyzes the cyclopropanation of alkenes, and studies to explore the scope of these cyclopropanation reactions are ongoing.

2) Hydroaminomethylation. In a second aspect of this program, we have continued to develop a dual catalyst system to convert *alpha*-olefins to amines by sequential hydroformylation and reductive amination. Hydroformylation occurs in the organic phase catalyzed by the combination of Rh(CO)₂(acac) and BISBI, a ligand developed by Eastman Kodak for hydroformylation with high selectivity for linear aldehydes. The aldehyde intermediate condenses with secondary amine reagents to form an iminium ion, which reacts with a metal hydride to afford the tertiary amine product. In prior years we showed the clean production of tertiary amines in high yield with very high (>50:1) linear/branched selectivity. During the past year, we have extended the scope of this work to the hydroaminomethylation of primary amines to form secondary amines. In addition, in work that has the potential to revolutionize the synthesis of primary amines, we showed that the reaction of NH₄OC(O)H as the nitrogen source provides formyl protected primary amines as product. By using ammonium formate as the source of ammonia, the primary amine product is protected *in situ*. The synthesis of linear primary amines from 1-alkenes has been a longstanding goal of catalysis for the synthesis of nylon monomers and many fine chemicals.

COMPUTATIONAL-EXPERIMENTAL STUDIES OF AEROSOL TRANSFORMATIONS FROM THE LIQUID TO GLASSY STATE

Principal Investigator: Frances Houle
Co-Investigator: Kevin Wilson

Project Description

Recent studies report evidence that some organic aerosols exist in the atmosphere not as well mixed liquids – the traditional description – but rather as highly viscous, glassy materials with extremely slow internal reaction-diffusion times and low evaporation rates. These observations suggest that the characteristics of organic aerosols currently used in regional and global climate models are fundamentally incorrect: viscosity affects reactivity and indeed, the models consistently under-predict the quantity of aerosol in the atmosphere by factors of 5 to 10. We are addressing this gap by developing a quantitative and predictive description of how aerosols are transformed, in particular by gas phase oxidants. Reaction-diffusion models that are chemically accurate and fully validated by experimental data have not been previously used in this field and hold promise for improving parameterizations in atmospheric models. Model simulations are performed using stochastic methods, which are well-suited to large dynamic ranges of conditions and capture fluctuations and rare events key to reactivity in these complex nanoscale systems. Our goals are to examine the complex coupling of oxidative ageing chemistry with environment- and history-dependent viscosity and to generate a comprehensive model that can be applied to a range of aerosol transformation chemistries. Our model design strategy is to develop key components of the model separately and merge them after validation. The main components required are (1) uptake of gas reactants, (2) a free radical chain over many product generations, and (3) dynamic perturbations by environmental factors such as temperature, pollutant plumes, and humidity and by internal factors such as immiscibility of products.

Accomplishments

In the third and final year of this LDRD we have continued work on a fully coupled reaction-diffusion mechanism for semi-solid aliphatic alkane oxidation by OH, on the chemistry of oxidation of aqueous citric acid by OH, and have carried out predictive studies using the models developed. Last year we reported that a semi-solid organic aerosol forms an unreacted core covered by an oxidized shell despite very high driving forces for diffusional mixing. This year we fully characterized the system. We determined that the shell is enriched in carboxylic acids, and that the progressive fragmentation of the oxidized material is driven by aldehyde chemistry. As fragmentation progresses the outer shell of the particle becomes plasticized, enabling a more rapid consumption of the aerosol material. Carboxylic acids are hydrophilic, therefore we examined citric acid chemistry for the case where water uptake is extensive due to their presence. The oxidation chemistry was found to convolve both free radical and acid-base chemical pathways. With these validated models, we have carried out predictive studies of oxidation of C₃₀ alkanes over a range of viscosities. Results for laboratory (high OH concentrations) and atmospheric (low OH concentrations) conditions have been compared. It was found that the relationship between mixing rates as the material spans liquid to solid states and oxidation rates over the large OH partial pressure range is not simple. This has important implications for the use of laboratory conditions to determine key processes in the atmosphere and for the need for quantitative models to connect laboratory work and environmental observations. Two final papers describing these accomplishments are in preparation.

Spotlighting Catalysis: *In situ* and *Operando* Characterization of Photoelectrochemical Assemblies

Principal Investigators: Francesca M. Toma, Ian D. Sharp, Mary K. Gilles, Shaul Aloni, Ethan Crumlin

Project Description

We propose to advance the state of the art of *in situ* and *operando* characterization by developing for the first time photoelectrochemical characterization over various length scales. A central aspect of this work is focused on the development of peak force scanning photoelectrochemical microscopy (PF-SPECM). This technique will combine scanning electrochemical microscopy with photoconductive atomic force microscopy for *in situ* and *operando* study of heterogeneous photocatalytic reactions at the nanoscale. We leverage recent advances in *operando* electrochemical characterization to extend these approaches to photodriven chemical transformations. Scanning probe measurements are complemented by study of identical photoelectrochemical assemblies using a suite of advanced *in situ* and *operando* characterization techniques, namely: i) high resolution transmission and scanning transmission electron microscopy (TEM and STEM), ii) scanning transmission X-ray microscopy (STXM), and iii) ambient pressure X-ray photoelectron spectroscopy (AP-XPS). The combination of these methods will enable unprecedented access to catalytic mechanisms, dynamic chemical and morphological transformations, and photocorrosion processes at the nano and mesoscale level.

This work will substantially advance the state-of-the-art by coupling light into *in situ* and *operando* electrochemical measurement systems, ultimately enabling mechanistic insights that will guide materials design and improve performance.

Accomplishments

The most significant accomplishments have been achieved in the development of *in situ* and *operando* PF-SPECM and STXM techniques. Specifically, to develop the SPECM technique, we have established a protocol for i) in-liquid electrochemical measurements, and ii) photoconductive measurements in air and controlled conditions. We used electrochemical atomic force microscope (EC-AFM) to monitor *in situ* degradation of BiVO₄ and gain information on the corrosion mechanism of this promising photoanode for solar-driven water splitting. This technique allows us to acquire time-lapse topography images of electrodes under active electrochemical conditions. In addition, we have also characterized the nanoscale heterogeneity of local conductive properties of BiVO₄ by photoconductive (PC) AFM, which simultaneously provides very high spatial resolution (~20 nm) for topology and photocurrent, as a function of wavelength and light intensity at an applied bias. We have observed a correlation between the topological features (grains) in the material and the photocurrent maps. Specifically, we find intragrain and intergrain inhomogeneity. The development of these protocols provides a critical foundation for ongoing work devoted to probing correlations between topological, electronic, and (photo-)electrochemical properties of individual grains on the nanometer scale. We are now combining EC and PC-AFM into PF-SPECM to perform *operando* measurements and gain nanoscale structure-activity information of photoelectrocatalytic systems.

Finally, we have monitored the V and O K-edges in BiVO₄ by STXM and found chemical inhomogeneity on pristine samples and as a function of the corrosion process. Such samples will next be used to monitor spectral and spatial changes in real time under *operando* conditions.

HARNESSING THE SOIL MICROBIOME FOR FOOD AND FUEL SECURITY

Principal Investigator(s): Eoin Brodie, Peter Nico

Project Description

Current crop yields need to be nearly doubled on a global scale to meet growing population demands; including increased utilization of marginal lands and better management of fertilizer inputs (Vance et al., 2003; Cordell et al., 2009). Phosphorus (P) is one of the most limiting plant nutrients, with yields on 30-40% of the world's arable land limited by P availability (Runge-Metzer, 1995). P deficiency is largely due to poor mobility of inorganic P in soil solutions, making it largely inaccessible to plants (Hinsinger, 2001). During soil formation and aging (pedogenesis) P transitions from a mineral form to a labile form that is available for plant uptake. However much of the labile P can be sorbed onto the surfaces of soil particles, immobilized into soil organic matter, or incorporated into recalcitrant inorganic forms. These processes result in eventual depletion of mineral P and labile P with an accumulation of the occluded and organic forms of P that are not accessible to plants (Izquierdo et al., 2013).

The soil microbiome has evolved the capacity to mine critical nutrients for its own benefit and potentially that of other system inhabitants, such as plants. This project aims to gain an understanding of the microbial mechanisms of soil phosphorus (P) solubilization and how those mechanisms can be harnessed and developed into robust plant-soil-microbe associations that deliver P to bioenergy crop plants growing on marginal lands.

Accomplishments

To date we have established a nutrient limitation observatory at the Ecological Staircase in Mendocino Co. Using analytical chemistry and spectroscopic methods we have characterized and quantified the key phosphorus chemical species across this extreme gradient in soil fertility. Available P declined significantly with soil age with aluminum and iron bearing phosphorus minerals becoming more prevalent. NMR spectroscopy identified phytic acid as the primary organic form and μ XRF at the Advanced Light Source demonstrated that hotspots of P in soil were organic. Progress to date strongly suggests a new mechanism of P control in which Fe minerals regulate the availability of organic P. This mechanism, if confirmed, is a novel observation with profound implications for the strategies organisms must employ to access that P. We have identified rhizosphere bacteria that have the physiological traits necessary to solubilize metal-organic-P complexes, have shown that these bacteria are enriched in P limited soils and are working to characterize their mechanisms of P solubilization. We have also developed a multi/hyperspectral imaging approach for real-time monitoring of plant tissue chemistry for early diagnosis of microbially-mediated growth promotion due to nutritional factors.

With new knowledge of metal-organic P forms we are designing new consortia of microbes that first dissolve iron and then hydrolyse phytic acid for plant uptake, combined with complementary microbes that solubilize P from aluminum minerals. These consortia will be tested at the greenhouse scale using model plants (*Arabidopsis* and *Brachypodium*), plus bioenergy feedstocks (*Switchgrass* and *Sorghum*) and a model food crop with a high P demand (*Soy*).

The Soil Metazoan Microbiome: A compartment of importance to soil nutrient cycling

Principal Investigator(s): Javier A. Ceja-Navarro

Project Description

The capacity of a soil to sustain food and fuel production derives from its physical, chemical and biological properties, which facilitate and regulate the availability of nutrients. Studies of the biological processes driving the cycling of soil nutrients have focused principally on free-living and plant-associated microorganisms. This approach has generated substantial strides in our knowledge of soil biology. However, most previous efforts have neglected the role of another important component of soil - its metazoans. Soil living eukaryotic organisms compose around 5% of the soil biomass, with multicellular animals reaching numbers of 500 to 200,000 individuals per square meter of soil, only for the case of arthropods. Hence, soil nutrient cycling models that neglect the role of metazoans are fundamentally incomplete. Furthermore, this highly diverse group of organisms carries an equally diverse collection of commensal microbes.

The main goal of this project is to study of metazoan-associated microorganisms with a focus on arthropods, with the application of a multi-scale approach that will enable the characterization of the contribution of soil metazoans, and their microbiomes to nutrient cycling, and a better understanding of the conditions in which the associated microbiomes are active.

We have studied the diversity of arthropods in the soils of the Ecological Staircase in Mendocino, CA and the composition of their associated microbial communities. For this, developed a strategy for the isolation of DNA from single arthropod specimens (100 microns and higher) in high-throughput mode that allows the extraction of 90 specimens at once. As part of our survey, we also worked on the isolation of plant polymer degrading and nitrogen fixing microbes from selected groups of arthropods that will later by use to test for the association between host and symbiont. Our research has also moved towards the study of functional role of arthropods and other metazoans in soil systems using artificial environmental settings where microbiome dynamics will be followed.

Accomplishments

After optimizing the protocols for DNA extraction in high-throughput we managed to characterize the microbiome of 400 isolated arthropod specimens, an accomplishment that represents the largest survey of host-associated microbial communities. The most abundant groups included Collembolans, Mites, Diplurans, Millipedes, Centipedes, and Termites. We succeeded in identifying their associated Bacterial and Archaeal populations by sequencing the 16S rRNA using the Illumina MiSeq platform. We have gathered a collection of 200 bacterial isolates from 13 different bacterial species. These bacterial isolates have the metabolic machinery to either degrade cellulose and lignin, fix nitrogen, or solubilize phosphorus. This work has been presented at the American Society of Microbiology meeting (ASM) and the ASIMOLAR meeting of microbial physiologist, and has allowed me to mentor 3 students from different Universities, including UC-Berkeley and the University of Puerto Rico.

**Ultra High Resolution Climate Projections
to Support Climate Readiness in the San Francisco Bay Area**

Principal Investigator: Andrew Jones

Project Description

The purpose of this project is to develop the scientific basis for understanding and predicting climate at decision-relevant scales in urban environments. Using the San Francisco Bay Area as a testbed, we will conduct ultra-high resolution climate simulations that examine interactions among existing microclimates, modifications to the built environment, energy and water use, and global climate change. The initial simulations are designed to determine how climate change will affect the risk of extreme heat events and how modifications to the built environment and landscape irrigation could ameliorate or enhance such risks at the neighborhood and regional scales. Urban modifications to be examined include the widespread adoption of white roofs, infrared reflective coatings, rooftop photovoltaics, and diminished water use for landscape irrigation. More broadly, this project will enhance basic scientific understanding of land-atmosphere interactions in urban environments and develop a standing capacity for addressing a range of climate-related urban risks such as flooding due to extreme precipitation, changes in energy and water demands, and changes in air quality.

The model system we will use consists of three components: (A. Meteorological boundary conditions projected for 2050 under business-as-usual scenarios using Earth system models, together with meteorological reanalyses for 2010; (B. The Weather Research and Forecasting Model (WRF), combined with a detailed urban canopy model; (C.. Detailed descriptions of the San Francisco and Bay Area built landscape; and (D. Our hypothetical modifications to the urban infrastructure for adaptation to climate change and likely resulting water shortages. The numerical experiments will focus on both the present day and the year 2050.

Accomplishments

Using satellite observations of land cover, albedo, green vegetation fraction, and sea-surface temperatures, we have successfully adapted our urban climate modeling system to the San Francisco Bay Area and are able to reproduce major features of the present-day Bay Area climate including temporal variations in temperature and evapotranspiration, as well as microclimatic variation across the 9 counties of the Bay Area. We have assembled a spatially and temporally dense database of meteorological observations that we are using to further evaluate the model's representation of fog, sea breeze, the effects of topography, and other local-scale features, which are essential for understanding how microclimates will change in response to global climate change and changes to the built environment. In addition, we have enhanced the model framework to include an urban irrigation module and have validated this module using data from irrigation-only water customers.

Most significantly, we have deployed this modeling framework to understand climatic controls on the demand for irrigation water in urban environments, initially focusing on the recent drought years of 2012-2014. We have shown for the first time that heat mitigation strategies, such as reflective roof coatings known as “cool roofs”, can substantially impact irrigation water demand. We showed that summertime irrigation demand could have been up to 10% lower in the Bay Area during the recent drought with widespread adoption of cool roofs. A manuscript on this has been submitted to *Nature Climate Change*.

**PREDICTING THE MAXIMUM RATE OF CARBOXYLATION BASED ON OPTIMAL LEAF
RESOURCE ALLOCATION**

Principal Investigator: Trevor F. Keenan

Project Description

The purpose of this project is to dramatically increase our ability to understand, from first-principles, the governing drivers of global photosynthesis, and how plants adapt photosynthetic capacity under a changing climate. Photosynthetic traits such as the velocity of carboxylation are known to vary with changes in climate and soil properties. These observed relationships have been included in land surface models through empirical equations. A fundamental mechanistic understanding remains lacking, however, making spatial and temporal extrapolation difficult at best. In addition, the current approach gives little, flawed (through empirical extrapolation), or no consideration for the known acclimation of photosynthesis to changes in growth conditions and climate. Recent advances in the theory of optimal resource allocation, along with technical advances that greatly increase the amount of data available, now provide a path through which to test hypotheses regarding the primary governing controls.

In this project, we propose to use recent theoretical developments to generate testable hypotheses as to the mechanisms governing biotic adaptation of photosynthesis. Ultimately, the project will provide a mechanistic predictive capacity for photosynthesis suitable for incorporation in the next generation of land surface models. This research will thus advance key tools used to quantify and predict long-term ecosystem changes.

Accomplishments

In the first year of this project, which started in March 2016, our efforts have been focused both on theoretical development, testing, and application. Our most significant accomplishment has been the development of a global database of plant trait observations, necessary to test the predictions generated from first-principles. In developing the plant trait database (published in late 2016) we used advanced methods to account for light-dependent trait plasticity through plant canopies, which revealed previously unaccounted for plant trait relationships. The results represent a significant advancement in the field and are currently in press in the journal *Nature Plants*. We envisage that this refined database will be key to enabling the further development and testing of theoretical advances.

We have also succeeded in applying the theoretical development of photosynthesis at global scales to examine changes in global ecosystem function, and implications for the growth rate of atmospheric CO₂. These results, published in *Nature Communications*, show an enhancement of the terrestrial sink and a decline in the fraction of anthropogenic emissions that remain in the atmosphere over the past decade, despite increasing anthropogenic emissions. As we had hoped, our theoretical advances enabled a significantly clearer and more detailed description of recent changes in the land sink.

In addition to the above we have established significant collaborations with leading researchers both in the US and internationally.

Assessing Microbial Functions at Terrestrial-Aquatic Interfaces by Metagenome-Based Metabolic Flux Analysis

Principal Investigator: Tas Baas, Neslihan; co-PI: Garcia Martin, Hector

Project Description

This project aims to define microbial functions and controls on turnover of soil carbon and nutrients at terrestrial to aquatic interfaces. 47-55% of the soil carbon from tropical, arctic or temperate ecosystems is transported into the rivers. Ever growing evidence suggests that microorganisms in these systems degrade terrestrial carbon and result in a significant CO₂ input to the atmosphere. Discretization of the microbial responses resulting in this feedback fills a big gap in our knowledge. Deciphering microbial responses requires differentiating amongst carbon and nutrient use and fluxes through microbial metabolism which cannot be measured directly and comprehensively.

In order to do address this bottleneck this project implements a novel metagenome-based metabolic flux analysis (MFA) approach. Genome-scale models provide the necessary elements to translate sequence information from metagenomes generated from community DNA to a set of possible metabolic reactions on substrate utilization and resulting products (metabolites and fluxes). One of the products of this project is a metagenome based diagnostic tool that can be used to answer challenging wide scoped questions in terrestrial and aquatic carbon cycling. While sequencing of community DNA metagenomics enables access to genes and functions, genomes assembled from metagenomes can be used for genome-scale models of cellular metabolism from which metabolic fluxes can be calculated. This project reflects a striking integration of metagenome data to genome-scale MFA in order to generate a next generation analysis approach and provides new avenues for data integration to larger scale modeling efforts.

Accomplishments

Our accomplishments are in multiple folds. Most significant is the development of protocols for DNA preparation from low biomass aquatic samples for metagenome sequencing. This method uses collection water through three filter sizes which allows us to differentiate micro eukaryotes and microbial communities attached to particulate matter (1.2μ) from benthic microorganism (0.2μ and 0.1μ). Moreover we developed a multi-method DNA extraction strategy that results in high species coverage. Currently with these methods we are analyzing river water and hyporheic samples collected between April and October 2015-2016 from selected East River, CO sites. Via detailed characterization of dissolved organic matter (DOM) chemistry, microbial community dynamics and functional diversity we aim to determine the linkages between DOM inputs, degradation and microbial functions of different organisms.

We have also succeeded in establishing lab-scale incubations in which we can mimic field conditions. To this end, we tested and optimized batch-scale installations that simulate diurnal cycles, mixing conditions and carbon inputs. Additionally, we are currently in process of transferring this knowledge to continuous systems in which we plan to use ¹³C-labeled carbon sources that are analogous to terrestrial DOM inputs characterized from the field. This installation will allow us to track carbon use through microbial communities and generate valuable ¹³C-CO₂ and -protein profiles for constraining fluxes in genome-scale models generated from assembled genomes of the microbial communities.

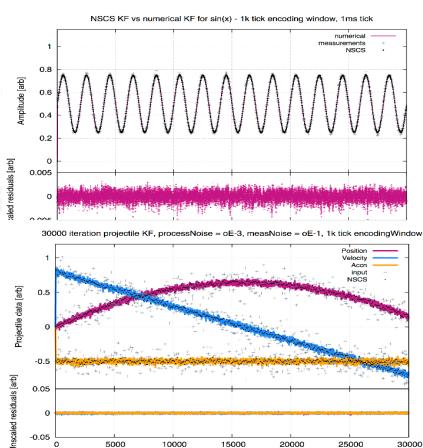
Kalman Filters on TrueNorth

Principal Investigator(s): Paolo Calafiura

Project Description

Neuromorphic computing is a low-power, alternative computing framework suitable to certain problems. Kalman filters are powerful mathematical tools used in a wide array of automation and tracking problems. Our specific goal is to implement Kalman filters in neuromorphic computing platforms for high-throughput, low-power, high-performance computing with continuous outputs. In year 1, we developed implementations of Kalman filters (KF) in spiking neural networks, achieved state-of-the-art decoding of human brain signals using DNNs, and uncovered critical bottlenecks in mapping software networks to IBM TrueNorth (TN) chip[TRN]. In year 2, we will leverage recent advances in deep learning to overcome the discovered bottlenecks, investigate alternative hardware implementations of neural networks using FPGAs, and evaluate both software and hardware implementations of neural networks on two domains: charged particle tracking for high-energy physics (HEP), and prediction of movement from neural signals for brain-machine interfaces (BMI).

Accomplishments



Our most significant accomplishment has been to implement for the first time a multi-dimensional steady-state Kalman Filter algorithm in IBM's TrueNorth neuromorphic architecture. The TrueNorth chip encodes data using spikes, and we implemented both a rate-encoded, serial version of the algorithm, and a rate-and-spatial encoded, parallel version to reduce latency. The algorithm has been successfully applied to track the time evolution of simple simulated physical systems and the performance of the algorithm has been compared to a traditional numeric Kalman Filter, whilst varying a number of parameters, including rate encoding, spatial encoding, sample rate, and the relative ratio of measurement errors and process noise. This allowed us to evaluate the pros and cons of the TrueNorth architecture and its potential in the two science domains we have investigated. We have presented our first year results at the Computing in High Energy Physics conference in Oct 2016.

We have additionally continued to investigate the utility of deep neural networks as an analysis tool for neural data. We have applied deep learning to human data during speech production and achieved state-of-the-art performance for classification tasks. We are preparing this work for publication this year.

Building on this work, in year 2 we will apply our TrueNorth implementation of the Kalman Filter to the interpretation of neurological data from human brain's speech generation area which are being collected at UCSF. We are on track to integrate our TrueNorth Kalman Filter into the clinical neural data acquisition system in the coming months, and hope to apply our system to a neurosurgical patient this summer. Finally, building on our success in speech classification with deep networks, we are working on using TN as classification system to take human brain signals into produced speech sounds. This will also be tested in the clinic over the summer.

Unconstrained Functionals for Massively Parallel Scaling of Conjugate Gradient Eigensolvers

Principal Investigator(s): Andrew Canning

Project Description

A large number of scientific applications require eigensolvers and in particular for applications where some smaller percentage of the eigenpairs are required, rather than the full spectrum, iterative eigensolvers are typically used. The scaling on modern massively parallel multicore computers of these types of iterative eigensolvers is limited by the reorthogonalization step which typically uses direct diagonalization of the subspace matrix, Cholesky or QR decomposition. The dimension of the subspace matrix is typically much smaller than the full matrix which is why operations on the full matrix scale efficiently while operations on the subspace matrix limit the parallel scaling. The main goal of this project is to develop a highly parallel scaling method, based on an unconstrained functional approach, which completely eliminates the reorthogonalization step. We plan to disseminate the results of our studies to the scientific user community of iterative eigensolvers as well as develop an open source library routine based on the best methods that can be used by the numerous application codes that require iterative eigensolvers. This will allow the scientific community to better exploit existing massively parallel multicore computers as well as future exascale machines. In particular this will greatly benefit the materials science and chemistry community, the majority of whose codes and computer runs use iterative eigensolvers.

Accomplishments

In addition to previously implementing the unconstrained method in the PARATEC materials science code the method was also implemented in the widely used publicly available materials/chemistry codes Quantum Expresso (QE) and we improved the implementation in the CP2K code so that we would also have an evaluation of the code for materials/chemistry codes that use a Gaussian basis. The main issue with the implementation in the CP2K code was that the preconditioner used in the code for the more standard methods already implemented in the code did not work well for the new unconstrained functional. This was not the case for the plane wave codes such as PARATEC and QE where the previous preconditioners work well for the new functional. Therefore a significant effort in the last year was the development of new preconditioners for the Gaussian basis set implementation in CP2K. We found a new preconditioner based on approximate form of the Hessian matrix gave good convergence for the new functional at a much lower cost than construction of the true Hessian matrix. Using the new preconditioner we have performed parallel scaling studies up to large core counts to compare the scaling to previously used methods. We find that our new method significantly outperforms previous methods in terms of parallel scaling to large core counts.

We will release our method as a library as well as put it into other widely used open source materials science and chemistry codes such as CP2K to benefit the materials and chemistry research communities.

ExaGrid: Large-Scale, Asynchronous Co-Simulation of Advanced Electric Grid Systems

Principal Investigator: Cy Chan

Project Description

Energy researchers require fast, efficient co-simulation platforms to study the interactions of the complex large-scale, distributed systems integrated in future smart grids. Current simulation tools focus on different aspects of smart grids without capturing the global picture. Our project examines the feasibility and techniques required to extend this capability to model areas as large as California and even the USA. To simulate such areas, there are thousands of nodes for the power system simulation, and millions of component controllers interconnected through communication systems. Current tools were not designed to achieve the scale of simulation that researchers will require to study the dynamic behaviors and advanced control strategies of the future electric grid.

Our project goal is to design and prototype a parallel simulation platform to evaluate hypothetical scenarios on large, integrated smart power grids, including advanced controllers, demand response, and high penetration of distributed generation resources. We are also exploring the simulation algorithms and system design to determine requirements for achieving scalability of the platform on current and future HPC systems. To do so we are leveraging our asynchronous execution modeling tools to extend the Virtual Grid Integration Laboratory (VirGIL), a non-HPC modular co-simulation platform. ExaGrid is building upon VirGIL to explore how using high performance computing systems and methods can accelerate the simulation and run experiments for much larger electrical systems.

Accomplishments

Through several consultations with members of LBNL's Energy Technologies Area, we have established a modular prototype design for the ExaGrid platform and are implementing it to satisfy the requirements of co-simulation of a large number of components (e.g. smart loads, generation, and storage) connected to a common power grid. Our modeling platform will leverage existing power component models, such as the Modelica building, battery storage, and electric vehicle models through the use of the Functional Mockup Interface (FMI). We have also investigated several techniques to parallelize and scale the power grid and network models.

We have identified solutions to two key challenges to enable parallel simulation of the power grid. One key challenge is the efficient simulation of systems of differential equations in a multi-scale environment. Our approach is to utilize a quantized-state system (QSS) technique to discretize the state space instead of simulation time to allow processes with different time scales to progress efficiently. The other key challenge is the coordination of time events across model components distributed across multiple compute nodes. We are employing parallel discrete event simulation (PDES) to allow components on different compute nodes to step forward in time asynchronously. We are leveraging our prior experience with execution modeling and studying the parallelism and asynchrony inherent in the power system models of interest.

We have implemented a parallel shared-memory power flow solver to handle local grid partitions and are extending it to handle the power flow problem across distributed memory. Furthermore, we are exploring how to efficiently partition and assign the smart grid components to processors on the machine in a way that reduces data movement costs, and thus simulation time, and examining whether advanced mapping strategies can provide the capability to adapt to dynamic load imbalance.

Exploiting Physics-Based Concurrency in Time-Dependent Extreme-Scale Multiphysics Simulations

Principal Investigator(s): Marcus Day

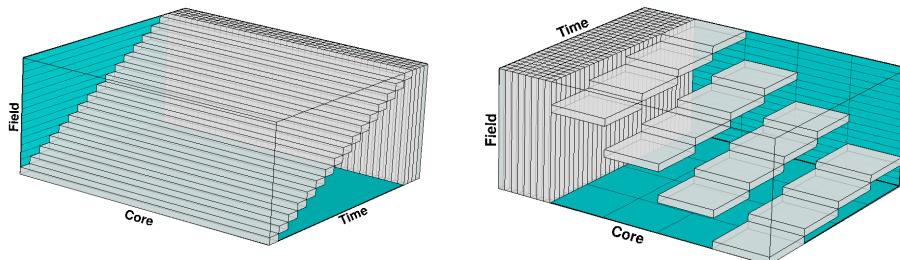
Project Description

Extreme-scale time-dependent multiphysics simulations of PDE-based systems will need to exploit an unprecedented level of algorithmic concurrency in order to make effective use of leading edge high performance computing hardware. A common approach to addressing this challenge involves streamlining and parallelizing the individual component kernels that comprise a large coupled solver in order that *each* scale effectively across the entire machine. We propose a novel alternative: **a global time stepping strategy for multiphysics applications that intertwines the simultaneous evaluation of constituent kernels having disparate, but complementary, computing resource requirements**. The key mathematical challenge is to develop an algorithm that performs robustly, independent of the order in which the component kernels are evaluated.

Asynchronous Spectral Deferred Corrections (ASDC) is based on a novel extension spectral deferred corrections. ASDC constructs highly accurate solutions via an iterative sequence of time step corrections that based on low-order incremental updates. For multiphysics applications this iteration can be used to orchestrate a lagged sequential coupling of the computational kernels which themselves can be implemented across a dramatically reduced pool of compute cores. There will, of course, be a tradeoff: increased the concurrency of the overall simulation vs. degradation of algorithm performance in terms of iteration count. However, there are important cases where this approach allows a net gain in efficiency - particularly if some of the kernels are communication bound, while others in the calculation require no communication (as is the case for many reacting flow systems - see figure below). The ASDC strategy can be applied to a wide range of multiphysics applications, from turbulent combustion to porous media flows.

Accomplishments

The basic methodology was first implemented on a representative model system and verified to be feasible (robust, simply implementable), in the context of a complex one-dimensional low Mach number combustion application. The strategy is now being reimplemented at scale for multidimensional, time-dependent reacting flow systems, where the constituent kernels include multigrid-based variable-coefficient Poisson solvers, and point-wise ODE integrators for reaction kinetics, all coupled to a hyperbolic integrator on many (tens of thousands) compute cores. The implementation is such that the iterative asynchronous time integration scheme can serve as drop-in replacements for the standard integrators in these applications.



Schematic of multiphysics timestep Left depicts bulk-sequential evaluation of disparate kernels during a timestep. At right, asynchronous kernel evaluations can be distributed across the machine with dramatically reduced communication requirements.

Design of Quantum Chemistry Simulations for Superconducting Circuits

Principal Investigator(s): Wibe Albert de Jong, Jarrod McClean

Project Description

The purpose of this project is to design and demonstrate quantum simulations of quantum chemistry problems using superconducting circuit simulation systems developed at Berkeley. Quantum simulations on quantum computers have the potential to revolutionize the field of computational chemistry and physics.

We will design quantum simulations to compute the energy spectrum for a small diatomic molecule analogous to earlier work by Lanyon and coworkers. We will pursue spectroscopy and electron dynamics of a diatomic system consisting of two different elements and more than one electron, which will require a different setup of the Hamiltonian and experiment. We propose to design a quantum simulation representing the chemical reaction dynamics of a one-dimensional proton shuttle or electron transfer process in a large biomolecule, akin to the work of Lu and coworkers.

This project will be a close partnership with the integrated experiment/theory quantum system LDRD of the groups of Siddiqi and Whaley from the Materials Science Division/UC Berkeley who have been focusing on building, controlling and analyzing the capabilities of the superconducting qubit circuit technology. This partnership has the potential to establish LBNL at the forefront of quantum computing from hardware to simulation.

Accomplishments

During 2016 the project has made great progress on both the theoretical development efforts and collaborating with experimental sides of quantum computing efforts to develop software and algorithms for quantum chemistry on superconducting qubits. First, a new theory work was published in collaboration with the Aspuru-Guzik group at Harvard to better quantify the capabilities of hybrid quantum-classical algorithms in quantum simulation, including new techniques which led to cost reductions of up to an order of magnitude. Building on these advances in collaboration with Google's Quantum AI group and the Aspuru-Guzik group at Harvard, an experimental demonstration in superconducting qubits was performed comparing a 3-qubit quantum phase estimation with a 2-qubit variational quantum eigensolver, meeting one of our year 1 objectives.

Additionally, an entirely new theoretical method was developed to extend the capabilities of hybrid quantum-classical variational methods to excited state energies and properties. Interestingly, this method was also found to correct decoherence based errors without the use of formal error correction, which yielded a novel error suppression method for more general computations. This work is available as a pre-print and currently submitted for publication. A new experiment to demonstrate this technique in a real system is nearing completion in collaboration with the Sidiqqi group in the Materials Science Division/UC Berkeley. This will yield the first scalable demonstration of molecular excited states and the new error suppression technique on a quantum device.

An open-source Python based fermion simulation package, FermiLib, is being developed in collaboration with Ryan Babbush at Google and Damian Steiger at ETH Zurich of the ProjectQ Team. The goal of this package is to eliminate the need for expert domain knowledge to engage in quantum algorithms research in chemistry and related fields. The goal is to release it under an open source license, and eventually package it with the ProjectQ software framework.

Modeling the Earth's Hydrological Cycle from Watershed to Global Scales

Principal Investigator(s): Hans Johansen, William D. Collins

Project Description

This project built a state-of-the-art prototype model of land-atmosphere hydrological cycle at ultra-high resolutions. Our hypothesis is that current models cannot accurately predict water resource availability, due to under-resolved simulation of precipitation events (such as cloud systems) interacting with orography (terrain), and leading to under-resolved hydrological predictions. The overall goal was to create a prototype capable of highly accurate short-term simulations of the hydrological system, driven from global climate scales, but validated against high-resolution data sets and regional observations. A National Academy report [*A National Strategy for Advancing Climate Modeling*, 2012, p. 89-91] has called for research toward this valuable capability, which is needed by federal and state agencies to answer science-driven policy and infrastructure questions.

Our approach for creating the prototype was to: (1) integrate software for state-of-the-art climate and hydrological simulation capabilities that capture the effects of high-resolution precipitation events; (2) generate ensembles of ultra-high resolution simulations on next-generation NERSC architectures; and (3) establish bounds on model uncertainties when compared with observational data. The mathematical research component of this project includes developing novel reduced-order models for the atmospheric-hydrological coupling. Typical regional atmosphere models under-resolve orography, so we will leverage our high-resolution simulations to create watershed-level hydrological modeling capabilities.

Accomplishments

Our most significant accomplishment has been in generating high-resolution, regionally-refined simulation results and comparing them to observable hydrological outputs. This is the foundation of being able to generate reduced-order models that can be used in watershed-level simulations.

Large-scale CESM simulations using regionally-refined meshes were completed on NERSC's Cori supercomputer. The "variable resolution" (VR) meshes that were used have finest resolution of 3.5km over areas important for hydrological simulation of California watersheds. The VR mesh workflow smoothes rough digital elevation model (DEM) orographic data to be compatible with CESM atmosphere models; initial simulations show that the orographic smoothing is both needed, for stability, and potentially detrimental to high-resolution simulations. Observational data comparisons (PRISM, MODIS) for seasonal averages have shown that results are severely resolution-dependent, and that the coupling of physics and dynamics transport can greatly affect leeward/windward precipitation and snow. The results of this analysis are being prepared for submission to a peer-reviewed journal.

In addition, we have begun comparison runs of a regional weather model to investigate the mountain hydro-climate and evaluate the source of precipitation and snow biases in VR-CESM. These simulations were integrated with watershed-level hydrological models to study the hydrologic processes in Sierra Nevada and California.

Fast numerical methods for Green's function in mesoscale simulation
 Principal Investigator(s): Lin Lin

Project Description

The purpose of this project is to develop a general methodology for coupling quantum physics and classical physics for multiscale systems, without introducing system dependent parameters, in the framework of Kohn-Sham density functional theory. We obtain various physical quantities such as energy, electron density and forces, by setting up an appropriate boundary condition at the quantum-classical interface. Our goal is to develop new numerical methods that can be used to treat large scale *ab initio* calculations for open systems with non-trivial boundary conditions, such as dislocations in materials, and further for systems at the mesoscopic level.

We develop Dirichlet-to-Neumann (DtN) map type techniques for formulating the boundary condition of Kohn-Sham density functional theory for an open system. The DtN map avoids the ill-defined problem of finding boundary conditions for individual eigenpairs of an eigenvalue problem, and consistently provide boundary conditions for the density matrix via a number of Green's functions. We can further capitalize the pole expansion and the selected inversion (PEXSI) method for efficiently solving the discrete linear systems with the non-Hermitian boundary conditions due to the DtN map.

Accomplishments

Our most significant accomplishment has been to develop the PEXSI-Sigma formulation for quantum-classical interface fully at the numerical linear algebra level. We demonstrate that consistent boundary conditions can be formulated using an auxiliary Green's function corresponding to a physical configuration. This formulation is particularly attractive for 2D and 3D systems, and can reduces the computational complexity to at most quadratic, thanks to its interface with the pole expansion and selected inversion method (PEXSI). Our preliminary result implemented in DFTB+ package has demonstrated promising results for systems such as dislocation dipoles in graphene sheets.

The decay property is a powerful tool for designing efficient numerical methods in science and engineering applications. In quantum physics literature, the exponential decay property of Green's functions and related physical quantities is referred to as the “near-sightedness principle” of electronic matters. We have studied decay properties of discretized Green's functions for indefinite Schrodinger type operators. We obtained sharp decay estimate for discretized Green's functions for the first time, in the sense that the asymptotic decay rate is independent of the domain size and of the discretization parameter.

The Fock exchange operator plays a central role in modern quantum chemistry. The large computational cost associated with the Fock exchange operator hinders Hartree-Fock calculations and Kohn-Sham density functional theory calculations with hybrid exchange-correlation functionals, even for systems consisting of hundreds of atoms. We developed the adaptively compressed exchange operator (ACE) formulation, which greatly reduces the computational cost associated with the Fock exchange operator without loss of accuracy. The ACE formulation offers orders of magnitude speedup for Hartree-Fock-like calculations. The method has been quickly adopted by the electronic structure community, and is now publicly available in the widely used Quantum ESPRESSO package.

Project Title Solving Problems in Materials Theory via Quantum Networks
Principal Investigator(s): Joel Moore

Project Description

This project concentrates on theoretical analysis of problems in quantum dynamics that are motivated by experiments on solid-state materials and atomic systems. Another goal of the project is to connect real-world problems to simulation by quantum networks of a few qubits, as created with superconducting devices, or by analog quantum emulators made from atoms. Specific examples to be studied were quantum dynamical processes ranging from transport of charge and energy in one spatial dimension, through non-abelian Berry phases in superconducting qubits, to optically generated dynamics in solids, and also questions about how the level of coherence in a set of qubits is degraded by the environment.

Accomplishments

The PI and postdoc Romain Vasseur completed a comprehensive paper (#1) combining and extending past results on several problems in quantum dynamics of one-dimensional systems, combining analytical and numerical approaches. One-dimensional systems are important in the development of quantum networks because they are the only systems whose quantum dynamics can be convergently calculated beyond the problem size accessible by exact diagonalization. The review covered both problems with disorder, such as the many-body localization transition that is a subject of active study, and far-from-equilibrium transport problems without disorder.

A problem more specifically motivated by solid-state experiments was to determine the limits on the "Floquet" description of topological surface states observed in an important recent experiment by the Gedik group at MIT (Science, 2013). The perfect separation between surface states and bulk states in topological insulators becomes only approximate under the time-dependent conditions of an optical pulse, and mixing between the two implies a limit on which pump pulse shapes can be described well by the Floquet picture. The first author on this paper, Michael Kolodrubetz, was supported by the LDRD. The dynamics of topological phases is an active topic beyond this specific problem, and the PI and postdocs (including one supported by the LDRD) studied "pumping" dynamics in Weyl semimetals (publication #4).

The postdoc primarily supported by the grant (Kolodrubetz) wrote a single-author paper, published in Physical Review Letters (#5), on how to use a few-qubit quantum emulator to create the same non-Abelian Berry phases that were previously studied by the PI in condensed matter contexts. Work continues in this direction to find interesting phenomena that can be created with existing systems of a few qubits and serve as benchmarks as the size of quantum networks increases.

Optimal Design for Computationally Expensive Black-Box Applications

Principal Investigator: Juliane Mueller

Project Description

The optimization of problems that involve computationally expensive black-box simulations for computing objective function values requires efficient algorithms that are able to find (near) optimal solutions within a very limited number of function evaluations. Derivatives are generally not available and automatic differentiation is often not applicable. Our goal is to develop algorithms that use surrogate model approximations of the expensive functions in order to guide the search for the optimum. In particular, we propose to develop new algorithms that are able to address problems for which the evaluation of the simulation model may fail (“hidden constraints”, missing function values). Secondly, our goal is to develop a surrogate model optimization algorithm for problems with multiple conflicting objectives.

We develop derivative-free optimization algorithms that reduce the computational expense in order to find (near) optimal solutions. We use computationally cheap surrogate models to approximate the objective function and to guide the search for the optimum. When facing “hidden constraints”, objective function values are missing and we cannot update our surrogate model. We develop an evaluability function to predict if a variable vector will be evaluable. We exploit this information to decide where to do the next expensive simulation. For multi-objective problems, we are looking for so-called trade-off (Pareto optimal) solutions. We fit a surrogate model to each objective function and we combine global and local search methods to explore the whole parameter domain and to zoom in on regions where good trade-offs have already been detected.

Accomplishments - Algorithm for Hidden Constraints Optimization

Hidden constraints arise when function evaluations fail, e.g., an underlying solver does not converge. We define an evaluability function (value 1 if a function value was obtained, 0 otherwise). We fit a piecewise linear approximation function to this evaluability function. Then, we use a surrogate model for the expensive simulation objective function to suggest promising new sample points. We combine the information from the objective function's surrogate model and the piecewise linear approximation of the evaluability function to decide where to do the next expensive evaluation. We developed a large set of benchmark problems for which we tested the algorithm. Finally, we successfully applied our algorithm to an application problem arising in combustion modeling.

Accomplishments - Algorithm for Multi-objective Optimization

We successfully developed a new multi-objective derivative-free surrogate model algorithm. We developed completely new sampling strategies that combine local and global search methods. We showed the efficiency and effectiveness of our algorithm on a large set of test problems and on applications arising in structural optimization and airfoil design. We considered problems with 1-35 decision variables and 2-10 objective functions, which are much larger problems than have been previously addressed. Our algorithm outperforms widely-used evolutionary methods with respect to the goodness of the solutions and the number of evaluations needed to find the solutions.

EXDAC – EXtreme Data Analysis for Cosmology

Peter Nugent

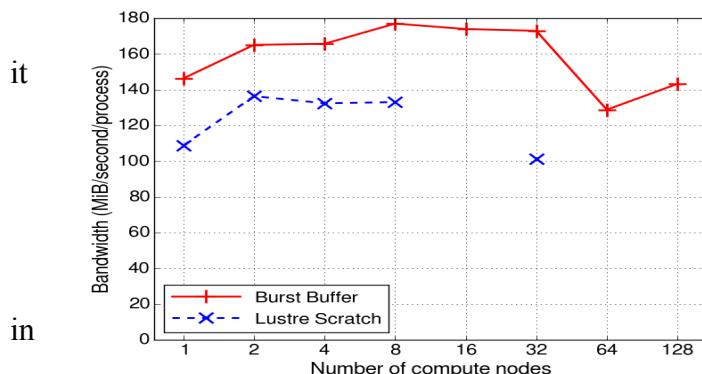
Project Description

In recent years astrophysics has undergone a renaissance, transforming from a data-starved to a data-driven science. A new generation of experiments — including Planck, BOSS, DES, DESI, Euclid, WFIRST and LSST — will gather massive data sets that will provide more than an order of magnitude improvement in our understanding of cosmology and the evolution of the universe. Their analysis requires leading-edge high performance computing resources and novel techniques to handle the multiple PB's of data generated throughout these surveys. Furthermore, interpreting these observations is impossible without a modeling and simulation effort that will generate orders of magnitude more "simulation" data — used to directly understand and constrain systematic uncertainties in these experiments and to determine the covariance matrix of the data.

The goal of this LDRD is to prepare for performing such analyses on the next generation of HPC data-focused resources and to generate feedback to HPC resource providers to enable their resources to be configured optimally for such analyses. In particular we will explore how best to leverage the value of BurstBuffer technologies on the NERSC Cori system by tying ourselves directly into the software NRE effort. DESI and LSST will come to fruition in the 2020 time frame. Thus we are at that critical juncture in time in which we have the ability to influence both the scope and scale of future analysis efforts — something that can directly lead to a greater scientific impact for these experiments. Our ultimate goal is to make the scientific case for the Extreme Data Science Facility for Cosmic Frontier research in High Energy Physics.

Accomplishments

Our most significant accomplishment this past year was to leverage our previous year's interface with the NERSC-Cori NRE effort and apply what we learned to Cori Phase I as that system came online. We carried out this research on two major efforts. The first was a Nyx simulation using the BurstBuffer to handle our I/O as well as our checkpoint restarts. The second was a processing run of the DESI *Tractor* code on the DECaLS data (<http://legacysurvey.org>). These results were presented at CHEP 2016 by Wahid Bhimji and showed how BurstBuffer is a highly relevant technology for HEP workflows. Both showed very nice performance on the BurstBuffer with the Tractor application runs maintaining over 120 MB/s I/O speeds through



it
in

128 compute nodes (see figure on left). Nyx had similar performance metrics. DESI will now use this as moves to Cori Phase II for their DR5 data release in July 2017. These efforts led to the creation of the Center of Computational Excellence (tri-lab effort in HEP computing) as well as formed a major segment of our ECP program cosmology.

Simulating Excited State Energies and Dynamics with Superconducting Qubits

Principal Investigators: Irfan Siddiqi and Birgitta Whaley

Project Description

The calculation of molecular properties from first-principles is a classically intractable problem due to the exponential scaling in computation cost with both the number of atoms and basis set size. For these reasons quantum simulations have been the subject of increasing study both theoretically and experimentally, with efforts to develop various approximate approaches that trade off reduced simulation accuracy for a lower burden of computational complexity. We will develop an experimental platform based upon a new hybrid approach known as the Variational Quantum Eigensolver (VQE) which makes efficient use of both quantum and classical computational resources to store and process data. Initially we plan to apply small scale superconducting qubit based simulators to model various known problems in quantum chemistry as a proof of concept of both experimental and theoretical techniques. Once completed we hope to scale the system to larger numbers of qubits allowing us to explore the application of this computing paradigm to cutting-edge problems in the field.

We also began developing a new platform for quantum simulation, in which ultracold, ground-state, polar molecules are used as quantum bits, held in an optical lattice potential, interacting via electric dipole interactions, and imaged at the single molecule level. This molecular quantum gas microscope will utilize LiRb molecules that are produced by coherent photoassocation from ultracold atomic gases of Li and Rb.

Accomplishments

Current work has focused on the simulation of the molecular orbitals of Hydrogen (H_2) using a 3D Circuit Quantum Electro-Dynamics (CQED) approach. Using this architecture we have successfully implemented the VQE using a two superconducting qubit system. We have used this quantum simulator to extract both the ground and, for the first time, excited states of the H_2 molecule. In addition, we have made significant progress characterizing the robustness of this algorithm to various noise channels as well as finding optimal ways in which to leverage classical resources. Progress has been made in designing, simulating and fabricating 2D coplanar qubit architectures that will allow scaling this algorithm to larger quantum system sizes. Prototype 10 qubit devices have been fabricated and measured which demonstrate coherence times sufficient to implement large scale VQE for processes such as ozone dissociation.¹

We have shown that our deterministic quantum feedback approach to joint measurement-based generation of pairwise entanglement of remote superconducting qubits is globally optimal, derived a generic upper bound on the rate of entanglement generation, and showed that a full-parity feedback protocol saturates this bound and is thus optimal among all measurement-based entanglement schemes.² We have made progress in design of implementation of a quantum circuit representing the MERA ansatz within the VQE framework, with the first goal of performing a proof-of-principle calculation of the ground state of an eighty-one spin Heisenberg chain. We have determined the difference between classical and quantum evaluations in 2- and 3-D lattice problems,³ and are now working on compilation software for implementation of a Solovay-Kitaev algorithm for quantum gates with guaranteed precision.

For the LiRb molecular quantum gas microscope, we have produced overlapped laser cooled gases of Li and Rb atoms. We implemented the newly proposed D1 dark-state laser cooling method to reduce the laser-cooled Li gas temperature (in 3D) to 40 microkelvin.

Open Framework for High-Performance Streaming Analytics

Principal Investigator(s): John Wu

Project Description

To realize the grand visions such as Smart Grid, Smart City, Smart Building and so on, we have to gather and analyze massive amounts of information, identify key signals in the data, and automatically respond to them appropriately. In this process, a large number of sensors produce constant streams of data that need to be integrated and organized before sophisticated pattern detection and discovery algorithms could be applied. This LDRD project is to develop a few key techniques for integrating these streams. The initial task will be focused on data reduction and local feature extraction. Ultimately, we foresee this project to establish a core set of techniques for a high-performance stream analysis engine that would ingest streaming sensor data from a variety of sensors, fuse data streams to form coherent sources of information, identify important events specified by users, and deliver the resulting signals according to common industrial standards. We plan to demonstrate the effectiveness of these algorithms on a set of microPMU data collected from LBNL's own electric power supply lines. This would serve as the basis of additional applications on Smart Grid, Smart City, Smart Building, and other environments that require real-time data analysis and control.

Accomplishments

In the past year, we have designed and implemented a novel data reduction technique named IDEALEM based on statistical similarity. The key feature that distinguishes this method is that it permits data blocks to be compared without regard to the relative positions of the values in incoming data. It represents similar blocks with a one that appeared earlier in the stream. Instead of measuring the similarity of two blocks based on traditional measures such as the Euclidian distance, we use a statistical tool known as Kolmogorov-Smirnov test (KS test). Through a careful design of the compression algorithm, we are able to keep distinctive features in a dataset, while significantly reducing the size needed to keep common and uninteresting data records. On data sets from power grid and brain wave measurement, IDEALEM can compress many of the variables by more than 100-fold, while capturing important features at the same time. This clearly demonstrates the usefulness of our new compression method [1, 2].

We have also worked on analysis techniques for streaming data [3, 4]. To understand the impact of a new pricing structure on the residential electricity demand, we need a baseline model that captures every factor other than the new price. The gold standard baseline is a randomized control group, however, a good control group is hard to design, and could only serve as a baseline for a group, not any individual household. To overcome these shortcomings, we developed a number of techniques that could predict the hourly usage years ahead. In particular, we developed a continuous prediction strategy that first forecasts lagged variables and then used them in further predictions, but we found that the prediction error increases over time. Based on an observed linear relationship between temperature and aggregate power (LTAP), we designed a new prediction method named LTAP that avoids this accumulation of prediction errors when forecasting usage of each household. In our tests, the average predicted usages by LTAP match the control group for all two summers the test data covered. The LTAP baseline also appears to be an effective way to address the self-selection bias in treatment groups in human subject studies[3].

Neuromorphic Image Analysis and Pattern Recognition

Principal Investigator(s): Chao Yang (CRD)

Other investigators: Karen Davies (MBIB), Alex Hexemer (ALS), Thorsten Kurth (NERSC), Xiaoye Li (CRD), Peter Nugent (CRD, NERSC), Dilworth Parkinson (ALS), Nicholas Sauter (MBIB), Daniela Ushizima (CRD, NERSC, BIDS), Singanallur Venkatakrishnan (ALS)

Project Description

The purpose of this project is to reformulate a number of image analysis and pattern recognition problems arising in DOE science applications as neuromorphic computing problems. In particular, we propose to use properly trained convolutional neural networks (CNNs) to solve a number image classification and feature extraction problems in the areas of structural biology, materials science and cosmology. We investigate the construction and architecture optimization of these CNNs and the feasibility of deploying these CNNs on new energy efficient computer architectures that are designed specifically to mimic this type of neural network. An example of such new computer architecture is the IBM's TrueNorth neurosynaptic system. We examine the effect of different depths for CNN architectures as well as the low precision arithmetic on the reliability of a CNN.

Accomplishments

We collected and prepared labeled data from diverse modalities: cryo-electron microscopy (cryoEM), X-ray diffraction, X-ray microCT of materials, and sky surveys for supernova identification. We produced simulated data for cryoEM and grazing incidence small angle X-ray scattering (GISAXS) image classification. We began to analyze micro-CT slices for composite materials to extract desirable features to be classified. A number of software tools (MatConvNet, CAFFE, TensorFlow etc.) were used to configure and train CNNs for both binary classification problems (X-ray diffraction and SuperNova images) and multi-class classification (CryoEM and GISAXS). Training was performed on CPUs and GPUs. We deployed one CNN to the IBM TrueNorth chip successfully.

For simulated cryoEM images, we were able to successfully classify up to 84 2D projection views using a moderate sized CNN. For simulated GISAXS images, we successfully classified 7 different crystal lattice types using a 3-layer CNN with accuracy ranging from 83% to 93% depending on the noise level, and choice of various parameters. We used a 2 layer CNN with fully connected layer and softmax classifier in the topmost layer to identify the presence of supernova in sky survey images and achieved 94-95% success rate. For X-ray crystallography image data, we were able to identify images with clear Bragg spots by using a two-layer CNN in 92% of the cases.

We experimented with lowering the precision of the CNN input and CNN weights *via* quantization and found that, for CryoEM projection view classification, a high success rate can be achieved even when the input image and CNN weights were quantized to 3 bits. This result was presented as a poster at the 2016 Supercomputing conference as part of a ACM Student competition.

In the second year, we will increase both the volume and complexity of the training / testing data for previously designed CNNs to account for different imaging conditions, detector types, noise sources, and image characteristics. We will also try to understand the constraints and limitations imposed by the current generation of neuromorphic chips and to seek ways to alter the CNN design to accommodate these constraints.

IDEA—The International Database of Efficient Appliances: A New Tool for Optimizing Energy Efficiency Policy
Principal Investigator: Brian Gerke

Project Description

The purpose of this project is to build the International Database of Efficient Appliances (IDEA), a flexible database for storing market and energy-performance data for a wide variety of appliances, electronics, and other consumer products sold worldwide. At present, the data required to understand the global impacts of national energy efficiency (EE) policies are almost hopelessly fragmented and disjoint. IDEA combines data from disparate sources, such as retailers, manufacturers, and government efficiency certification databases, to produce a unified record for each product. Retail data can be collected on a regular cadence to allow tracking of product price and availability in real time. These features make IDEA a powerful tool for policy development and evaluation. The LDRD project will complete a pilot research project comparing EE policy impacts across markets, and IDEA's data-collection capacity will rapidly enable new research projects beyond the LDRD scope. The IDEA framework is sufficiently flexible that it need not be limited to appliances. In the longer term, IDEA will evolve into IDEE—the International Database of Equipment Efficiency—encompassing vehicles, building components, solar equipment, and other products, in addition to appliances and electronics.

IDEA is the first full-scale implementation of a conceptual database framework that the PI helped to develop in 2013. The work in this LDRD program builds on a partial, US-only implementation of the framework that the PI has developed in support of DOE's Appliance Standards program. IDEA is developed in the Python language, under the Django web framework, which enables a flexible approach to database design and easy implementation of a web interface.

Accomplishments

In this year we have made upgrades to the IDEA prototype we constructed in the first year of the LDRD, to yield a fully functional production version of the database that can produce analysis-ready data to support a variety of specific projects. Data collection has now occurred in China, India, Indonesia, South Africa, Mexico, the United States, Canada, Saudi Arabia, and Indonesia. IDEA has incorporated data from a wide variety of sources, including retail and manufacturer websites, online and privately shared government certification databases, and even market research data on products available for sale in physical stores in Indonesia. IDEA data collected in Indonesia are being used to inform the evaluation and development of energy efficiency standards, under the auspices of the Super-Efficient Appliance Deployment (SEAD) initiative of the Clean Energy Ministerial.

We have also developed new analytical methods to use IDEA data for analysis of the costs and benefits of energy efficiency upgrades, in a manner that allows for comparison of cost-effectiveness across different appliance categories and across different markets. By making use of statistical tools including multilinear regression and modern machine-learning techniques, we can account for the effect on appliance price of features other than energy efficiency, allowing the price impacts of efficiency to be revealed and compared directly to the energy savings they can yield. Some of these techniques were presented at the 2016 Summer Study conference hosted by the American Council for an Energy Efficient Economy (ACEEE). The machine-learning approach holds promise as a semi-automated and unbiased approach to cost-benefit analysis that can be applied across a wide range of appliances and markets.

Transportation System Science for Energy Savings

Principal Investigator(s): Anand R. Gopal, Alexandre Bayen

Project Description

Passenger transportation is responsible for 25% of US greenhouse gas emissions. Current use-phase energy consumption patterns in the transportation system are very inefficient. Nominal vehicle occupancy is less than 25% of capacity and the mode share is dominated by inefficient road transport. New scientific modeling techniques and network optimization methods are necessary to achieve long-term behavioral and technological shifts toward an energy efficient transportation system. To meet this need, this project aims to develop an urban-scale, agent-based microsimulation transportation system model with millions of agents.

The agent-based model, named *Behavior, Energy, Autonomy, Mobility Model (BEAM)*, will model the behavior of individual travelers and the effect of their short and medium term choices on the transportation system as a whole. Initially, the model will be developed to simulate choices and trips of all travelers in the nine-county San Francisco Bay Area. To achieve such ambitious scale and resolution, BEAM will be the first transportation system model to be implemented entirely in a high-performance computing environment. The goal of developing BEAM is to identify opportunities for behaviorally-aware incentives and policies to substantially improve transportation system energy efficiency. The model will also be able to look at scenarios that can assess the impacts of various new technologies in the transportation system, like vehicle connectivity and automation, electric vehicles and app-based ridesharing. The project team estimates that transportation energy use could be reduced by as much as 50% if aggressive use-phase efficiency measures are implemented.

Accomplishments

First, we developed the overall architecture of the BEAM model. Next, we began implementation by focusing on building and calibrating baseline system mobility for the Bay area. We then implemented the plug-in electric vehicle module. Each of these steps are explained below. The BEAM model architecture is massively parallel and modular. Code performance and efficiency are critical and the entire model will be implemented on either NERSC or a cloud-based HPC system. Ultimately, the goal is to implement BEAM in cities all around the country in order to maximize transportation system energy efficiency.

Travel behavior and transportation system simulation for the Bay area was developed, calibrated and validated from numerous data sources. Personal vehicle trips were modeled with data from surveys implemented by the state of California and by the Metropolitan Transportation Commission (MTC) and were supplemented with cellular tower call detail records. The transit trip module is under development based on data streams from BART as well as MTC. The road and rail network details were developed using OpenStreetMap.

A module that simulates plug-in electric vehicle (PEV) trips was developed, calibrated and validated. The module also included optimal siting of PEV charging infrastructure in order to service charging demand at lowest cost. We published a paper in the IEEE Transaction on Transportation Electrification on the infrastructure siting model. Spatially explicit PEV adoption was derived from SERA, a vehicle stock turnover model developed by NREL. The PEV trips and charging were calibrated and validated using data on public charging sessions from a variety of EVSE service providers. PEV travel and charging behavior were modeled at the level of individual drivers.

Behavior Analytics
 PI: Annika Todd, Co-PI: C. Anna Spurlock

Project Description

The purpose of our projects is to conduct research in the emerging space of data science that interfaces with human behavior, or what we are calling “behavior analytics.” Our goal is to develop techniques to enable energy policy makers and other industry stakeholders to make evidence-based and data-driven decisions.

We are working towards the completion of several flagship projects, described in more detail below, to be completed with the LDRD funding. These projects involve diving deeply into highly disaggregated smart meter data to gain insights about the nature of household energy consumption behavior, and to understand the nature of energy-use heterogeneity across households. These insights will help program administrators and contractors implement more cost-efficient programs, inform policy makers on how to quickly and successfully achieve energy reduction goals, help industry leaders develop new techniques, and increase utility customer satisfaction. These projects are being done using currently available data consisting of hourly energy use observations for hundreds of thousands of households spanning three years. Within the period during which these data were collected, time-based rate programs were implemented. Importantly, these programs were designed as randomized control trials, something that is very rare in the program pilot space, and is the gold standard for causal inference of program impacts.

Accomplishments

Our primary accomplishments include several publications/conference papers. Along with collaborators in the Computational Research Division at LBNL, we have completed a paper entitled “Extracting Baseline Electricity Usage Using Gradient Tree Boosting.” This paper was presented at IEEE’s 2015 International Conference on Big Data Intelligence and Computing (DataCom 2015), and was published through the conference proceedings. This paper won the Best Paper Award for DataCom 2015. In addition, following this line of identifying improved baseline methods, we completed a paper entitled “Predicting Baseline for Analysis of Electricity Pricing” which is forthcoming in the International Journal of Big Data Intelligence. Finally, our paper “Comparison of Clustering Techniques for Residential Energy Behavior using Smart Meter Data” has been accepted to the 2nd Association for the Advancement of Artificial Intelligence (AAAI) Workshop on Smart Grid and Smart Building. In addition, we’re in the process of revising two additional papers that we’re preparing for publication.

Our work has caught the attention of industry and other researchers. We are in the process of securing a contract with PG&E for \$340K to implement several of our methods; we’ll be testing the effectiveness of evaluation methods augmented by several of the methods we’ve developed in our LDRD work. In addition, we’ve received funding from the SGIG project to implement some of our Baseline methods in a paper for that DOE project.

Advanced In-Situ Experiments for Understanding Induced Seismicity
Principal Investigator: (Yves, Guglielmi)

Project Description

The topic of induced seismicity has been hotly debated in recent years, as subsurface energy activities involving injection of large volumes of fluids have increasingly led to the reactivation of existing faults (NAS, 2012). Despite concern about induced seismicity, the role of fluids in seismic nucleation remains poorly understood, in part because there is a lack of designated field experiments with controlled injection into faults and real-time monitoring of fault slip behavior. The scientific goal of this project is to develop new instruments and methods to evaluate the critical coupling between injected fluids, effective stresses, evolving fault properties and seismicity via intermediate-scale fault reactivation experiments conducted in underground mines and deep boreholes. The project positions LBNL as a premier research organization for induced seismicity research: (1) It provided partial support for the strategic hire of Dr. Yves Guglielmi of University of Aix-Marseille, a world-renowned expert on fault hydrogeomechanics, and (2) it supports further development, testing and application of Dr. Guglielmi's new high-resolution borehole packer-system for in-situ characterization of hydromechanical properties (deformation, seismicity, permeability) from semi-controlled fault activation.

Accomplishments

In 2016, Dr. Yves Guglielmi developed a field experiment of fault reactivation using a new high-resolution borehole packer-system prototype that allows to characterize the fault three-dimensional movements during fluid injections. First key achievement is to show that the prototype measured both axial and radial displacements at the borehole wall with a 3-to-5 micrometers resolution, while monitoring downhole fluid pressure, flow rate and seismicity. Second achievement is that a systematic protocol has been developed (using Matlab routines) to extract the three-dimensional fault elastic response and the inelastic slip from the experimental data, leading to an estimation of fault compliance, permeability and stresses variations associated to fault rupture. Third achievement is that a millimeter scale seismic fault slip was triggered, measured by both the instrument prototype and a network of seismic sensors. These experiments will help improving the knowledge about fluid injections induced seismicity, and developing a deeper-borehole probe to capture the phenomena at the depths of fluids manipulations in reservoirs. In the second year, the project goals are to build and test this upgraded probe.

Multi-Scale Modeling of Geochemical Impacts on Fracture Evolution

Principal Investigator(s): Bhavna Arora and Sergi Molins

Project Description

The objective of this project is to develop a multi-scale model for the simulation of geochemical impacts on fracture evolution. The model will combine a pore-scale description with a Darcy-scale continuum representation within a single adaptive simulation framework. The motivation behind this work is that current geochemical modeling of fractures is limited to either a continuum or pore-scale representation. Relying exclusively on a Darcy-scale representation implies that modeling of fractured systems has been limited to using a treatment that may oversimplify geochemical parameters and flow within complex fracture geometries. While a pore-scale representation is suitable for the fractures, the pore-scale resolution required for the reacting rock matrix makes this approach extremely expensive computationally.

The model developed in this project will dramatically increase our ability to understand fracture evolution combining the rigorous pore scale treatment with the computational advantages of a Darcy-scale treatment. Understanding fracture evolution is essential for many subsurface energy applications, including subsurface storage, shale gas production, fracking, CO₂ sequestration, and geothermal energy extraction.

The model we are developing in this project can be further used as a general framework to combine subdomains using different scale characterization or even to combine sub-models implemented in different codes, an approach applicable to other Earth Sciences problems.

Accomplishments

Our most significant accomplishment has been the development of the computational framework that implements our multi-scale conceptual model. The development has built upon an existing pore scale code, Chombo-Crunch, which is based on an embedded-boundary finite-volume adaptive mesh refinement method. In this framework, embedded boundaries represent the boundaries between the fracture pore-scale domain and the rock-matrix domain. The two mutually exclusive embedded boundary domains communicate transport information from one model to the other at the embedded boundary via a flux matching condition or boundary condition swapping.

We have also succeeded in bringing to bear the adaptive mesh refinement technique to adaptively refine the resolution of the domain based on pore scale geometry and concentration gradients that develop within the porous continuum domain.

We are in the process of extending this adaptivity to time stepping incorporating sub-cycling within our framework and documenting the model in a manuscript.

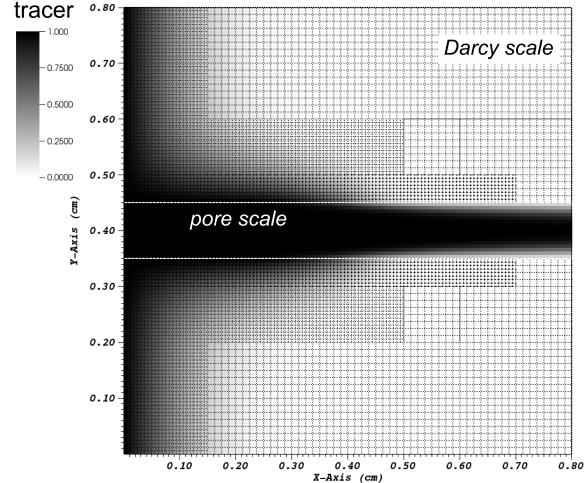


Figure 1. Parallel fracture simulation of infiltration of a conservative tracer that is diffusing into the rock matrix across the embedded boundary (dashed white line), i.e. the boundary between the pore scale and Darcy-scale continuum domain. Dotted lines show the grid cells in the adaptive discretization of the domain

EVALUATING THE EFFECTIVENESS OF METAL ISOTOPES TO FINGERPRINT REDOX REACTIONS IN THE ENVIRONMENT

Principal Investigator(s): John Neil Christensen

Project Description

The purpose of this project is to identify and quantify the mechanisms of metal isotope fractionation during reduction-oxidation reactions using carefully planned laboratory experiments. The existence of isotope fractionation during these reactions has been widely observed in laboratory and geologic environments for more than 25 years, however the understanding of why there is isotope fractionation and what mechanisms are most important in producing isotope fractionation at environmental conditions is still minimal. The data from the study will provide some of the first experimental observations of uranium and iron isotopic fractionation during reduction-oxidation transformations. The data will also allow us to create computational models that will be used to interpret the rates and efficiencies of reduction-oxidation reactions relevant to field scale environmental questions such as transport of organic carbon in soils and radionuclide contaminant transport.

We will develop a new protocol for quantifying metal redox reactions at aqueous fluid-mineral surface interfaces and we will directly probe the role of metal speciation in solution as a control on redox transformations. A recent study by Stylo and coworkers (2015) and 2 earlier studies (Rademacher et al., 2006; Stirling et al., 2007) suggest that uranium isotope fractionation only occurs due to microbially mediated redox transformations and that inorganic transformations result in no fractionation. This result is interesting because it is in conflict with underlying theory that uranium isotope fractionation is an equilibrium process and that most microbially mediated redox reactions are thought to be irreversible kinetic reduction reactions. Our new experiments are designed to test whether there is truly a difference between microbial and inorganic reduction or if the earlier works misinterpreted the meaning of their experimental results.

Our hypothesis is that the degree of uranium isotopic fractionation during reduction is controlled by the relative flux of uranium atoms to and from the reductant surface. In the case where the lifetime of an U(VI) atom at the reductant surface is short there is a relatively low probability that any specific atom will be reduced. This, in turn, gives rise to the possibility of isotopic discrimination in the reduction reaction. In contrast when the lifetime of U(VI) at the reductant surface is long there is less isotopic discrimination in the reduction reaction. The relative time an atom spends at the reductant surface could be controlled by the likelihood of sorption preceding reduction, for example.

Accomplishments

Our most significant accomplishment has been to develop a method for testing uranium isotopic fractionation during reduction by iron sulfide. Our preliminary findings suggest that when aqueous uranium speciation is dominated by calcium uranyl carbonate complexes there is very little sorption to the iron sulfide mineral surface and the reduction of uranium favors the ^{238}U isotope compared to the ^{235}U isotope as predicted by nuclear volume theory. In contrast when uranium is complexed with just bicarbonate sorption reactions dominate the experiments and there is no measurable isotopic fractionation. We reported some of our early results at an international research conference (Brown et al, 2016) and are now working on a publication.

Clay Interlayer Stratification:
Deconstructing Drivers of Mass Transport in Shales
Principal Investigator(s): Laura Nielsen Lammers

Project Description

Clay minerals are ubiquitous in the geosphere and serve numerous critical energy functions due to their colloidal size, layered structure, and strong affinity for both ions and organic molecules. The ions located in the interlayers of high structural charge clays have long been considered fixed and non-exchangeable, but recent high-resolution imaging suggests that they can undergo exchange reactions that are slow on laboratory timescales but likely influence mass transport on the field scale. Currently, both the overall exchange capacity and the dynamics of exchange reactions for ions and organic molecules in high structural charge clay interlayers are unknown.

The objective of this project was to develop a mechanistic understanding of mass transport driven by ion exchange in the high structural charge clay mineral illite, which is the dominant clay phase found in shale rock. In particular, we investigated the dynamics of ion exchange in interlayers starting from an initially collapsed or anhydrous state. We developed a multi-scale modeling approach that uses inputs from atomistic simulation to model the collective diffusion of ions in the interlayer leading to ion exchange on the continuum scale. Large-scale kinetic Monte Carlo (kMC) simulations were parameterized based on single event kinetics derived from *ab initio* density functional theory (DFT) and classical molecular dynamics (MD) simulations. The properties of the exchange front predicted by our kMC and continuum models are consistent with those observed experimentally.

Accomplishments

The key accomplishments of this project in FY2016 were to (1) validate atomistic simulation results using DFT calculations and (2) develop methodologies to up-scale molecular simulation results to describe ion exchange as a continuum process. Following on results from FY2015, we used DFT calculations to determine energy barriers for Cs and K interlayer ion migration in illite. The DFT calculations confirmed that K^+ ions in the vicinity of larger Cs^+ ions in the interlayer have dramatically lower migration barriers than K^+ ions in pure K-illite. These calculations underscore our preliminary finding that the dynamics of interlayer ion diffusion are highly sensitive to interlayer spacing. Clay ion exchange phenomena thus exemplify strong coupling between interlayer chemistry and layer structure and mechanics.

To up-scale single ion migration dynamics, we developed a kMC model that simulates the collective dynamics of interlayer ion diffusion and mass transport. Our kMC model treats interlayer ion diffusion as a Poisson process, with characteristic diffusion timescales of ions that are informed by our atomistic simulation results. These simulations have provided unique insights into emergent phenomena that arise from the collective motion of diffusing ions.

Finally, we have developed a preliminary continuum model for interlayer ion exchange reactions based on the mechanisms identified using atomistic and kMC simulation methods. This model can be used to predict exchange rates over the large length scales and long timescales relevant to mass transport phenomena in shale rock. The results of this model demonstrate that both the dynamics and structure of the exchange front depend strongly on the molecular environment of the exchanging ion.

Frequency-Modulated Hydraulic Fracturing for Secure and Efficient Reservoir Permeability Enhancement

Principal Investigator(s): Seiji Nakagawa, Valeri Korneev (deceased), Kurt Nihei, and Timothy Kneafsey

Project Description

Hydraulic fracturing or “fracking” is an indispensable tool for producing oil and gas, and geothermal fluids for energy production, from deep subsurface reservoirs. The proposed technology involves finite-frequency modulation of pressure pulses applied at the borehole, to initiate and propagate a hydraulic fracture. By altering the amplitude and frequency of the dynamic pressure pulses superimposed on the background static pressure, we attempt to manipulate the extent and orientation of hydraulic fracture propagation. Alternatively, the viscosity of the injected fluid can be changed (modulated) which may have a different impact on the fracture propagation. Laboratory hydraulic fracturing experiments are conducted under true-triaxial stresses, using small rock and transparent, glass cubes containing an analogue borehole. The geometry of the fractures as they propagate is imaged visually for transparent samples, and by using X-ray CT for opaque rock samples. Numerical modeling is conducted using finite element models, to examine how the magnitude and location of the stress concentration within a system of hydraulic fractures vary with the frequency-modulated pressure applied at the borehole, leading to further fracture growth.

Accomplishments

We conducted a series of laboratory hydraulic fracturing experiments, using a combined, optical and acoustic-emission visualization system which has been developed in our laboratory. In FY2016, a new controlled fluid injection system which drives the fluid was developed. The effect of two types of injection pressure/flow modulation was examined: continuous sine waves superposed on background DC flow, and “boxcar” functions with alternating zero and a constant flow rate. High-viscosity fluid was used as the fracturing fluid. The results from the sine-wave modulated injection tests for altering the behavior of hydraulic fractures were ambiguous. However, the latter tests resulted in a fracture network more complex than the fractures produced by constant-rate injection of fluid (either fast or slow).

The experiments were conducted also on natural rock (granite) samples which were heat treated to increase the grain-scale heterogeneity and the microcrack population. Unfortunately, the high permeability and the resulting fluid leakoff made these samples not suited for the same experiment as the glass blocks. As an alternate solution, we modulated the viscosity of the injected fluid (fracturing fluid) by cyclically injecting low-viscosity liquid metal and high-viscosity glycerol. Because the high-viscosity glycerol formed an impermeable “shell” around a borehole, subsequent fast injection of low-viscosity metal was able to fracture the rock without strongly affected by the leakoff. Once the fracture was formed, the high-viscosity fluid was injected again to form another layer of shell around the fracture, and this process was repeated for several times. Interestingly, the fracture formed by this method did not follow the direction of the maximum principle stress applied on the sample, unlike hydraulic fractures produced by conventional methods. The evolution of the fracture and the distribution of the injected metal were visualized via X-ray CT, at several injection stages during the experiment.

Dynamic Fracture Simulation in Geomaterials at Multiple Length Scales

Principal Investigator(s): Jonny Rutqvist, Kunhwi Kim, Alejandro Queiruga

Project Description

The purpose of this project is to develop large scale simulation capabilities for the prediction of three-dimensional fracture initiation and propagation of which the process is coupled to flow and mass transfer in various geomechanics applications (e.g., hydraulic fracturing, enhanced geothermal, subsurface disposal and storage). Two tracks of design and development for individual geomechanical methods are pursued: a discrete modeling approach based on the Rigid-Body-Spring Network (RBSN) framework and a continuum-based method using peridynamics. Both of the methods are developed by adoption of the common code base for large scale parallel computations in mind, and eventually interfaced with TOUGH2 code which handles flow analyses. Verification and validation of the resulting algorithms are performed based on available analytical solutions from the literature.

Accomplishments

The aforementioned numerical methods, the RBSN and peridynamics, have been developed separately at the initial stage. The development procedure for each method involves (1) the implementation of time integration algorithms with parallelization schemes, and (2) verification of the codes against available analytical and experimental results of crack propagation.

For the RBSN method, fracture models, based on elemental stress tensors/vectors, have been implemented in the developed code framework, so they can be selectively applied to simulate fracture processes under various loading conditions. The serial code has been modified into an initial version of parallelization, where OpenMP directives are used and tested for the performance gains on a single workstation. The current code will continue to be transformed into a massively parallel simulator using message passing instead of threading. In TOUGH-RBSN linkage, computational efforts have been made to implement fracture aperture dependent hydrological properties (i.e., porosity, permeability) for more rational simulations. However, unascertained numerical instabilities have arisen at times during test simulations, which need to be remediated for large-scale computations.

Extensive development and analysis was performed for the peridynamics-based fracture propagation code. A new Python/C framework was developed that can solve general nonlinear peridynamics models statically or with fully-implicit Runge-Kutta time integration using tangents obtained by symbolic differentiation of the force states. The mechanical fields are fully coupled to a new thin-film flow model along a fracture mesh. We performed a thorough analysis of the accuracy, stability, and rate of convergence of three different state-based peridynamic constitutive responses found in the literature, with further variations on the formulations. By applying the peridynamics models to standard mechanics problems, we have determined that the best-case formulation for peridynamics obtains linear convergence with an instability in the displacement field. The work was submitted to Computer Methods in Applied Mechanics and Engineering (Queiruga and G. Moridis, 2016)

Project Title: Characterizing the Environmental Impact of Chemical Compounds Used in O&G Development

Principal Investigator(s): William Stringfellow

Project Description

Oil and gas (O&G) development in the USA has expanded rapidly over the last decade and there is growing public concern about the environmental impacts of oil-field chemical additive use and water management practices. Rapid growth has alarmed the public in part because O&G chemical additives have not been sufficiently characterized to allow for an analysis of their environmental impacts. In this study, we are conducting a systematic investigation of the environmental profiles of O&G chemicals, including properties related to contaminant mobility, recalcitrance, and toxicity. Developing a better understanding of the properties of O&G chemicals will allow the selection of chemicals with improved environmental profiles, that are more acceptable to the public, and can improve the sustainability of O&G development. The characterization and development of fate-transport properties for these chemicals will allow for the application of predictive models in the context of local and regional groundwater investigations, while providing a critical service in protecting groundwater resources in California.

Accomplishments

Major accomplishments of this LDRD include an evaluation of the types, frequency of application, and quantities of chemicals used in O&G development. It was shown that chemical additives used in hydraulic fracturing, which is a tightly regulated O&G field activity, are also widely used for other O&G development activities, suggesting that green chemical alternatives should be considered for all O&G field activities, not just hydraulic fracturing (manuscript submitted). Using data science approaches, it was calculated from fundamental physical and chemical properties which O&G additives could be treated using existing water-treatment technology and which could not. It was demonstrated that a class of commonly used biocides called quaternary ammonium compounds (QACs) were poorly characterized and needed further study (Camarillo, et al. 2016). Laboratory studies are in progress to develop technology for the treatment of QACs in water produced from O&G fields. There is intense interest in reusing O&G produced water for irrigated agriculture and we are negotiating with industrial partners for scale up of laboratory studies to pilot-scale applications.

Low-energy, low-cost water desalination

Robert Kostecki

Project Description

This project was rescoped in February 2016 into three separate research tasks: (1) enhanced seawater desalination from materials architectures derived from porous aromatic frameworks (J. Urban, J. Long, MSD), (2) synchrotron x-ray spectroscopic investigation of iron-based homogeneous hydrosilylation catalysts via micro-droplet reactors (M. Ahmet, CSD), and (3) plasma processing methods critical to the advancement of a high-impact desalination technology (C. Subban, ESDR). The purpose and goals of these projects is to enable new paradigms in desalination and separations:

1. Design a new class of porous aromatic frameworks (PAFs), optimized for seawater desalination by the capture of NaCl ions from aqueous solution. To accomplish this goal new densely functionalized with oxygen-containing moieties PAFs are designed and synthesized, which can potentially desalinate seawater with as little as 60 g of polymer per liter. PAFs are studied for system regeneration using renewable sources such as thermophotovoltaics (TPV).
2. Explore the physical and chemical properties of nano-confined water via a unique blend of inorganic synthesis, and spectroscopy coupled to novel micro-droplet and aerosol methods. Inorganic micelles with hollow cores of several nanometers in diameters are synthesized and filled with aqueous electrolytes to monitor changes in basic physic-chemical properties by X-ray & Infrared spectroscopy coupled with mass spectrometry and other analytical methods.
3. Develop inexpensive ion exchange resins (IER), which are compatible with *in situ* electrochemical regeneration of IER. Develop novel low-temperature plasma processing method to obtain an electrically conductive and ion-porous carbon layer on the surface of the milled IER powders.

Accomplishments

1. 18 functionalized polyarylimide and poly(aryleneethynylene) PAFs were synthesized via diverse synthetic routes. The synthesized polymers contain sodium-binding groups, including carboxylic acids, phenols, alcohols, and ether chains of varying lengths. These materials were tested for desalination performance using a salinity meter (based upon conductivity) and in some cases inductively coupled plasma mass spectrometry (ICP-MS). Results ranging from no effect to a 14% decrease in salinity were observed, using 20 mg polymer in 7 mL of 3.5 g NaCl/L aqueous solution. Upon scaling up the leading material's desalination performance was not reproduced, and efforts to effectively reproduce the synthesis of this compound and to verify its NaCl capacity are ongoing.
2. Preliminary results were obtained at O and Mg K absorption edges from aqueous solutions of Mg(NO₃)₂ using continuously flowing micro-droplets at the ALS demonstrating the promise of this micro-droplet reactors for use with soft-X-rays. Higher X-ray flux and smaller beam size in the beamline 11.0.2 and improved detection configuration in the present endstation will render possible much improved sensitivity and detectability of coordination complexes and even intermediate species at short contact times, down to milliseconds, which will be obtained using continuously flowing micro-droplets. Cl K and Co K absorption edges were also successfully monitored using our micro-droplet reactor and photodiode detection scheme.
3. The existing vacuum chamber was reconfigured for the treatment of powder substrates (milled IER). Various sample holder designs were fabricated and tested to ensure uniform exposure of IER powders to plasma. The most promising results were obtained using Ar plasma generated with a graphite cathode held parallel to the sample tray. Using this configuration, a series of experiments were conducted to access the impact of plasma on IER powders as a function of time. The samples when tested for surface hydrophilicity and ion-exchange capabilities showed no noticeable changes. Although these preliminary results are promising, extensive characterization of the treated surfaces is still necessary.

VOLUMETRIC ABSORPTION OF SOLAR RADIATION IN LIQUIDS AND GASES BY TUNING THE EMISSIVITY OF SURFACES

Principal Investigator: Robert Kostecki

Project Description

Solar-to-thermal energy conversion is important for many renewable energy applications, such as concentrated solar electricity production, water desalination, thermochemical reactions, water heating, and thermal storage. All of these applications involve the heating of liquids and gases. Currently, solar heating of the heat transfer fluid in all these applications is achieved through surface-based methods, where the heat is transferred via convection using heat exchangers to the fluid. This results in a solar-to-thermal energy conversion efficiency between 40–60% depending on the temperature. One potential way to significantly increase the solar-to-thermal energy conversion is to volumetrically absorb solar radiation directly into the fluid. Various researchers have tried to solve this problem by seeding heat transfer fluids with nanoparticles, thereby making the fluid black, leading to volumetric absorption of solar. This approach has not been successful in spite of ~30 years of research because the nanoparticle-laden fluid affects the performance and reliability of the pumps that pump the heat transfer fluids.

The goal of this project is to develop a new method to volumetrically heat fluids while reducing the complexity of the system. We propose to design and fabricate a device that efficiently absorbs solar radiation and selectively emits thermal radiation that matches the absorption spectrum of a liquid or gas. This will represent a paradigm shift in solar heating of fluids with the potential to scale up in a wide range of applications.

Accomplishments

The first accomplishment of this project has been to develop a theoretical model that determines the spatial temperature distribution in a fluid subjected to a spectrally selective thermal radiative heat flux. This model accounts for non-gray absorption, extinction, and scattering within both non-particulate and particulate-laden liquid films. Based on this model we have been able to design selective emitters for highly efficient steam generation of water and volumetric heating of Therminol (a common industrial heat transfer fluid). Currently, we are preparing a manuscript for submission that details our theoretical model and compares the benefits of surface and volumetric heating of liquids under various conditions.

To experimentally demonstrate volumetric heating of fluids, two experimental systems had to be fabricated and assembled. The first was a custom designed Fourier transform infrared (FTIR) spectrometer that has the ability to measure both diffuse and specular reflection and transmission over a wavelength range of 400 nm to 20 μm and over a temperature range of 300 K to 1000 K. This FTIR allows us to measure the emissivity of our spectrally selective emitter films over a wide range of temperatures and determine their thermal stability (a major problem in solar-thermal applications). The second experimental setup that was built was our solar simulator experiment that has the ability to apply an external radiative heat flux that mimics the sun and can concentrate sunlight between 1 sun and ~70 suns. This experiment allows us to experimentally validate our novel approach to volumetric heating of fluids. In addition to these two experimental setups we have also refurbished a reactive sputter machine and are using the sputter to design and fabricate selectively emitting films. Currently, we have designed and fabricated selectively emitting films for heating of water, Therminol, and near infrared applications and are now in the process of acquiring data that will demonstrate the advantages of our novel method of volumetric heating of fluids.

Accelerating Technology Development by Disruptive Scaling and Manufacturing processes.

Principal Investigator(s): Gerd Ceder, Vivek Subramanian, and Venkat Srinivasan

Project Description

The overarching goal of this project has been to advance the science of manufacturing, with an initial focus on battery material and devices. The LDRD has developed three core competencies, (i) predicting synthesis conditions (ii) visualizing processing of materials into electrodes and (iii) developing new modular manufacturing methods based on additive manufacturing. The core competencies have allowed the program to establish a unique capability at LBNL, and has attracted funding from the Advanced Manufacturing Office in DOE. The project allows LBNL to expand from traditional materials discovery and build the continuum from discovery to devices by accelerating the synthesis of materials, their incorporation into components and devices and finally into novel processing for next generation devices. Although the accomplishments, listed below, are specific to batteries, the capabilities are cross cutting and impact a variety of fields.

These electrodes consist of dried porous slurry coatings on metal foil current collectors. This project has specifically focused on the understanding the slurry drying process. Drying slurry drops were studied as a model of the edges of drying slurry coatings. While the 3D structural information provided by X-ray tomography would be desirable, significant drying on the time scale of the data acquisition sequence would lead to extremely distorted results. Instead, radiography, involving only the collection of 2D transmission images from a single direction through the sample, was used in conjunction with a data analysis procedure developed for this project to extract the dynamic spatial distribution of active material particles.

Accomplishments

Predicting synthesis conditions: With the establishing of the Materials Project, the prediction of new materials with unique properties has undergone a transformation and significant acceleration. However, the bottleneck has moved to synthesis of the materials with the phase purity needed to integrate them into devices. In order to fill this continuum we have used first principle calculations to predict the effect of pH on the morphology of LiFePO₄ particles. The study, one of the first reports in the literature, is the expected to be combined with machine learning to establish the science of material synthesis.

Visualizing processing: Once new materials are synthesized, the bottleneck moves to the integration of these materials into components, for example into battery electrodes. Herein, the process conditions (e.g., viscosity, volume fractions, drying time etc. for slurry drying) can impact final morphology and performance. We have, for the first time, used X-ray tomography and tomography at the ALS to study the slurry drying process under Operando conditions. Using SiO_x microparticles/Super C 45/carboxymethyl cellulose/deionized water on an aluminum substrate as an example battery system, we have learnt under what process conditions uniform film formation can be expected. This study brings, for the first time, science to the art of processing of batteries.

Modular manufacturing: We have been developing, in collaboration with LLNL, unique additive manufacturing methods to build flow batteries. Our approach is to start with a microfluidic device as a proof-of-concept and then expand into larger devices once the capability is established.

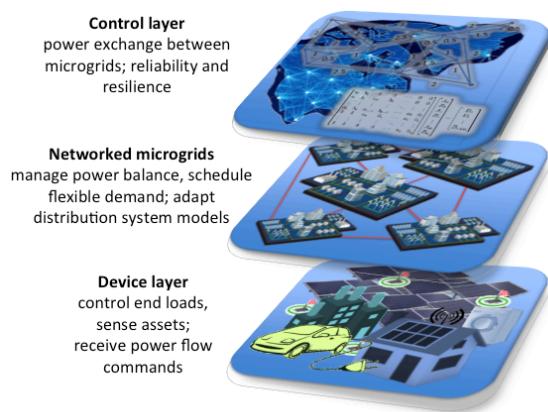
Intelligent Distribution Grid Analytics: Distribution Phasor Measurement Unit and Operational Data (The Grid Initiative)

Principal Investigator: Emma Stewart, CO-PI: Michael Stadler

Project Description

California has set ambitious sustainability goals targeting 50% penetration renewable generation by 2030, including behind the meter distributed and transmission side resources. These goals offer blueprints to the rest of the US and the world, with California leading the way in advanced inverter deployment, micro-grids, and storage. The Grid Initiative perceives our distributed energy resource (DER) future as a collection of interconnected micro-grids. These include behind the meter, and grid connected resources, combining storage, photovoltaics, electric vehicles, and flexible demand, to reduce reliance on the legacy bulk centralized generation and transmission. In our vision, customers are transformed from passive recipients of electricity to active participants in our sustainable energy future. Challenges for a 50% distributed grid include:

- 1) Dramatic increase in uncertainty and variability in generation
- 2) Aging transmission and distribution infrastructure
- 3) Poor visibility in distribution grid; inaccurate models
- 4) EV, PV, Storage presence straining distribution assets.



1) Dramatic increase in uncertainty and variability in generation
 2) Aging transmission and distribution infrastructure
 3) Poor visibility in distribution grid; inaccurate models
 4) EV, PV, Storage presence straining distribution assets.

To solve these issues we propose a Coordinated Grid Operating System, which accounts for flow of power, data and money, between consumers and operators. We consider this coordinated system to be structured in layers and the grid initiative LDRD is developing projects and expertise within these layers, with the ultimate vision of a coordinated operating platform.

Within the first year of this LDRD project we seek to address the first stages of the grid operating system architecture, with focused projects in the device and feeder/networked microgrid layers. The team combines multidisciplinary expertise in Grid Integration, Buildings Technology, data analytics and cyber security.

Accomplishments

In year 1 the research approach is to monitor the distribution grid condition and detect anomalies, leveraging distribution micro-synchrophasor technology (μ PMUs). Using analytics derived from μ PMU data we foresee a significant improvement in anomaly prediction speed and accuracy. We then couple this and algorithms directly related to this, to a simulation tool, developing controls and accounting for sensor latency, to allow reconfiguration and re-dispatch of high renewable penetration microgrid technologies to absorb variability caused by things such as cloud cover and grid events. In addition to this the team have developed algorithms, which can represent the controllability of the feeder network. Optimal power flow techniques are used to define bounds of operations and controllability of voltage and phase angle of the feeder. The last activity within the grid initiative LDRD is developing inverter controls which can be tuned for performance in high penetration clusters, to control a variable to a global goal, such as phase angle difference across a point, enabling seamless, economically and technically viable feeder reconfiguration. The power flow control method will mitigate impacts of large reverse power flow and utilize fast data and controls which are condition based, not "set and leave" enabling less curtailment (a method often used to mitigate reverse power flow) and enabling further markets for behind the meter control.

Neuro/Nano Technology for Brain Mapping

Principal Investigator(s): Peter Denes, Kris Bouchard, Chris Chang, Bruce Cohen, Jim Schuck
Terumi Kohwi-Shigematsu

Project Description

The purpose of this project is to lay the foundations for next generation neurotechnologies responsive to the Presidential *BRAIN* Initiative. Our 4-prong approach is to advance electrical, optical, acoustical and chemical tools for recording and stimulating brain activity. Underlying many of these techniques is also the incorporation of high performance computing and advanced algorithms to understand the data collected.

Accomplishments

We have developed a multi-channel electrocorticography readout system, implemented in a single integrated circuit. Readout electronics and a data acquisition system have also been developed. A method for patterning and depositing inert metal electrodes has been implemented. In-vitro tests have shown that the circuit works as predicted. Current efforts are aimed at in-vivo measurements.

As optical probes, we have paired organic biosensors (from C. Chang) for detecting neural ions and metabolites with upconverting nanocrystals (UCNPs), which absorb in the near infrared (NIR) and emit in the visible to couple to the biosensors. We have now shown that upconverted energy transfer (UET) significantly increases biosensor stability—so much so that no photobleaching is observable after hours of continuous excitation—in addition to facilitating imaging through tissue with benign NIR light. UCNPs optimized for efficient UET of fluorescent sensors have been developed. For sensor targeting, we have developed methodology for the attachment of nanocrystals to antibodies to UCNPs surfaces. Current efforts are geared toward imaging these nanocrystal-sensor conjugates in neurons, controlling cellular localization to membranes, vesicles, and synapses to monitor the ion flux underpinning neural activity.

We have continued advancing high-performance computing for both ‘off-line’ and ‘on-line’ data analysis. We have: (a) engineered a data storage system based on the HDF5 format in order to leverage the computing resources of NERSC and are extending it to other use cases, (b) developed a scalable framework for statistical data analysis that gives more accurate and interpretable results than the state-of-the-art algorithms in machine learning. Current efforts are focused on HPC implementations of data analysis methods on NERSC, and applying our framework to other data analytics challenges.

Novel Magnetic Field Mapping Technology For Small And Closed Aperture Undulators

Principal Investigator: Erik Wallen

Project Description

The objective of this project is to develop a magnetic measurement technique that will enable the magnetic characterization of undulator and accelerator magnet geometries where there is only access along the narrow vacuum chamber of the accelerator. Technological developments involving optical methods and sensor technology are required to map magnetic fields accurately on a straight path in closed aperture insertion devices and other magnets. It is critical that this technology is in hand to properly produce optimized insertion devices for accelerator applications such as ALS-U, Bella, and beyond, where closed small bore devices are appropriate.

This key technology has not been fully developed yet at any other national laboratory in the US. To achieve this objective, we identified 4 components or systems that need to be developed: 1) ultra-compact magnetic field sensor package, 2) a position acquisition system using laser technology, 3) a transverse positioning system for the magnetic field sensors, and 4) a magnetic sensor transport mechanism concept.

Accomplishments

1) Ultra-compact magnetic field sensor package. A miniature measurement system with 2 Hall probes and on-board voltage source and analog digital converter (ADC) has been developed. The unit fits into a 5 mm diameter tube. The ADC has 24-bit resolution and the signal is digitized at the source, very close to the Hall probes inside the 5 mm diameter unit.

2) Position acquisition system using laser technology. A laser system capable of resolving the position of the Hall probe sensor unit with approximately 15 μm resolution in all three dimensions inside a 5 mm inner diameter tube has been procured, assembled, and commissioned.

3) Transverse positioning system for the magnetic field sensors. Micro Electronic Motion System (MEMS) components have been integrated in the Hall probe sensor unit in order to make it possible to rotate the Hall probe sensors around the axis of the Hall probe unit. By making measurement of the magnetic field on a circle, the magnetic fields at any point inside the circle can be derived from the measured values at the edge of the circle.

4) Magnetic sensor transport mechanism concept. The magnetic field sensor head is pushed and pulled along the tube that is simulating the circular vacuum of an insertion device. A drive 3.25 m long drive belt system has been assembled, which makes it possible to measure the magnetic field along 3 m long tubes.

A measurement system consisting of the 4 components listed above has been fully assembled and a series of initial measurements in a 5 mm inner diameter tube have been carried out with promising results. The results from the magnetic measurements with system will be presented at the 16th International Superconductive Electronics Conference in June 2017 (ISEC 2017), in the section Readouts & Detectors.

At the ALS-U it will be possible to install insertion devices, either Delta-type undulators or superconducting undulators, using small aperture vacuum chambers with cylindrical cross section. The magnetic characterization of the insertion devices to be installed is an absolute necessity. It is also necessary to carry out magnetic measurements on accelerator magnets for the ALS-U with closed apertures. The promising results from the LDRD project has led to that further financing on the level of 50% of a postdoc position for year 2017 has been obtained from the ALS-U.

**HIGH-PERFORMANCE CHEMICAL IDENTIFICATION FOR HYPERSPECTRAL
DATA SCIENCE**
Principle Investigator: Benjamin P. Bowen

The aim of our OpenMSI research program is to develop open tools for the analysis of very large mass spectrometry imaging (MSI) datasets. This LDRD in particular is focused on providing chemical tools for transforming raw mass spectra into chemically informative patterns of identified *molecules* and *molecule classes*. This research will lead towards establishing OpenMSI as a new science resource, centered at LBNL and used by thousands of researchers around the world.

A central challenge in mass spectrometry imaging (MSI) is the identification of molecular identities from spectra, i.e., which molecule(s) constitute a particular peak. Molecular identification is complex and time-consuming so that often only a small fraction of peaks are identified in practice. This progress demonstrates how OpenMSI can be utilized for compound identification and multimodal data analysis. Our progress includes:

- (i) Utilizing Cori, NERSC's newest supercomputing system to build over 170,000 theoretical fragmentation trees for molecules. The majority of the OpenMSI allocation at NERSC was used to compute the complete enumeration of 171494 molecular structures. These “pactolus trees” are the foundation for statistical scoring algorithms that can assign a putative identity from an observed mass spectrum.
- (ii) Integration of all known, publicly available biomolecule databases into a Metabolite Atlas compound database at NERSC. We designed a custom MySQL database and Python API to store and access the integrated totality of publicly available compound databases. The integrated reference data was drawn mainly from ChEBI, LipidMaps, HMDB, MetaCyc, and a few small databases.
- (iii) Development of analysis capabilities within the OpenMSI platform for next-generation screening assays. The OpenMSI Arrayed Analysis Toolkit (OMAAT), is a software package that addresses the challenges of analyzing spatially defined samples in MSI datasets. We demonstrate the utility of OMAAT by analyzing an MSI dataset of a high-throughput enzyme activity screen comprising 384 samples arrayed onto a NIMS surface at a 450 micron pitch decreasing analysis time >100 fold while maintaining robust spot-finding.

Much of the power of chemical imaging is due to the fact that the images are of intact biomolecules. Automatic annotation will greatly increase the accuracy and throughput of MSI *through in silico* annotations and collaborative sharing of verified annotations. Our research will enable scientists to leverage simulation and information from previous experiments by automatically and intelligently propagating quantitative, probabilistic annotations to peaks across datasets. This capability will enable faster and more accurate annotation of the data and ultimately enable more complete analysis and annotation of spectra than is currently possible. These capabilities are important not just to MSI but spectral imaging methods at large.

REINVENTING PRE-CLIICAL AND ENVIRONMENTAL TESTING PARADIGMS

Principal Investigator(s): Brown, James Bentley

Project Description

Motivation: Pre-clinical drug development of lead therapeutic compounds usually begins with rodent models and ends with non-human primates prior to phase I trials. This process is now producing on average ~7 drugs per year (94% failure rate) at a combined cost of over \$60B (\$850M per drug). Our long-term goal is to reduce the societal and economic costs of drug development and biological risk assessment by two orders of magnitude in the next twenty years. This aim will require input from many disciplines; in this project, we will provide new statistical methods that are needed to facilitate large- and multi-scale studies in ensembles of biosystems, from invertebrates, to human tissue mimetics, to mammalian models.

Aim 1) New approaches to identify causal (epi)genetic variants in functional population studies. Our goal remains to generate a suite of statistics sufficiently powerful to study large groups of functional variants at potentially distal genomic loci, thereby enabling the reliable detection of compound and *trans* effects.

Aim 2) Develop new dimension reduction techniques for biological data. Develop a new paradigm in statistical machine learning based on the idea that any prediction or regression model based on ensembles (e.g. deep learners, Random Forests (RFs), probability machines) can be interrogated by mapping path predictors take through the ensemble during fitting. This approach relies on the idea that ensembles like RFs implicitly fit “interactions” of arbitrarily high order, and hence capture data structure in the natural dimension.

Accomplishments

Aim 1: Our NIH R01 application last year was unsuccessful, but we have re-submitted. We have obtained an STTR from the ASCR in the DOE to develop some commercial applications of some of the technology we have developed, funding starts in Feb 2017. We continue to work on a primary publication despite some obstacles, including staff changes. We are confident that a primary publication will be forthcoming in the first half of this year. GWAS does indeed work well with our method, and we’re coining the phrase “Genome-Wide Epistasis Study” (GWES), to distinguish our statistical procedures that identify nonlinear interactions, indicative of epistasis, as opposed to main effects. We’re now collaborating with Dan Jacobson at ORNL, and Kris Bouchard here at LBNL.

Aim 2: We have a distributable software package for Introspective Learning Machines implementing iterative Random Forests (iRF) and “Unconstrained Surface Mapping” (USM) that will be made available. This is a general tool for supervised, unsupervised, and semi-supervised machine learning. The key feature of our algorithm is superb interpretability: it is not a black box – the explicit goal is to understand how the predictor is working and what it can tell us about the data it is modeling. We have completed an algorithm to integrate iRF with boosting to generate a new class of learning machine. We are working to identify patentable components of this technology.

MICROBIOME ADAPTATION IN RESPONSE TO ENVIRONMENTAL CHALLENGES

Principal Investigator(s): Susan Celniker

Project Description

The purpose of this project is to characterize the role of the microbiome in adaptation to environmental challenges. The microbiome has been linked to brain health, liver function, bowel disease, and many other physiological and behavioral phenotypes in a growing number of studies. However, the response of the microbiome to chemical perturbations is poorly understood. Accidental human and animal herbicide exposures to agricultural chemicals remain a serious problem in the United States, which accounts for 32% of the total global pesticide market. Here, we will characterize the role of the microbiome in adaptation to chronic pesticide exposures at environmentally relevant doses. By using both invertebrate and mammalian models, we will elucidate the impact of the gut microbiome on host health and generate the first atlas of microbiome chemical interactions in any organism.

We plan to measure the immediate and long-term responses of the gut microbiome to the top ten most utilized herbicides in the United States using the model organism *Drosophila melanogaster*. By utilizing both gnotobiotic and wild-type flies in our perturbations, we will isolate effects specifically due to the microbiome. In the mouse, we will study three compounds, informed by our fly model, in pre-adolescent exposure scenarios and long-term effects. As in the fly, we will use genomic and metabolomics techniques. Detailed, life course assays throughout a 12-week span will provide an extensive map of the dynamic composition of mammalian gut microbiomes. Utilizing the collaborative cross mice and also specified microbial compositions will enable the identification of microbiome chemical and genetic interactions.

We will be able to correlate pesticide-induced changes in behavior with changes in the microbiome, while controlling for genetic background. Importantly, we propose to establish a mammalian gnotobiotic resource facility at LBNL, an expertise that remains in short supply in the US and which is a critical component of the 'Microbes to Biomes' initiative necessary to make the transition from correlative science to causal proof.

Accomplishments

Using PacBio technology we sequenced eight species and for six (*A. tropicalis*, *L. brevis*, *B. kochii*, *E. durans*, *L. plantarum*, *A. pomorum*), we identified a large core circular genome in a single gapless contig assembly. Two others (*P. taichungensis*, *B. flexus*) are in three contigs. In the case of one species, this greatly improved assembly (the previous assembly was in hundreds of small contigs and revealed >1000 new genes and fundamentally new metabolic potentials. It has long been suspected that fruit flies receive folate (vitamin B12) from their microbiomes, since feeding antibiotics strongly reduces growth and survival on folate-free media. We found that the genome of *Acetobacter tropicalis*, one of the most abundant species in the fly gut, includes a complete folate synthesis pathway. Further, in all eight species sequenced, we identified complete plasmid and viral sequences that expand the metabolic potential of these microorganisms.

In one case, we found a complete set of enzymes required for metabolism of a known pesticide. This led us to hypothesize that gnotobiotic flies lacking this pathway should be significantly more susceptible to toxicity from this pesticide than our wildtype strain. We generated axenic adult flies and recapitulated exposures. As expected, germ free (GF) flies exposed died earlier than control flies with wild-type microbiomes. Further, we were able to fully rescue GF flies and restore wildtype survival curves by feeding flies the bacterial culture prior to exposure. We attempted similar rescue experiments with other microbes, none of which rescued, as expected. We illustrate that the GF condition does not make flies uniformly more susceptible to toxic compounds, as the wildtype microbiome offers no protection against certain toxicity. These studies were presented for an invited talk at the Society of Environmental Toxicology and Chemistry (SETAC) meeting in Orlando Florida (Nov 7, 2016).

Discovery and transfer of novel pathways for phosphate solubilization
Principal Investigator(s): Matthew Blow

Project Description

High yield agricultural plant growth is currently dependent on costly and environmentally damaging phosphate fertilizers. One approach to alleviating this dependency is to convert existing phosphorus sources in the soil into soluble forms available for plant uptake. A potential target is phytic acid, a plant phosphate storage molecule that accounts for 50% of total phosphate in some soils but is inaccessible to plant roots. Phytase enzymes catalyze the hydrolysis of phytic acid, and thus may be a means to liberate plant available phosphate from accumulated phytic acid in soil. The goal of this proposal is to transfer phytase genes and functions to the genome of a plant root associated bacterial host, and demonstrate a benefit to plants grown with phytic acid as the sole phosphate source. Towards this goal we will i) mine genome sequence databases for diverse phytase gene sequences; ii) synthesize these sequences and integrate them into the genome of the plant-root associating *Pseudomonas simiae*; iii) evaluate the ability of engineered strains to hydrolyze phytic acid in liquid culture; iv) test the ability of engineered strains to colonize and promote growth of *Arabidopsis thaliana* and model biofuel plant *Brachypodium distachyon*.

Accomplishments

We computationally identified 100 phylogenetically diverse phytase genes, with representatives from each of three distinct phytase gene families. We refactored these gene sequences for optimal expression in *P. fluorescens* and synthesized them using capabilities of the JGI DNA synthesis group. We transferred these genes into the genome of *Pseudomonas simiae*, to generate 88 candidate novel phytic acid hydrolyzing strains.

We next tested the ability of engineered strains to hydrolyze phytic acid in liquid culture and found 25 / 88 strains release substantial free phosphate, with five strains releasing at least 50% of total available phosphate. These include representatives of two of the three types of phytases tested. Importantly, for several active strains we observed no differences in growth rates to wild-type *P. fluorescens* when grown in rich media.

To test the potential benefits of phytate hydrolyzing strains to plants, we selected two engineered *P. fluorescens* with high activity in liquid culture, and inoculated *Arabidopsis* plants grown with phytic acid as the only phosphorous source. Compared with plants inoculated with wild-type *P. fluorescens* we observed a small but significant increase in dry weight and rosette size, providing preliminary evidence that these strains may confer a benefit to plants under phosphate limiting conditions.

We are currently performing biochemical characterization of the phytase enzymes, engineering phytases into alternative host strains, and expanding tests of plant growth promoting phenotypes in *Arabidopsis* and in the model biofuel plant *Brachypodium distachyon*.

Identification, Biomanufacturing and Characterization of Cyclic DiPeptides (CDPs), a diverse family of chemicals involved in mediating microbial interactions

Samuel Deutsch

Project Description

With this project we aim to develop methods to identify, activate and characterize microbial pathways involved in the production of secondary metabolites, a diverse group of molecules that have been broadly useful in multiple fields of application. For example, secondary metabolites have been shown to have important roles in shaping microbial communities in plant roots (rhizosphere), leafs, soil, marine environments and the human microbiome. In addition, some of these molecules have been commercially developed for agricultural or pharmaceutical applications and represent a potential source of growth for the US bioeconomy.

The sequencing of microbial genomes has revealed large numbers of novel predicted pathways for secondary metabolites, but the molecules that these pathways produce and their potential activities remain unknown. Thus there are clear opportunities for the discovery for new and potentially valuable compounds.

This LDRD will specifically support efforts to: (i) Re-engineer pathways identified through the analysis of sequencing data, predicted to produce a class of secondary metabolites called Cyclic dipeptides (CDPs) that are particularly tractable to these approaches. (ii) Develop workflows that make use integrated multi-OMICS approaches to activate silent secondary metabolite clusters from recently sequenced microbes.

Accomplishments

To date, we have identified 10 novel CDP pathways by analyzing genomics and metagenomics data. Using synthetic biology approaches we were able to re-engineer 9 of these pathways and to integrate them into a microbial production host. We have started our characterization efforts with one of these pathways and were able to optimize the culture, extraction and analysis protocols for the identification of the relevant molecule. We are now extending these approaches for the characterization of the remaining pathways.

We have also developed a pipeline for the culture and co-culture of newly sequenced actinobacterial genomes that were identified on the basis of their high content of secondary metabolite pathways. We performed genomics, metabolomics and are currently performing transcriptomics analysis on 25 samples, which has so far led to the identification of over 100 new metabolite peaks (that likely correspond to at least 10 new compounds). We have started preliminary purification for one of these molecules for full characterization. We expect to continue with these promising efforts for year 2 of the project.

Plant Growth Promoting Microbes: Signaling and Mechanisms

Principal Investigator(s): John Vogel

Project Description

Plant growth promoting microbes hold tremendous potential to greatly increase crop yields by stimulating plant growth and preventing disease. Despite their enormous potential, beneficial microbes are not widely deployed in large-scale agriculture because of their unpredictable performance. Thus, fundamental systems level knowledge about all aspects of the interaction between plants, beneficial microbes and the microbiome is needed to harness the benefits of the microbiome. The extreme complexity of the soil microbiome is a major impediment to acquiring this knowledge. This project seeks to establish a simplified experimental system to rigorously study the interaction between a model plant and a defined root microbiome and then use this system to identify plant genes required for beneficial plant-microbe interactions and/or microbial colonization of roots. We will use a forward genetic screen to identify plant mutants that affect microbiome composition or function and we will use transcriptional profiling to identify candidate plant genes involved in the interaction. Mutants and candidate genes will be characterized using the large amount of experimental tools that have been assembled in the lab over the past 14 years (e.g. sequenced mutant collections, sequenced natural accessions, efficient transformation and CRISPR, etc.)

Accomplishments

We have assembled a defined microbiome consisting of 60 bacterial strains including 23 strains known to promote the growth of *Arabidopsis thaliana* and 30 strains isolated from a microbiome selected to promote the growth of *Brachypodium distachyon*. We have demonstrated that the many of the isolates colonize *B. distachyon* roots, some to high levels, and that the community enhances plant growth. We have tested the ability of 30 individual isolates from the selected *B. distachyon* microbiome for their ability to promote plant growth and found that 6 isolates increased biomass, however, this has yet to be replicated. Experiments to determine the reproducibility of colonization have been conducted and we are waiting for the sequencing results. Similarly, we have begun screening for plant mutants that affect microbiome composition and are waiting for the sequencing results from the first 92 mutants. Through a separate CSP project 430 plant mutants have sequenced so we know the mutations can be quickly examined to identify candidate causal genes.

Previously, we observed that some strains of the beneficial fungus *Trichoderma harzianum* strains greatly increased plant biomass, up to 2.5 fold. We identified *B. distachyon* lines that vary in the degree to which *T. harzianum* promotes growth including some lines whose biomass actually decreases when inoculated with *T. harzianum*. An experiment to look at the effect of the bacterial microbiome on growth promotion by *T. harzianum* in three *B. distachyon* lines is underway.

We established collaborations with several researchers to use our defined microbiome or techniques. The two most significant are with two researchers at UC Davis who are using the defined microbiome to look for plant genotypes (*Setaria viridis* and corn) that affect microbiome composition. The corn work is part of a 2017 LDRD awarded to Trent Northen.

Tackling microbial-mediated plant carbon decomposition using ‘function-driven’ genomics
 Principal Investigator(s): Tanja Woyke, Devin Doud

Project Description

The principle goal of this research project is to advance our understanding of the role and mechanisms microbial communities have in carbon cycling by developing a “function-driven” genomics approach. Specifically, we developed a pipeline for single-cell and mini-metagenome sequencing of uncultivated organisms actively involved in the decomposition of crystalline cellulose, a primary component of plant biomass, and an attractive target for biofuels. This “function-driven” approach identifies and isolates only those members engaged in the activity of interest. We developed and benchmarked this cellulose-degrading single-cell genomics pipeline in the lab with synthetic microbial communities before applying it to a range of environmental ecosystems for identification of uncultivated environmental cellulose degraders.

Accomplishments

Our most significant accomplishment has been the development and validation of a fluorescent-based assay for detecting adhesion of single cells to crystalline cellulose particles using a flow cytometry platform. This assay is sensitive and specific, demonstrating high levels of enrichment (>90% relative abundance) of model cellulose degraders from a low starting abundance (<1%) in a synthetic microbial community. This method thus allows high confidence in the specificity of cellulose-degrading activity of recovered environmental microbes. In addition, the ability to enrich microbes from low abundances demonstrates that this tool may be able to recover rare microbes whose genomes may be lost in bulk metagenomic surveys. This function-based assay was demonstrated compatible with the downstream single-cell genomics pipeline that has been established at JGI, allowing for seamless integration of the cellulose-deconstruction screen with single-cell sequencing.

We then applied the entire function-based single-cell genomics pipeline to fresh environmental samples relevant to the biorefinery model (i.e. geothermal hot springs and alkaline lakes) for recovery of environmental microbes actively engaged in cellulose deconstruction under these conditions. By sequencing the genomes of positively screened cells, we were able to link the identity of these populations to the activity of cellulose deconstruction. This link provides insights into the *in situ* function of those populations in their native environment, and also allows predictions as to which genes they may have been using to accomplish deconstruction under these extreme environments. The recovered genes that we postulate were encoding the activity of cellulose deconstruction are fairly divergent from the amino acid sequences of known cellulases, suggesting these uncultivated microbes may possess untapped suites of enzymes for plant biomass deconstruction under extreme conditions.

We are currently in the process of sequencing a large number of genomes that were recovered from these environments using the cellulose-based selection approach, and moving forward with genomic analysis and functional validation of the putative cellulases recovered.

DESIGN OF HIGH-ENERGY DENSITY LITHIUM-ION SYSTEMS

Principal Investigator(s): Gerbrand Ceder

Project Description

Li-ion batteries provide the highest energy density of any rechargeable battery system, and as such have become the technology of choice for everything from portable electronics to electrical vehicles. Solid-state Li-conducting electrolytes have the potential to radically transform the Li-battery industry by significantly enhancing energy density, and eliminating safety concerns. Today, most incidents in Li batteries are caused by combustion of the electrolyte, which is an organic carbonate based liquid with high flashpoint. Replacing this flammable liquid with a solid-state conductor would make Li-ion batteries a highly safe technology and thereby accelerate its deployment in critical energy technologies where safety is a major concern, such as electrical vehicles and large-scale energy storage. To further improve energy density we are pursuing a novel class of cathode materials. We have recently shown that disordered rocksalt materials can function as cathode materials with very high energy density. By designing the appropriate state of order the Li composition of these materials can be adjusted so that diffusion through low activation-energy channels becomes percolating. These materials can achieve capacities > 250 mAh/g and achieve energy densities approaching 1000Wh/kg.

Accomplishments

We have developed the capability to make fully solid-state devices without any flammable liquid electrolyte. Using a thio-phosphate solid-state conductor as separator and as additive to the cathode, pellet based cells have shown very good initial performance. The solid-state conductor is mixed with the cathode and pressed to very high pressure. A pellet of conductor is similarly fabricated and added to this in a pressurized cell. We are currently investigating how to lower the operating pressure of the cell. We have also looked into boundary layers and coatings to prevent reaction between the solid-state electrolyte and the cathode. Initial attempts with fluorination have shown some success.

Hard X-Ray Photoemission for Materials Science

Principal Investigator: Charles S. Fadley

Project Description

Our goal is to significantly advance a newly established type of spectroscopy for materials science: hard x-ray photoemission (HXPS, HAXPES, HX-PES,...) with excitation energies above about 2 keV and enhanced bulk and buried interface sensitivity, to bring its benefits to a broader spectrum of users at LBNL and elsewhere, and to apply it to a broad range of forefront problems in materials science. An additional element is using standing-wave (SW) effects in both HXPS and soft x-ray photoemission (SXPS-with energies from a few hundred to 1.5 keV), as well as angle-resolved photoemission (SW-ARPES) to probe buried layers and interfaces in multilayer nanostructures with much higher sub-nm depth resolution . Exploiting the complementarity of hard and soft x-ray photoemission is a key strength of this program, based on extensive experience in the Fadley Group. The status of HXPS and standing-wave photoemission is reviewed in recent articles and book chapters [1,5,6], and I am co-chairing a major conference on this technique to be held at LBNL in 2017: <https://sites.google.com/a/lbl.gov/haxpes2017/>.

Accomplishments

We have carried out studies on several different materials systems, with collaborators at LBNL and elsewhere; see publication list, with numbers referenced here in brackets.

- With Bluhm (LBNL CSD), we have in the prior year for the first time combined SW excitation with HXPS and ambient-pressure photoemission at up to tens of Torr pressure in the study of solid-liquid films, opening a range of applications for the technique in energy & environmental studies. This collaboration continues, now involves work with the CAMERA project to greatly enhance the speed of data analysis, and will be the topic of an LDRD proposal in FY17.
- With Stemmer et al. (UCSB) and Chakhalian et a. (Rutgers), we studied multilayer oxide systems composed of: • LaNiO₃ and SrTiO₃, which show insulating behavior in thin LaNiO₃ layers [2], • GdTiO₃ and SrTiO₃, of interest because they exhibit a two-dimensional electron gas (2DEG) and ferromagnetic order at the interface between these two insulating materials [3], and a metal-to-insulator transition in ultra-thin manganite-cuprate superlattices [4].
- With Javey et al. (LBNL MSD, UCB), we used soft x-ray photoelectron microscopy to study single-layer transition-metal dichalcogenide semiconductor membrane structures that are very promising for future photovoltaic devices. We have also obtained additional HXPS and SXPS and ARPES data for these systems that are being analyzed and written up [7].
- With Chambers et al. (PNNL MSD), we combined SXPS, HXPS and SW-ARPES with local-density theory to study the interface-induced ferroelectricity of LaCrO₃/SrTiO₃ [8].
- With co-workers at the ALS, we have used Bragg reflection from crystal planes in the high-TC superconductor BSSCO to generate standing waves and for the first time measure the atomic-layer-resolved densities of states in this material [9].
- In work at the ALS and the Diamond Light Source, we have used hard x-ray Bragg reflection from crystal planes to generate standing waves in GaAs and in Mn-doped GaAs and thus via angle-resolved photoemission (HARPES) to determine for the first time element- and momentum- resolved densities of states in these materials [10], with broad future applications.
- In work at the ALS and at the European Synchrotron Radiation Source, we have for the first time used standing-wave excitation to provide depth resolution in resonant inelastic x-ray scattering [11], also with broad future applications.

Exploring Strong Visible Light-Matter Interactions in Correlated Oxide Materials
 Principal Investigator(s): Lane W. Martin

Project Description

Next-generation electronic and energy systems will have stringent performance requirements that may necessitate the development of a new set of materials. Complex oxides represent a class of candidate materials, but one that remains relatively poorly understood. Such applications require the identification of and control of materials that exhibit a variety of inter-related properties. For instance, an effective photovoltaic or photocatalytic material must possess a diverse set of electronic, optical, and chemical properties including strong absorption of sunlight, proper band alignment to drive charge separation/electrochemical reactions, *good* charge transport, long-term stability in air/solution, and low-cost. The search for a perfect material possessing all of these qualities has not been successful.

The proposed research aims to advance the mesoscale science of how to produce and control light-matter interactions in complex materials. We seek to discover, observe, characterize, understand, and ultimately control light-matter interactions at the mesoscale using advanced thin-film synthesis, structural and chemical analyses, and probes of optical, electrical, and other properties. The program provides an in-depth understanding of the structural and chemical nature of oxide films and interfaces and, in turn, how this impacts the ultimate performance of energy-systems and has implications for controlling fundamental energy transfer processes in devices.

Accomplishments

During this program, we have accomplished a number of important outcomes. First, we examined the evolution of the structural motif (*i.e.*, lattice parameters, symmetry, and octahedral rotations) of the interesting optical material SrRuO₃ as thin films grown on substrates engineered to have the same lattice parameters, but different octahedral rotations. This change in substrate changed the structural symmetry as well as the electrical transport and magnetic properties. Synchrotron-based quantification of the octahedral rotation network reveals that the tilting pattern in both film variants is the same and the abnormal rotation pattern observed in tetragonal SrRuO₃ indicates a possible decoupling between the internal octahedral rotation and lattice symmetry, which could provide new opportunities to engineer thin-film structure and properties. Studies of optical property evolution are ongoing.

Second, we explored the effect of growth conditions on the cation and anion chemistry, electrical leakage, conduction mechanisms, and ferroelectric and dielectric behavior of the interesting optically-active material BiFeO₃. Large variation of cation chemistry and cation gradients gave rise to marked differences in surface and domain morphology and electrical, dielectric, and ferroelectric properties. Studies of optical property evolution are ongoing.

Third, we explored the optical properties of a self-assembled metamaterial based on the innate spinodal decomposition of the VO₂–TiO₂ system wherein the metal-to-insulator transition in VO₂, and thin-film epitaxy enable the production of self-organized nanostructures with coherent interfaces and a structural unit cell down to 15 nm (tunable between horizontally and vertically aligned lamellae) wherein the iso-frequency surface is temperature-tunable from elliptic to hyperbolic dispersion producing metamaterial behavior. These results provide an efficient route for the fabrication of nanostructured metamaterials and other nanocomposites for desired functionalities. Additional studies of these structures are under way.

**Project Title: DEFECT DYNAMICS AND SURFACE EVOLUTION OF TUNGSTEN
STUDIED WITH ULTRAFAST ELECTRON DIFFRACTION**

Principal Investigator(s): (Andrew Minor, Daniele Filippetto, Andre Anders, Thomas Schenkel)

Project Description

We proposed a pilot project to investigate ultrafast processes responsible for the degradation of Tungsten thin films using both ultrafast electron diffraction (UED) at the APEX beamline and multiscale characterization at the National Center for Electron Microscopy (NCEM) in the Molecular Foundry. Our project involved the initial implementation of an *in situ* pump-probe experimental setup at the APEX beamline and correlative high resolution characterization at NCEM. The initial year of this project was intended to investigate the electron transparent materials as well as to build imaging components for the High Repetition-rate Electron Scattering (HiRES) beamline to take advantage of our unique high flux electron source for ultrafast imaging, not just diffraction. If successful, the use of HiRES for imaging would be a dramatic first step towards picosecond imaging with nanoscale resolution.

Accomplishments

In the initial year of this project, the main experimental chamber was designed and installed and alignment of the beam for ultrafast electron diffraction experiments was accomplished. To do this, the dipole junction, that steers the beam down the UED beamline away from the APEX high energy acceleration line, was installed. The necessary beam pipe, view screens, cameras, vacuum pumps, and support structure were also installed. The entire line maintained high vacuum, electrons were transmitted and initial ultrafast electron diffraction experiments commenced. Within the sample chamber, we installed a sample positioning assembly with two linear and two rotation stages for alignment of the multi-sample cartridge to the laser and electron beams. All four of the in-vacuum motors required for the sample manipulation were installed to enable sample positioning.

During the first year of this project we actively worked on acquiring, preparing and characterizing materials for UED studies of 2D materials. This included rhenium disulfide and tantalum disulfide bulk single crystals from 2D Semiconductors and CVD graphene samples from Fudan University. The rhenium disulfide was initially characterized at NCEM on TEAM 1 and the TitanX microscopes. Through collaborators we also have prepared graphene and Black Phosphorus samples.

The UED team successfully modeled the dynamics of the beam shape, time evolution, and maximum dose from the RF electron gun, through the entire beamline, and to the sample plane. From beam dynamic simulations, it was determined that a spot size of approximately 18nm will be possible with a proposed future upgrade to the UED line. In addition, dynamic electron diffraction simulations were performed on monolayer graphene upon heating by a pulsed heating source.

UNDERSTANDING RADIATION-INDUCED PHOTO-ELECTRON CHEMISTRY IN HIGH-CROSS SECTION ORGANOMETALLIC RESIST MATERIALS

Principal Investigator(s): Patrick Naulleau, David Prendergast

Project Description

The purpose of this project is to gain fundamental understanding of extreme ultraviolet radiation chemistry thereby accelerating the development of novel photoresist materials crucial to maintaining the long term viability of the semiconductor industry. The transition from 193-nm to 13.5-nm lithography brings with it a fundamental change in exposure mechanics, yet these new exposure mechanics are not understood. At 193-nm, the photoactive components in resist specifically absorb the DUV photons, at EUV however, the photons do not preferentially interact with the photoactive components and without understanding the actual mechanism, it is not possible to direct the development of new photoresist materials or concepts. This lack of knowledge has manifested itself in a stagnation of progress in EUV resist. In fact, in the past four years, no improvements have been made in the achievable resolution limits for EUV resists which are stuck at 16 nm compared to long term targets on the order of 5 nm. Moreover the sensitivity of these materials is 2x too slow to be commercially viable. The fundamental understanding sought here will enable development of materials specifically tailored to EUV and meeting the nanoscale patterning challenges.

Accomplishments

Our LDRD project has demonstrated new experimental and theoretical tools to investigate EUV photon-molecule interactions. Using synchrotron tools developed for chemical dynamics, we have correlated photo-absorption efficiency with molecular structure, measured the energy distribution of photo-emitted electrons and followed the post-excitation fragmentation of molecular targets. A velocity map imaging photoelectron spectrometer, built during the first year of the project has been utilized to collect photoelectron and mass spectra of the gas-phase molecules after EUV irradiation. Mass spectrometry coupled to electron ionization has been applied to understand the response of the molecules on the interaction with EUV emitted electrons. This data demonstrates the ability of molecule to emit more than one electron per absorbed photon, affords the possibility to tweak molecular absorption cross-sections, as well as generate significant fragmentation of the molecules, and finally to understand the important role of low kinetic energy electrons.

In a parallel effort theoretical simulation tools have been developed for EUV molecular photo-absorption and relaxation. These new capabilities have been used to demonstrate that molecules containing atoms with 4d orbitals accessible to EUV ionization such as iodine have significantly stronger absorption, and that only part of the incident energy is carried away by the photoelectron. Additional secondary electrons are emitted during Auger relaxation of the molecular photo-ion, followed by molecular fragmentation. Increasing molecular EUV absorption changes the nature of the radiation-induced chemistry, producing more electrons, ions and radicals. The toolset we have developed promises to enable intelligent design of optimized EUV resist systems.

Computational Design of Smart Complex Oxides with Tunable Quantum Phases

Jeffrey B. Neaton

Project Description

In this project, we develop and use computational approaches for discovery and design of complex functional materials for next-generation energy, computing, and information technologies. We will use a combination of state-of-the-art ab initio computational approaches – including density functional theory and many-body perturbation theory within the GW approximation and the Bethe-Salpeter approach – and high-throughput techniques to perform informed, comprehensive searches to identify new tunable and topological materials of technological relevance. Importantly, we will also understand and develop design rules for how atomic-scale structure and chemical composition conspire to give rise to tunability of novel quantum phases, providing a blueprint for future efforts to synthesize new materials in this and related classes.

Accomplishments

This past year, we have developed a workflow to identify new tunable and topological phases. Through collaborations with the BES-funded Materials Project Predictive Modeling Center, we have built a multi-layer computational screening workflow – including methods to efficiently evaluate wavefunction parity, band structure, and other topological properties – to search for new topological insulators and Dirac semimetals in a large compound space. Our focus has been on a class of topological materials, nodal semimetals – materials systems with nodal-point or -line Fermi surfaces – that are much sought after for their novel transport and topological properties. We recast the previously-derived constraints on the allowed electron fillings for band insulators in the 230 space groups into a new form, which enables effective screening of materials candidates based solely on their (1) space group, (2) electron count in the formula unit, and (3) multiplicity of the formula unit. This criterion greatly reduces the number of candidate materials in a database of previously-synthesized compounds, and helps us to efficiently identify a handful of candidates, from sampling only a few nonsymmorphic space groups.

Another exciting near-topological hybrid system where spin-orbit interactions are strong is MAPbI₃ and related compounds. Photovoltaic devices based on MAPbI₃ have exceeded 22% efficiency due to high charge-carrier mobilities and lifetimes. In collaboration with Alex Weber-Bargioni, we interpreted measurements that map the local short-circuit photocurrent, open-circuit photovoltage, and dark drift current in state-of-the-art MAPbI₃ solar cells using photoconductive atomic force microscopy. Our first-principles density functional theory calculations establish how Rashba-type energy band splitting in the hybrid organic–inorganic halide perovskites APbX₃ (A = CH₃NH₃⁺, CH(NH₂)₂⁺, Cs⁺, and X = I, Br) can be tuned and enhanced with electric fields and anisotropic strain. Further, our calculations quantify the degree to which this effect can be tuned via chemical substitution at the A and X sites, which alters amplitudes of different polar distortion patterns of the inorganic PbX₃ cage that directly impact Rashba splitting. In addition, we have made predictions regarding the polar phases of CsPbI₃ and (CH₃NH₃)PbI₃ with R3c symmetry possessing considerable Rashba splitting.

Project Title (A stochastic approach to calculate Auger recombination and impact excitation rates: Application to core-shell nanocrystals and seeded nanorods)
Principal Investigator(s): (Eran Rabani)

Project Description

The main goal of this project is to understand the Auger process in confined semiconductor nanostructures in the crossover region from zero-dimensional (quantum dots) to one-dimensional (quantum rods) and in heterodimensional nanostructures with mixed dimensionality such as dot-in-rod semiconductor heterostructures. The scaling with size and number of excitations of the Auger process is well understood in quantum dots and quantum wires, but poorly understood in the crossover region between the two confined geometries. Moreover, little is known on how coupling zero- and one-dimensional structures affects the Auger process.

We will develop an efficient *linear scaling* computational approach for calculating the Auger recombination rates to address the above challenges. This will be achieved by developing a stochastic approach to obtain the Auger rates based on our recently developed stochastic impact excitation rates and stochastic GW formalism. Extensions of the approach will focus on describing Auger rates in strongly confined excitons and the crossover to strongly interacting excitons, which correlated with the crossover from zero- to one-dimensional confinement.

Accomplishments

Our most significant accomplishment has been to develop stochastic Auger and implement it to study the process in system exceeding 50,000 electrons. This has been done for strongly confined system where the Auger process can be described by lowest order perturbation theory which neglects electron-hole interactions as well as for weakly confined system in one-dimension, where electron-hole interactions are considered within the Bethe-Salpeter equation.

In addition, we have also implemented the approach to quantum dots (CdSe), to core-shell quantum dots (CdSe/CdS), and to CdSe/CdS seeded nanorods within the lowest order stochastic perturbation theory, and to CdSe quantum rods within the weakly confined approach considering the electron-hole interactions. These preliminary results illustrate the strength of the stochastic Auger approach in describing Auger processes in extended nanostructure with open boundary conditions and diverse dimensionality. Future work will be devoted to uncover the scaling of the Auger process in the aforementioned crossover regime.

Project Title: Controlling Quantum Phenomena in Van der Waals Heterostructures
Principal Investigators: Feng Wang, Alex Zettl

Project Description

This project aims at understanding and controlling novel quantum phenomena and excited state properties in van der Waals (vdW) heterostructures. The successful isolation and manipulation of atomically-thin sheets of 2D crystals has ushered in a new era of basic scientific research and technological innovation: 2D layers of wide-ranging properties can now be grown separately and then simply stacked together to form a new class of materials (van der Waals-bonded heterostructures) with unprecedented flexibility and control. This enables the design and creation of functional 2D materials combining extremely different properties, which were simply not possible before. A large variety of 2D layers exist, ranging from semiconducting MoS₂ and insulating boron nitride to metallic TaS₂ and superconducting FeSe, that can be stacked, one on top of the other. The different quantum phenomena available to vdW heterostructures, such as superconductivity, magnetism, and charge density waves, can interact and couple to each other in ways that are not possible in other systems. Additional unprecedented control of physical properties in 2D vdW heterostructures can be achieved through electrostatic gating, mechanical strain, and substrate engineering. We propose to explore the enormous research opportunities that are manifest in atomically-thin vdW heterostructures. Specifically, we will develop ultraclean vdW heterostructures using micro-exfoliation and mechanical transfer in a controlled environment, and explore their novel electronic and optical properties. This LDRD builds upon and greatly expand the existing collaboration between Wang and Zettl. It will draw upon the unique capabilities of these two groups by combining the advanced device fabrication, electron microscopy, and transport expertise of Zettl and the ultrafast laser spectroscopy and optoelectronic expertise of Wang.

Accomplishments

Our most significant accomplishment has been to develop a reproducible protocol for preparing ultraclean Van der Waals heterostructures. Our method uses mechanical micro-exfoliation of atomically thin transition metal dichalcogenide (TMDC) crystals and hexagonal boron nitrid (hBN) crystals. Such two-dimensional crystals are stacked in a controlled environment to form high quality heterostructures with almost atomically clean interfaces.

Based on such ultraclean TMDC/hBN crystals developed in the LDRD effort, we are able to explore novel interlayer interactions between the 2D materials. We observed for the first time the interlayer electron-phonon couplings in van der Waals heterostructures.

The LDRD project also leads to a successful follow-on FWP project funded by the department of energy.

Sequence and Codes in Multivariate Metal-Organic Frameworks (MTV-MOFs)

Principal Investigator(s): Omar M. Yaghi

Project Description

The Yaghi group has previously demonstrated the capability of assembling linkers with different functional groups to construct single-phase metal organic frameworks, which have multivariate (MTV) functionalities. The sequence of such functionalities and the spatial arrangement where certain ones appear inside the pores, along with selective post-synthetic modifications (PSMs) on specific functional groups, will achieve a new level of complexity. This MTV approach allows fine-tuning of the pore environment with desirable implications on properties, *e.g.*, heterogeneous catalysis.

A general synthesis and characterization routine of building MTV-MOFs will first be established. Since fully functionalized MOFs are known to have decreased surface area and limited pore access, unfunctionalized struts will be mixed during synthesis to dilute the functionalities. The ratio of these two kinds of linkers can be modified to study the effect on surface area on resulting MOFs and consequential PSM reaction yield. The crystallinity and other properties will be analyzed using X-ray diffraction, spectroscopic, elemental, and gas adsorption analyses, and SEM/TEM observations. Two-dimensional NMR will be utilized to examine the spatial distribution of functionalities in nanoscale. Catalytic studies will be performed in collaboration with research groups of expertise.

Accomplishments

Post-synthetic Covalent Reactions in Tandem Leading to Enzyme-like Complexity within Metal-Organic Framework Crystals. The design of enzyme-like complexity inside MOFs requires multiple reactions to be performed on a MOF crystal without losing access to its interior. Up to seven post-synthetic reactions were successfully performed within the pores of a multivariate MOF, MTV-IRMOF-74-III, to covalently incorporate tri-peptides that resemble the active sites of enzymes in their spatial arrangement and compositional heterogeneity. With precise control over the type and ratio of the functionalities, high yields could be achieved of the seven post-synthetic reactions while retaining the porosity and crystallinity, leading to highly selective catalytic activity that were previously accomplished only in the presence of enzymes.

Photocatalytic CO₂ Conversion within Metal-Organic Frameworks Under Visible Light. Catalysts for carbon dioxide reduction with good reactivity, selectivity and durability are in great need. A CO₂-to-CO conversion photocatalyst Re^I(CO)₃(BPYDC)Cl, BPYDC = 2,2'-bipyridine-5,5'-dicarboxylate was incorporated into a zirconium MOF, UiO-67 (Re_n-MOF), which prevents the dimerization of the molecular catalyst and its deactivation. The photocatalytic activity can be tuned by precisely controlling the catalyst-containing/unfunctionalized linker ratio (the MTV approach) to adjust the density of covalently attached photoactive centers within MOF interior. Such catalytic units can also be spatially identified; structural analysis of Re-MOFs suggests that a fine balance of proximity between photoactive centers is needed for cooperatively enhanced photocatalytic activity, and that an optimum number of Re complexes per unit cell should reach the highest activity.

Project Title: Optical and Electrical Characterization of 2-Dimensional Nanosheets without Naturally Layered Structure
Principal Investigators: Jie Yao

Project Description

The purpose of this project is to explore new material phases that are only stable in ultrathin layers, namely, the 2D form. In particular, we synthesize and characterize sub-nm sheets of ZnO with h-BN like phase as an example. Our synthesis approach allows the exploration of physical and chemical properties of such new phases and enables novel device applications.

The samples are grown using a graphite oxide template method. The templates provide sufficient confinement for reduced thickness growths. This size of sample synthesized with our method is orders of magnitude larger than previously reported ones and is sufficiently large for performing characterization on single sheets. Optoelectronic characterization will be performed in order to understand how the new phase differs from its bulk wurtzite phase and verify its intrinsic behavior. Additionally, structural measurements will confirm the phase and provide high resolution information to assist in theoretical studies. This information will allow us to develop devices using these materials, both intrinsic and as part of heterostructures with other 2D materials.

This method can be utilized to reliably create large sheets of hBN – ZnO for studies and applications of this unique phase by itself, as well as in combinations with other nanoscale layered materials. This technique can also be extended to doped and alloyed versions of the new ZnO phase, and potentially to other material systems. The data from characterization will be useful in determining the potential uses of this phase of ZnO, which has been predicted to be useful for many applications.

Accomplishments

Atomic force microscopy (AFM) measurements have confirmed successful high-yield synthesis of sub-nm thick ZnO sheets with lateral sizes that reach up to 30 μm , allowing direct optical characterization and fabrication of devices for the first time. From TEM measurements, it was confirmed that the samples are polycrystalline with good crystalline quality, with a grain size ranging from 5-25 nm. Energy Dispersive X-ray spectroscopy also confirms the samples are primarily Zn and O, with minimal carbon left after the removal of the template. Thickness dependence photoluminescence shows a change of optical response near 1 nm in thickness, from a strong emission near the typical ZnO emission peak at 3.3 eV to a weak emission peak at 3.45 eV, which suggests the formation of the hBN phase. Additionally, after a high temperature (800°C) anneal in air, thicker samples were found to coarsen to nanoparticles where sub-nm samples remained flat, also suggesting the formation of the hBN phase. A manuscript has been prepared based on our discovery and will be submitted for publication soon.

Further explorations are going to be conducted on the new phase of ZnO. Structural characterization using Extended X-ray Absorption Fine Edge Spectroscopy (EXAFS), Grazing Incidence X-ray Diffraction (GIXD), and cross-sectional TEM will create a complete view of the hBN-ZnO structure, including any possible distortions caused by the stabilization of the new phase. Additionally, electronic transport measurements will be performed in order to determine the conductivity of the samples and their suitability for applications.

Advanced Computational Tools for High Resolution Cryo-Electron Microscopy

Principal Investigator(s): Paul, Adams

Project Description

The availability of direct electron detectors places single particle cryo-EM at a transformative point in its development. These detectors have made it possible to collect higher quality data and also apply newly developed methods to account for drift in the experiment. This now makes it possible to obtain single particle density maps that can be interpreted *ab initio* to generate atomic models. Reconstructions at resolutions comparable to X-ray crystallography (3Å to 4.5Å) will likely become more commonplace. Advanced computational tools for analyzing cryo-EM data will differentiate LBNL as a center for atomic resolution electron microscopy. Our high-level goals are:

- Extend our algorithms for the **optimization of atomic models** from X-ray data to make **direct use of cryo-EM density maps**. Biological insight from atomic resolution imaging relies on accurate, chemically reasonable structures. Current methods fail to do this, greatly limiting the value of the resulting models. Progress in this area may eventually lead to pharmaceutical industry use of the cryo-EM facility.
- **Apply these new developments to real-world biological problems** in collaboration with local researchers.

The resulting computational tools will provide a powerful platform for a proposed cryo-EM imaging facility at LBNL, enabling researchers to maximize the information they can obtain from challenging experiments. The ability to obtain atomic resolution structures in this way, especially for large molecular complexes, will be transformative for problems in human health, bioenergy, and systems & synthetic biology.

Accomplishments

In the last year we have made excellent progress in developing new computational algorithms and software to enable new workflows for the interpretation of cryo-EM maps. We have focused on the problem of model optimization, as this is new territory for cryo-EM practitioners. It is often the case that models built, automatically or manually, at low resolution start refinement with significant distortions from ideal geometry. We have therefore developed algorithms to automatically idealize secondary structure elements in models by local rebuilding. In this approach we use secondary structure identification and validation algorithms to locate distorted parts of the model that are then replaced by idealized versions. The resulting model is then refined with additional restraints to maintain secondary structure, torsion angle restraints on the protein main chain, and reference model restraints to the starting structure.

Idealization of protein loops differs from secondary structure idealization because of the large number of potential backbone conformations. Loops with poor geometry, in particular those with Ramachandran outliers can be readily identified using standard validation tools. However, correction of a Ramachandran outlier often requires significant changes in nearby backbone torsion angles to maintain the corrected loop spatially close to the initial loop and also to avoid introducing new outliers. We have developed an approach that detects Ramachandran outliers, corrects their backbone torsion angles and then use the cyclic coordinate descent algorithm to find appropriate values for nearby torsion angles. After backbone correction, side chains are restored in idealized conformations based on testing rotamers against the density. Initial tests show that a significant fraction of Ramachandran outliers can be corrected this way, leaving the main chain atoms within the convergence radius of current refinement methods.

Interfacing Chemical and Biological Catalysis for Solar-to-Fuel Conversion

Principal Investigator(s): Michelle Chang

Project Description

The purpose of this project is to develop approaches to integrate chemical and biology catalysis for solar-to-fuel conversion consisting of light-harvesting materials functionalized with hydrogen-producing catalysts and living microbes as an autotrophic chassis for the production of value-added fuels and other chemicals from CO₂ and photogenic H₂. Specific aims include (i) development of photocatalytic H₂-producing inorganic platforms that can operate in aqueous media at physiological pH and ionic strength, as well as (ii) metabolic engineering of H₂-metabolizing organisms to divert carbon fluxes to value added carbon products. In the past year, we have focused on developing methanogens as a synthetic biology platform for this goal.

Accomplishments

We have initiated work with the methanogen, *Methanococcus maripaludis*, which is capable of fixing carbon dioxide to produce methane as a product (*Figure 1A*). In this pathway, acetyl-CoA serves as a key intermediate and could possibly be tapped for the production a value-added compounds such as isoprenoids, polyketides, fatty acids, and a variety of other targets. In the past year, we have developed approaches for genetic engineering of *M. maripaludis*. In order to probe our ability to tap into the acetyl-CoA pool, we have constructed a series of pathway

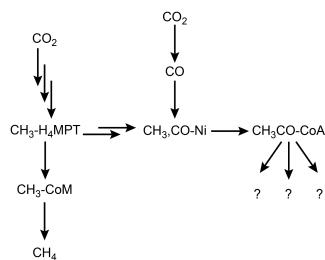


Figure 1. Developing *M. maripaludis* as a synthetic biology platform. Pathways downstream of carbon dioxide produce methane and acetyl-CoA.

variants for the production of 3-hydroxybutyrate. In testing this pathway, we have found that we can obtain high expression of the first gene in the pathway but the expression of the remaining genes are low. Upon further exploration, we attribute this behavior to differences in the 5'- and 3'-untranslated regions of the mRNA transcripts of archaea compared to other canonical hosts. We are currently working to address this limitation and have designed new constructs. In addition we are addressing other limitations in the metabolism of archaea that would need to be addressed when using enzymes from other hosts.

Designing Efficient Energy Conversion Pathways for Synthetic Organisms
Principal Investigator(s): Karen M. Davies

Project Description

The purpose of this project is to dramatically increase our understanding of how nature converts sunlight and other natural energy resources into the cellular energy units, ATP and NADPH, required for biomass or biopolymer production. The ultimate aim is to combine the most efficient natural energy converting pathways into synthetic organisms to improve the productivity of designer compounds e.g. Xylene, Polylactic acid, or Ethene, in large-scale industrial growth vats. To achieve this aim, we are comparing how the structure and *in situ* organization of proteins involved in both photosynthesis and oxidative phosphorylation from various species change with different growth conditions and how this influences the efficiency of the energy converting pathways.

Our approach involves two new revolutionary imaging techniques, which have not been routinely performed at LBNL. These techniques are: electron cryo-tomography and electron cryo-microscopy. Electron cryo-tomography allows a researcher to directly visualise the inside of cells at a resolution where both protein structure and membrane morphology is easily observed. This technique enables scientists to assess how proteins interact in cells to execute a function and how the efficiency of this pathway could be improved. Electron cryo-microscopy provides close to atomic details of macromolecular complexes allowing scientists to decipher atomic mechanisms of many enzymatic reactions aiding in the development of synthetic biocatalysts. One of the key aims of this LDRD project is to establish these two novel imaging techniques as a mainstay technique for all LBNL scientists in order to assist in the execution of DOE-directed research.

Accomplishments

Accomplishments to date involve primarily the installation and modernization of existing infrastructure to allow the routine execution of electron cryo-tomography and electron cryo-microscopy at LBNL. These include: repair of the house coolant systems and air condition units, replacement of antiquated windows computers, establishment of fast data transfer networks, installation of new computation resources, and the installation of the new ground-breaking direct electron detector (developed at LBNL) on our high-end transmission electron microscope.

Other accomplishments include hiring of new personal, establishment of scientific collaborations and protein purification protocols. To this end, I have hired a full-time postdoc, who, after several months of obtaining sufficient biomass, is establishing protein purification protocols to isolate membrane proteins involved in energy conversion from several species. Our most promising results are from a cyanobacteria where we have isolated a membrane protein complex involved in the energy conversion pathway to a purity which is almost sufficient for structure determination by single particle electron cryo-microscopy.

Robust Synthetic Membranes for Microbial Electrocatalysis: Separating Electron-Generating Organisms from the Catalytic Reaction Environment

Principal Investigators: Heinz Frei and Caroline Ajo-Franklin

Project Description:

Biohybrid technologies that combine bacterial and inorganic catalysts have been touted as a means of converting the dilute energy contained in wastewater or light to fuels and chemicals. Despite recent leaps forward, biohybrids need several major breakthroughs to become viable and, in particular, scalable on a scale that will have an impact on chemical manufacturing or fuel consumption, largely because of limitations at the abiotic/biotic interface. The goal of this project is to couple the incompatible inorganic and biological environments on the shortest possible length scale – the nanoscale – under membrane separation. Our approach consists of creating a single integrated biohybrid assembly composed of solid-supported inorganic catalysts separated from microbial catalysts by a nanometer-thick functionalized silica membrane.

Accomplishments:

We have designed in the first 12 months a novel biohybrid assembly, synthesized new molecular components tailored for it, and integrated these components into subsystems which we show have the desired functionality. These accomplishments poise us for demonstrating in the coming year the first nanoscale biohybrid assembly. Main features are the molecularly defined electronic properties of the interface and the modularity of the synthetic approach allowing the facile tuning of energetic and chemical properties for optimizing biohybrid function.

The integrated biohybrid assembly must chemically separate the microbial and inorganic catalysts while still electrically connecting them on the nanoscale. To enable spontaneous electron flow, new molecules and new synthetic methodologies needed to be developed. We synthesized novel wires based on *para*-oligo(phenylene vinylene) backbone and showed via cyclic voltammetry that addition of electron withdrawing groups to this backbone raises the redox potential to the desired range. We synthesized novel anchor moieties, including ‘spiders’ (e.g. $(BrCH_2)_3C-NH_2$) and $H_2N-Ph-Si(O)_3$ tripods to enable the covalent attachment of these molecular wires to energetically-matched inorganic supports. New amide coupling methods were introduced that afford a modular approach for wire assembly on these oxide surfaces.

In parallel, we have integrated several subsystems of increasing complexity and demonstrated the desired functionality. We verified that the subsystem of the microbial catalysts and the silica membrane are functionally compatible, i.e. the membrane supports attachment and growth of the cells, and the cells do not disrupt the structural or chemical properties of the membrane. We also demonstrated functionality of the inorganic catalysts: Upon injection of electrons into WO_3 conduction band, Au nanoparticles were able to catalytically convert O_2 to H_2O_2 , an important industrial oxidizing agent.

We have integrated and tested a 3-component subsystem composed of *S. oneidensis* microbial catalysts, the silica membrane with or without (non-optimized) embedded wires, and a WO_3 inorganic support. Using a specially-designed home-built electrochemical cell, we find that significantly more current is collected from the inorganic support when the molecular wires are present ($1 \mu A/cm^2$) than when they are not ($0.1 \mu A/cm^2$). In line with this observation, there is roughly an order of magnitude more living microbial catalysts on the wire-containing surface than the surface lacking wires. Taken together, these experiments suggest that we can electrically connect inorganic supports and microbial catalysts via nanoscale silica membranes.

Life Science applications of X-ray scattering at ALS-Upgrade

Principal Investigators: Greg L. Hura & John A. Tainer

Project Description

We see transformative advantages for our field through coordinated upgrades of the Advanced Light Source and its beamlines. We aim to accomplish both short and long term plans for enhancing existing capabilities and introducing new ones for the characterization of structure in biology. Central to our aims is experimentally demonstrating requirements on a light source for optimal implementation. Our proposal further optimizes what we have available now and defines light source upgrades which will have significant impacts. Our goals address the following two biological challenges 1) Building intuition on the large networks and multi-level feedback loops in cellular systems requires many measurements which current capabilities cannot deliver 2) Engineering biologically inspired macromolecules requires a rapid means to compare design relative to reality. By coordinating efforts to address these challenges we will ensure the ALS upgrade has high impact for the biosciences.

Accomplishments

With 6 months of funding left we are seeing the final steps in completing our goals as part of this LDRD. We have now installed a new liquid handler on the SIBYLS beamline. We took advantage of a 3 month shutdown of the ALS so as to have no impact on our user community. We are currently performing tests of the system *in situ*. We have begun to reengineer our beamline to accommodate the new system and integrate its control with other beamline equipment.

The new robotics will increase our throughput and will also mean significant investments in control and error checking. High throughput data collection can also be a tremendous waste of sample if controls are not in place. For biology, sample is limiting so significant continued effort is required in this area.

We have also re-designed sample delivery and estimate that we will exceed the ten-fold increase in speed promised in our proposal. This is not only due to the new robotics but also do to new sample delivery methods. The amount of decrease in sample requirements is still unclear. However we are certain that there is at least a two fold decrease. These two features together should be a tremendous advance for the application of SAXS at the ALS. We anticipate new science that will guide applications for ALS-U.

An example publication that will further motivate high throughput SAXS has been accepted. We have published an article titled “Designing and defining dynamic protein cage nanoassemblies in solution” in the journal *Science Advances*. In this publication we report a designed 600kDa macromolecular complexes and comprehensively asses their structure in a variety of solution conditions. We seek to build on this publication with our new instrumentation.

Codesigning Big Iron for Big Data - ‘Designing High Performance Computing Resources to Meet the Needs of Data Intensive Science’

Principal Investigator(s): Nicholas J. Wright,

Project Description

The purpose of this project is understand

1. How do the new and emerging data intensive workloads require fundamentally different computer architectures from those traditionally deployed at HPC centers?
2. How should we co-design, with our HPC vendor partners, computer architectures to meet the needs of data intensive users and ensure the DOE is able to meet its mission need in this important and emerging area?

Our overarching goal is to rigorously characterize the computing resource requirements of the emerging ‘big-data’ workload, and use that information to drive the design and configuration of advanced computing architectures to meet the needs of this emerging set of application use-cases. This will require we place special focus upon storage architectures, as the extensive use of these is perhaps the principle-defining feature of data intensive workloads today. To achieve this goal we will analyze representative applications and workflows of today. Additionally, we will engage strategically with emerging areas to ensure we meet the needs of applications and workflows of tomorrow. We will then use detailed performance analysis of these applications combined with advanced architectural simulation of future computing system options to understand the correct set of architectural trade-offs for the design of future data-intensive computing systems.

Accomplishments

We have extended our I/O analysis to include a detailed breakdown of time spent in each POSIX I/O call. The results show that some data analytics applications are more limited by metadata performance than data transfer performance. The metadata costs are found to originate from SQLite database updates, Python initialization, and opens of many small scientific data files. Other applications perform parallel reads from a single shared file and are more limited by I/O read bandwidth. These conflicting requirements make it difficult to deliver an ideal storage subsystem for all applications. However, we have demonstrated that there are mechanisms within the DataWarp Burst Buffer that allow the storage subsystem to be tuned for the current I/O workload. In particular, the private namespace feature of DataWarp significantly reduces metadata costs associated with SQLite database accesses. This indicates that capable Burst Buffer software can enable both data and metadata heavy workloads to run efficiently on a single HPC storage subsystem.

We studied the communication requirements of parallel data analytics applications and find 1) some use collective MPI communication with a fixed message size of 4 bytes and 320 KiB, and 2) others use variable-sized non-blocking point-to-point messages to exchange data between many MPI pairs. This second class of applications make use of a distributed k-d tree data structure and are found to have similar communication requirements to simulation science AMR applications. This means data analytics applications can also benefit from hardware features enabling asynchronous progress, MPI tag matching, and network topologies that do not significantly penalize long-range communication.

We analyzed runtime in external libraries and find that simulation science and data analytics applications often use the same libraries and spend significant time in the libraries.

Toward Next Generation Gamma-Ray Tracking Arrays: Development of Inverted Coaxial Segmented HPGe Detector Technology

Principal Investigator(s): Heather Crawford and Reynold Cooper

Project Description

This project is aimed at characterizing a novel next-generation high-purity Ge detector technology, and to better understand the performance limitations for gamma-ray energy tracking detectors. The large-volume inverted coaxial HPGe segmented point contact detector has unique properties associated with the low electric field strength, long charge drift times and highly localized weighting potentials within the detector. These characteristics provide potential for discrimination of single vs. multi-site gamma-ray scattering interactions and outstanding position resolution, but also introduce challenges associated with charge trapping along the drift path, and an associated degradation of energy resolution.

Within this LDRD we will characterize a prototype inverted coaxial segmented point contact detector, and explore the performance limitations associated with this technology. We will perform controlled scanning measurements using highly collimated gamma-ray sources to systematically construct an experimental basis of signals corresponding to gamma-ray interactions localized within the crystal volume. With this experimental signal basis, we will develop pulse shape analysis algorithms to determine, event-by-event, the location of individual gamma-ray interactions. We will explore limitations on the position resolution of such a detector, and on the energy resolution following development of charge-loss correction algorithms. In parallel, we will pursue realistic simulations for this detector geometry, refining the description of signal shapes, etc. in response to the scanning data sets obtained.

Accomplishments

The most significant accomplishment associated with the first year of this LDRD effort has been to improve the energy resolution from the full-volume point-contact signal on the prototype detector. A comprehensive set of collimated beam measurements using a ^{137}Cs source was made to characterize the detector response in two dimensions – namely in depth (z) and in azimuthal angle around the cylindrical axis of the detector. From these measurements, sets of basis signals for the rear segments, which provide information on the azimuthal angle, were produced as a function of charge drift time, serving here as a proxy for depth in the crystal. A pulse-shape analysis was developed to extract for each event the depth and azimuthal angle, allowing a refined correction to the observed energy.

With this two-dimensional position localization and energy correction routine, we have shown one potential drawback of this detector technology to be a correctable quantity. We have also already shown reconstruction in azimuthal angle to be better than 1mm, confirming the potential for position resolution with this technology.

We have now begun work on extending the pulse shape analysis to extract the third dimension in the crystal, namely the radial position. Beyond this, the pulse shape analysis and energy correction developments will be expanded to include more complex events with multiple gamma-ray interaction sites.

COMPUTATIONAL NUCLEAR PHYSICS CODE DEVELOPMENT FOR FUNDAMENTAL INTERACTIONS/ASTROPHYSICS, SUPPORTING FRIB

Principal Investigators: Wick Haxton, Dan Kasen, Thorsten Kurth, NSD
Ann Almgren, John Bell, Esmond Ng, Sam Williams, Chao Yang, CRD

Project Description

The project goal is to develop next-generation codes to support fundamental nuclear physics important to FRIB, the Facility for Rare Isotope Beams. This report describes second-year progress on the project's two foci:

(1) Three-D models of core-collapse supernovae (CCSN) that combine realistic treatments of the nuclear equation-of-state, shock wave generation and propagation, and energy and lepton number transport are typically integrated to one second after core bounce, determining the initial conditions for the star's subsequent mantle ejection and neutrino-driven neutron-rich wind. Our goal is to produce an integrated code framework for propagating the explosion to later times, coupling explosion codes like CHIMERA, the compressible hydrodynamics code CASTRO, and the radiation transport code SEDONA.

(2) FRIB's rare isotopes, if captured in atom traps, can open up new opportunities to test fundamental symmetries such as CP and parity. We are computing the low-energy, symmetry-violating NN interactions probed in such tests, by finding numerically exact solutions of the strong interaction by discretizing time and space on the lattice (LQCD).

Accomplishments (Year Two)

Previous work on parity-violating NN interactions in QCD has been restricted to s-wave interactions due to the use of local multi-nucleon operators. Our group developed new code and successfully performed the first LQCD calculations of the phase shifts for p, d, and higher waves (and for s-wave interactions beyond the scattering length approximation), now published in Phys.Lett.B. We also evaluated neutrinoless double beta-decay amplitudes for lepton-number violating mechanisms mediated short-distance 4-quark operators.

The direct calculation of CP-violating processes with lattice QCD is very challenging. However, the CP-violating pion-nucleon couplings, which dominate the EDMs in large nuclei, can be determined from spectroscopic lattice QCD calculations, a much simpler task. We recently obtained an improved value for the QCD theta-parameter coupling through the most precise lattice QCD calculation of the neutron-proton mass splitting.

In astrophysics we continued development of the 3D CCSN code CHIMERA, including its integration with the local CASTRO/SEDONA suite. Chimera simulations for a variety of initial conditions, reflecting differences in possible progenitors. We explored the yields of radioactive isotopes such as ^{44}Ti , comparing results in 1D to those for 3D.

New code was developed for importing results from Chimera CCSN models into the CASTRO AMR hydrodynamics code. Our implementation properly conserves mass and energy. Differences between the dynamical evolution predictions of CASTRO and Chimera are being studied. Once the evolution to late times is complete, the final ejecta structure will be feed into the SEDONA radiation transport code, allowing us to predict the emission across the electromagnetic spectrum (from gamma-rays through optical).

The work provided the foundation for our recently funded award in the DOE Exascale Computing Project. The project "Exascale Models of Stellar Explosions: Quintessential Multi-Physics Simulations" is led by LBNL with partners at ORNL, ANL, and Stonybrook.

Topmetal Charge Readout Plane for Neutrinoless Double-Beta Decay Searches
 Principal Investigator: Yuan Mei

Project Description

The purpose of this project is to develop a direct charge readout plane that is suitable for high-pressure gaseous Time Projection Chamber (TPC), operating in either electron drifting or ion drifting mode, for the search of Neutrinoless Double-Beta Decay ($0\nu\beta\beta$). A positive observation of $0\nu\beta\beta$ would signal violation of the lepton number conservation, confirm that the neutrino is its own antiparticle, and provide support for the lepton-aided mechanism of generation of the matter-antimatter asymmetry in the early universe. It will also provide insights into the mechanism responsible for non-zero neutrino mass. It has recently been demonstrated that certain high pressure gas such as Xenon exhibits excellent intrinsic energy resolution in the $0\nu\beta\beta$ energy range by ionization alone. When instrumented as a TPC, it enables charge track imaging capabilities that provide extra handle for discriminating $0\nu\beta\beta$ signals against backgrounds. TPCs are also easily scalable to large mass provided there is an accompanying charge readout scheme.

Leveraging the recently developed CMOS direct charge sensor *Topmetal*, we envision the realization of a charge readout plane with a tiled array of CMOS charge sensors, without gas-electron multiplication. Charge collection electrodes, front-end amplifiers, as well as data processing circuits, are integrated in the CMOS sensors placed directly at the site of charge measurement. The plane will simultaneously achieve the necessary low electronic noise for energy resolution and the high spatial resolution for ionization charge tracking, while satisfying the stringent radio-purity and scalability requirements for a future tonne-scale experiment.

Accomplishments

We established the feasibility of direct charge collection in gas without avalanche gain using an earlier version of pixelated low-noise sensor *Topmetal-II*.

Through simulations of both gas properties and electronics, we have completed a parametric optimization of a ~10cm sized prototype plane, which resulted in the full specification of the new *Topmetal-S* CMOS chip that will be tiled on the plane. Working with collaborators, we have completed the circuit design of *Topmetal-S* and have submitted the design to the foundry for production.

We are in the process of characterizing the *Topmetal-S* sensors, designing and constructing a ~10cm sized array, as well as producing readout and analysis firmware/software. These tasks are the main focus of the 2nd year continuation of the project.

Next-Generation Neutrino and Rare-Event Detection

Principal Investigator(s): Gabriel D. Oreb Gann

Project Description

The ability to separate the Cherenkov component from the dominant scintillation signal in organic liquid scintillator detectors would open up the possibility for a new kind of large-scale experiment capable of a very broad program of physics. The program would span both nuclear and high-energy physics, including a next-generation neutrinoless double beta decay search, ultra-precise solar neutrino measurements, geo- and supernova neutrinos, nucleon decay searches, and measurement of the neutrino mass hierarchy and CP violating phase with long-baseline neutrinos. The primary goal of this project was an explicit demonstration of this separation in a range of scintillating target materials.

An apparatus has been constructed at LBNL to perform this characterization, including determining the light yield and timing properties for various target cocktails in order to enable optimization of target choice in large detectors for particular physics goals. Successful separation of prompt Cherenkov light from delayed scintillation would enable significantly enhanced background rejection through a combination of ultra-low energy thresholds (below Cherenkov threshold) and directional information in such experiments.

Accomplishments

With this LDRD we have constructed a sophisticated, high-precision apparatus capable of robust, reproducible measurements of the intrinsic light yield and timing properties of a range of target materials. The CHESS (CHErenkov / Scintillation Separation) experiment employs an innovative detector design with an array of small, fast photomultiplier tubes and state-of-the-art electronics to demonstrate the reconstruction of a Cherenkov ring in a scintillating medium based on photon hit time and detected photoelectron density. A 200-ml vessel constructed from UV-transparent acrylic houses the target, which can be excited either: i) by a low-energy beta emitter (a ^{90}Sr source attached to the vessel), with a fast PMT attached to an adjacent side to provide a “tag” for source events; or ii) using two 1-cm scintillator paddles to tag cosmic muons travelling within 6 degrees of vertical. An array of 12 fast (300ps TTS) 1-inch H11934 Hamamatsu PMTs positioned vertically beneath the target are used to image the Cherenkov ring and to measure the time profile of emitted light. Scintillator panels provide a 4π veto for cosmic shower events. A complete simulation allows fine-tuning of the design, and calibration has been completed using a pure water target, which can be modeled exactly, allowing a full understanding of the apparatus.

The ability to reconstruct Cherenkov rings has demonstrated in a water target, and used to determine the time precision of CHESS as 338 ± 12 ps FWHM. CHESS has also been used to demonstrate the separation of Cherenkov and scintillation light in both linear alkylbenzene (LAB) and LAB with 2g/L of PPO as a fluor (LAB/PPO). This is the first such demonstration for the more challenging LAB/PPO cocktail and improves on previous results for LAB. The fast time resolution results in an efficiency for identifying Cherenkov photons in LAB/PPO of $70 \pm 3\%$ and $63 \pm 8\%$ for time- and charge-based separation, respectively, with scintillation contamination levels of $36 \pm 5\%$ and $38 \pm 4\%$. LAB/PPO data is consistent with a rise time of 0.75 ± 0.25 ns.

This apparatus can now be used to characterize alternative target materials, such as the newly developed water-based liquid scintillator (WbLS). This provides an excellent basis for future R&D and detector development.

Upgrade to the Relativistic Heavy Ion Collider Accelerator
 Principal Investigator(s): (Sichtermann, Ernst and Jacak, Barbara)

Project Description

The purpose of this project is to develop a program investigating the gluonic structure of dense matter. Cold, dense matter will be probed using electron-ion collisions at a future collider, while the gluonic structure of hot, dense matter can be studied by measuring direct photons produced in heavy ion collisions at the LHC. The first goal of this proposal is to establish a leading role in physics at the EIC. This will provide a basis for continued and enhanced block funding for NSD research, and will attract external funding for EIC detector R&D and construction. The second goal of this project is to produce physics now, studying the structure of hot, dense matter using the ALICE Experiment at the LHC. First data will be taken in late 2015.

We will simulate electron-nucleus collisions and determine requirements for detecting the scattered electron and produced particles. We will use these studies to develop a role for LBNL in designing, and eventually constructing, an experiment for the EIC. In ALICE, we join international collaborators for calorimetric direct photon measurements. We will calibrate the EMCAL, understand the energy scale, and characterize the calorimeter performance, producing calibrations to be used by the entire ALICE collaboration. Our goal is to analyze neutral meson and inclusive photon production, finally combining the information to extract the direct photon spectra.

Accomplishments

In January 2016, we hosted the first meeting of the new EIC Users Group in Berkeley. We collaborated with colleagues from UCB, Davis, UCLA, Riverside, LANL and LLNL to prepare a UC consortium aiming at EIC science.

Sichtermann, Klein, and Jacak have identified key observables to study two exciting topics at EIC. One is the gluonic structure of heavy nuclei, where the gluons carry at most a few percent of a nucleon's energy. The other is the spin structure of polarized nucleons probed with electron beams; we aim to quantify how much of the nucleon spin is carried by the spins of soft gluons and how much by orbital angular momentum of quarks and gluons. We devised a concept for a silicon pixel tracker based upon the LBNL group's work on the ALICE inner tracker upgrade. Sichtermann imported MATLAB-based softward to simulate the kinematics of eA collisions and create a concept for a barrel tracker + forward silicon pixels to track the scattered electron. Due to their compact size and position near the beam pipe, forward and barrel trackers must be designed together.

Postdoc Yue Shi Lai and Jacak worked on calibrations of 2015 and 2016 data in the ALICE EMCAL and a new calorimeter, DCAL, using techniques developed for PHENIX to extend ALICE capabilities. While gain calibrations from reconstructing neutral pions from photons detected in calorimeter towers were provided by ALICE collaborators, Lai calibrated those towers with insufficient reconstructed pions by matching the slope and level of the energy spectra to known good towers. This allowed recovery of a substantial number of uncalibrated DCAL towers. In addition, we investigated the calorimeter response in p+p and Pb+Pb collisions, and studied how best to perform shower shape analysis. This will be important for separating single photons from double photons arising from the decay of high momentum neutral pions.

Multi-disciplinary Research to Enhance Understanding of Transport, Risks, and Mitigation of Radioisotopes for Improved Radiological Resilience

Principal Investigator: Kai Vetter

Project Description

The purpose of this project is to enhance the technologies and understanding in the assessment, prediction, remediation, and impact of releases of radioactive materials into the environment with the focus on the unique opportunities provided by the Fukushima Dai-ichi Nuclear Plant accident. Teams composed of scientific technical staff and postdoctoral scholars from four divisions focused on the four priority areas: (i) measuring and assessing the distribution of relevant radioisotopes, (ii) modeling and predicting their interactions and their transport, (iii) estimating and mitigating their impact on the environment and human health, and (iv) developing new remediation strategies through physical and chemical treatments of contaminated soil.

Accomplishments

- i) Improvements were made to the High Efficiency Multimode Imager (HEMI), including integration with a LiDAR sensor to enable real-time 3-D scene reconstruction and gamma-ray fusion to enhance radiation mapping capabilities. HEMI was deployed in a handheld configuration during a measurement campaign in June 2016 in the exclusion zone within Fukushima Prefecture. We were able to demonstrate a vastly improved ability to visualize, localize, and characterize sources/hotspots in real-time in 3-D.
- ii) High resolution, high fidelity integrated hydrologic simulations of a contaminated Fukushima watershed were conducted to assess cesium decontamination scenarios and to manage the potential risks of secondary contamination. A number of numerical experiments including various magnitudes of forest thinning were implemented in the model, providing quantitative measures of the tradeoffs between the removal of contaminated trees and the potential for an increase in erosion and thus transport of cesium. Geo-spatially distributed results can be used to aid in remediation decisions such as the relocation of communities and agricultural activities in the Fukushima prefecture. Additionally, benchmarking of two integrated hydrologic models (one developed by LLNL and one used by the Japan Atomic Energy Agency) was used to build confidence in both simulators for use in numerical prediction in Fukushima remediation efforts.
- iii) Cs uptake profiles and viability upon exposure were confirmed for cells exposed to both cold and radioactive cesium. To evaluate cell death, clonogenic survival was determined upon exposure to external Cs-137 sources as well as upon contamination with cold and radioactive Cs. Live cells exposed to different levels of acute or chronic doses were monitored in real-time while placed inside our microscope. Our bioinformatics pipeline has determined the chemical and radiological impact of chronic exposures on cell proliferation, cell death and homeostatic levels for DNA damage. Kinetic measurements from acute data enable the validation of mathematical models to predict the response to chronic exposure.
- iv) A basic soft X-ray absorption spectroscopy study of Cs incorporation into clay minerals was completed. Protocols for rapid characterization of Cs-contaminated soils by soft X-ray scanning transmission X-ray microscopy (STXM) were developed. Procedures are now in place to pre-screen relatively large quantities of soil and mineral samples in advance of STXM analysis to locate micron-scale particles with high Cs content; autoradiography (using an image plate and particle manipulation system provided by JAEA) can be used to identify high-activity soil samples, and microprobe X-ray fluorescence imaging can be used to quantitatively measure the spatial distribution of Cs.

The Next Generation Low-Mass Solid-State Pixel Detector

Principal Investigator(s): Nu Xu

Other investigators: Eric Anderssen, Xin Dong, Leo Greiner

Project Description:

The idea of the proposal is aimed at key technological R&D to enable a next-generation low-mass solid-state pixel detector with a five to ten-fold faster readout time. The faster pixel detector, HFT⁺, will allow us to sample almost all 200 GeV *Au+Au* collisions, provided by RHIC, in order to precisely measure the small bottom hadron production cross sections at RHIC. The physics program with the proposed HFT⁺ is complementary to the heavy flavor program at the LHC. Furthermore, HFT⁺ pixel technology is fast, thin and radiation hard, hence, it is of great interest in many other applications. This newly developed fast MAP can be readily used as the inner-tracker for the proposed sPHENIX. Both barrel- and forward-tracking at a future Electron-Ion-Collider detector are among the longer-term opportunities. One of the present spin-offs, the TopMetal detector, is part of an LBL/CCNU R&D effort into use in a future neutrinoless-double-decay experiment. In addition, the fast pixel detector can also be used for beam microscopy in experiment at 88" cyclotron at LBNL.

Accomplishments:

According to the original plan, we structured the proposal into two parts: First year we focus on trigger developing, assuming the success of the fast heavy flavor tracker in the future. This is achieved by using the collected data from STAR and simulations. In the second year, we planned to involve LBNL mechanical engineer(s) to design a plan to install the new/fast low-mass solid-state pixel detector in a detector at RHIC. Since the second year was not founded, this report will focus on the achievements from the first year's efforts.

Result (1): At RHIC the production cross section for bottom quark hadrons in the 200 GeV *Au+Au* collisions is relatively low. One would benefit greatly if a fast trigger detector with precision on the secondary vertex measurement. The fast HFT⁺ is precisely aimed for this physics. From the collected data, we have tested the decay channel B-hadron => D⁰. The first result of the measurement is shown at the recent QM2017 conference.

Result (2): With the project, the simulated result of the B-hadron =>D⁰ measurement is also done. At the relatively low transverse momentum region, p_T < 6 GeV/c, the fraction of the bottom-hadron decayed charm-meson is about one to two orders of magnitude lower than that of the total charm-hadrons. So the newly proposed fast heavy flavor detector is absolutely necessary for future measurements at RHIC. This result has already included in the vertex detector proposal in sPHENIX experiment [2].

In summary, from the one year LDRD effort, our most significant accomplishments are: (1) From data developed a possible trigger of B-hadron => D⁰ for future measurements at RHIC; (2) From simulation, determined the significance for the measurement of B-hadron => D⁰ in the top 10% central *Au+Au* collisions at RHIC. Both of the results will be implemented in the future sPHENIX experiment.

Enabling Big Science with High Throughput Methodologies Year 1

Principal Investigator: Carl Haber

Project Description

This LDRD proposal is aimed at evaluating and acquiring technical concepts and capabilities which could be crucial aspects of future efforts to construct large particle detector systems at the Laboratory. These efforts address, in particular, particle physics and nuclear physics experiments which require large area arrays of precision sensors.

The particular technologies and methods proposed for study here involve precision electrical and mechanical assembly, inspection, and testing, which require high throughput and very repetitive and reproducible procedures. The throughput requirement derives from schedule and cost drivers. Indeed, the labor costs of these large projects could be reduced dramatically as a result of these methods.

The goal of this LDRD project is to identify prototypical processes which are general enough to apply to many future fabrication efforts. A set of structures were chosen and a corresponding high throughput assembly, test, and inspection process was designed. In Year 2 this is extended into the actual fabrication of the process and its evaluation.

Accomplishments

In Year 1 we looked at a tracking stave concept, consisting of a thermal-mechanical carbon fiber core, co-cured low mass copper-kapton "bus" tapes, and sensor modules. The sensor modules consist of a silicon sensor, hybrid printed circuit boards holding front end readout electronics, and a new multi-function bias, multiplexer, monitoring and control circuit. The latter provides a highly efficient low voltage, high current regulation function, remote multiplexed control of high voltage, low current sensor bias, and real-time monitoring and control capabilities. Typical experiments require 10-20 thousand of such elements, which must be of extremely high reliability and radiation resistant.

Considering the various challenges and requirements we decided to focus on the new multi-function board as the target of the design and evaluation study which will extend into Year 2. In Year 1 we designed a full assembly and test process. We began the design work on both the circuits and the floor plan. (This is continuing into Year 2 with parts fabrication underway and software development).

In Year 1 we also developed a variety of inspection and measurement tools which we have applied to sensor module and stave metrology. Most significant here is a full 1.4 meter long optical scanner for both 2D and 3D imaging and metrology. We also studied optical inspection issues for cosmic microwave bolometer arrays: We applied a number of optical profiling techniques to measure the surface quality of ceramic lenses and tested these on a measurement station assembled as part of this work.

In Year 2 we will complete the design of, and fabricate, and test the multi-function board array, in a scalable system. We will develop the control and acquisition tools required to operate this process, in scalable way. We will continue the bolometer scanner to conclusion including analysis algorithms.

Searches for the Supersymmetric Particles at the LHC in Run-2 and Beyond

Principal Investigators: *Ian Hinchcliffe and Beate Heinemann*

Project Description

The purpose of this LDRD is to search for supersymmetric partners of Standard Model particles. There are strong theoretical and experimental reason why supersymmetry might exist in Nature and run 2 at the LHC, starting in 2015, provides an excellent opportunity to search for them. The proposal focuses on two different kinds of particles and the analyses searching for them have different challenges.

The search for the top squark relies on being able to identify jets originating from bottom quarks based on the high precision silicon tracking detectors. The search for charginos requires the efficient detection of leptons. This proposal includes also a component about the longer term future for which it is critical to ensure the ability of triggering on leptons in the 1020GeV range.

An idea of installing double silicon layers to trigger such leptons will be evaluated in the context of this work.

Accomplishments

Several publications have resulted from this work. These publications used data collected at the LHC in 2015 and 2016. Although no new particles were observed, these searches have greatly extended the limits on the masses on such possible particles. The work is ongoing supported by DOE HEP research funds as data taken in the last quarter of 2016 and data to be taken in 2017 and 2018 will continue to be analyzed by the ATLAS collaboration using methods developed from the support provided by the LDRD.

Enabling Technologies for Next Generation Receivers to Measure the Polarization of Cosmic Microwave Background

Principal Investigator(s): (Akito Kusaka)

Project Description

The cosmic microwave background (CMB) is a unique tool to approach some of the most important questions in cosmology and fundamental physics: inflation, dark energy, dark matter and neutrinos. The P5 subpanel of the HEPAP committee has recommended that the DOE support an ambitious next-generation experimental concept called CMB Stage 4 (CMB-S4), and LBNL is poised to play a leading role in this program. This proposal encompasses key technologies that will enable next generation receivers for such future CMB experiments: a cryogenic half-wave plate (HWP), advancement in detector technology, and an optimization of high-throughput optics system. These will not only enhance CMB experimental sensitivity, but also minimize project cost and greatly simplify construction of the instruments.

The required detector count for CMB-S4 is more than 20 times of that for experiments under construction, while the cost increase is restricted to only 5-10 times that of current experiments. The goal of this proposed research is to develop three key technologies that will enable a cost effective leap in experimental sensitivity for CMB-S4: (1) A continuously rotating cryogenic half-wave plate (HWP) for maximally efficient polarization modulation. While technically challenging, the cryogenic temperature of the HWP suppresses the excess thermal emission from the HWP and prevents the detectors from sensitivity degradation. (2) Improvement of CMB detectors by reducing the operating temperature of the transition-edge sensors (TES). The TES operating at lower temperature (~ 70 mK) has a suppressed level of thermal noise, which contributes to lower level of the detector noise as well as higher fabrication yield.

Accomplishments

The cryogenic HWP development has made significant progress. We have fabricated, evaluated, and concluded a small-scale prototype. This system employs mag-lev bearing with high-T_c superconductor ring and an electromagnetic drive, and designed to operate at a cryogenic temperature below 77K. This system was demonstrated and evaluated using liquid nitrogen, and we achieved low level of friction and desired rotation stability. Based on the lessons learned from the prototype design, fabrication and operation, we are making progress on the full-scale system with inner diameter of 46 cm, which is applicable for CMB-S4. We also developed an inductively-coupled non-contact thermometry. Since the mag-lev bearing and electromagnetic drive systems offer zero contact, thermometry with zero contact is desirable to monitor the temperature of the rotor. A prototype thermometry system is demonstrated, and will be integrated into the full-scale system. We also made progress in understanding the requirement regarding the rotation stability and possible systematics of the HWP.

We have also developed a cryostat as a test-setup for a 70 mK bolometers for the next-generation CMB instrument. The cryostat is equipped with a two-stage pulse-tube cooler to achieve 4 K, and an adiabatic demagnetization refrigerator (ADR) on the 4 K stage to achieve ~ 50 mK temperature. We have completed the design of the cryostat, and fabricated most of the parts for this cryostat system. The system is under commissioning and evaluation. We are also setting up a sputter machine dedicated to fabricating the superconducting layer for this TES. The machine was donated by SFSU and refurbished under the support of this LDRD.

Next Generation Cosmic Microwave Background Detector Arrays Enabling a Factor 10-100 Increase in Array Size

Principal Investigator: Adrian T. Lee

Project Description:

The purpose of this project is to develop scalable technology for next-generation Cosmic Microwave Background (CMB) polarimetry experiments. Primordial gravitational waves produced during inflation and gravitational lensing by large-scale structure imprints unique polarization patterns on the CMB. Amplitude of polarization signal from primordial gravitational wave constrains model of an inflation and its energy scale. A detailed characterization of the small angular scale polarization pattern would allow us to constrain the sum of the neutrino masses and the evolution of dark energy by cross-correlating with optical surveys. CMB experiments with order $\sim 10,000$ detectors are now just getting deployed. CMB community is gaining momentum for next stage of CMB experiment. Goal for the next generation CMB polarization experiment is to characterize polarization with an unprecedented accuracy with $\sim 500,000$ detectors. Desire to increase detector count by more than an order of magnitude requires fresh approaches. We identified components in current detector systems that are currently not scalable, and we came up with a method to improve their scalability. This year we studied increasing detector fabrication throughput by working together with commercial foundry. Focal plane integration throughput could also be increased by lithographing detector and readout electronics on a same wafer. We made key progress to integrate detector and readout electronics on a single wafer by developing resonators for frequency division multiplexing readout at higher frequency.

Accomplishments:

During FY15, we identified two promising commercial fabrication foundries that could fabricate CMB detectors. This year, we worked closely with both foundries to fabricate multi-chroic antenna coupled TES detectors. Given the success of the first round, we continued on to fabricate detector array with a commercial company. Fabrication of the detector array also went well. Detector yield was 97% with uniformity of detector properties within our specification. Figure shows fabricated detector array and measured detector performances.

During FY15, we successfully fabricated monolithic superconducting resonators for frequency-division multiplexing readout that has 40 ~ 70 resonators between 1 MHz ~ 5 MHz. However, resonators were too big to be integrated on a detector wafer. This year, we fabricated superconducting resonators that resonates at 50 MHz ~ 100 MHz. Such resonators have small enough foot print to be able to get integrated on a detector wafer as shown.



Ultrahigh Voltage and Light Collection in Liquid Xenon Dark Matter Experiments

Principal Investigator(s): McKinsey, Daniel

Project Description

Efficient light collection and adequate electric drift field are both essential for achieving the best sensitivity of liquid xenon (LXe) to dark matter interactions. The best evidence that sufficient light collection and drift field can be achieved comes from LUX, where 11% light collection and 200 V/cm drift field were demonstrated. Compared to LUX, the goals for large future detectors are currently more modest for light collection ($> 7.5\%$) and more ambitious for drift field (> 700 V/cm). There is a bit of a tradeoff here; it is believed that the larger LXe detector will result in more light being lost due to finite reflectivity and absorption by impurities in the LXe, while it is also believed that the LUX drift field was limited by dust or asperities on the cathode and anode grids, and that additional engineering and quality control will allow better high-voltage (HV) performance. At the same time, there is little basic understanding of what fundamentally limits light collection or HV. This lack of basic understanding creates additional risk: if it is not known what physical mechanisms actually limit light collection and drift field in practice, then there is a danger that that incorrect quality control and quality assurance metrics will be applied, and final detector performance could suffer. At the same time, a better understanding of these topics may enable enhanced performance above baseline assumptions. In this LRD project, both of these topics are studied so as to enable optimization of LXe-based dark matter experiments. Berkeley is a leader in dark matter experiments using LXe, and this work will help maintain Berkeley's leadership role.

Accomplishments

The xenon gas handling and purification systems have been designed and all components purchased. The high voltage testing apparatus has been designed, purchased, and assembled, including electric field simulations of the overall apparatus and Rogowski electrodes. An existing cryostat has been modified for this study. A purity monitor has been designed, built, and successfully tested; this will be used to verify that electron lifetime in the LXe is sufficiently high for high-voltage breakdown tests to be meaningful. High voltage feedthroughs and monitoring systems have been designed, fabricated, and assembled.

The light collection apparatus has been fully designed, including an optical cell that can be filled with LXe, and into which 175 nm light may be introduced. An existing cryostat has been modified to suit this experiment. Measurements of internal reflectivity from PTFE surfaces covered with water and mineral oil have been compared to measurements without liquid, in preparation for studies in which PTFE will be immersed in LXe.

We are now focusing on the exploitation of both of these systems. HV studies will quantify the effects of electrode gap size, electrode size and shape, electrode surface treatment, and liquid purity. Reflectivity studies will quantify the dependence of reflectivity on wavelength of light, surface treatment, angle of incidence, and LXe purity.

**CONFRONTING BEYOND THE STANDARD MODEL THEORIES WITH NEW LHC
AND ASTROPHYSICAL DATA**
Principal Investigator: *Michele Papucci*

Project Description

The purpose of this project is to leverage the present and upcoming data coming from the Large Hadron Collider, Dark Matter detection searches and particle astrophysics experiments to gain knowledge of new particle physics beyond the Standard Model (BSM). The use of novel software tools the PI is currently developing will improve the effectiveness of comparing theoretical models to the LHC data and allow more extensive studies of the implications of the experimental results for BSM models. In particular this project will focus on searches for models of Dark Matter, models addressing the naturalness of the electroweak scale and any possible new physics signal that may show up in the upcoming data.

Accomplishments

The results of the work supported by this LDRD focused on study of the 750GeV LHC di-photon excess in the 2015 data, on supersymmetric gauge-mediated models, natural Higgs sector models of “Neutral naturalness”, novel searches for new particles in heavy ion collisions, on Dark Matter signatures in gamma ray data and on the connection between the Standard Model Higgs and inflation.

One of the first (and highest cited) studies characterizing and laying out the possible BSM interpretation of the 750 GeV di-photon excess was performed with the support of this LDRD. Further studies of models giving rise to di-photon signals at the LHC were performed. Motivated by this research program, S.Knapen proposed a novel way to search for light axion-like particles produced in photon fusion in ultra-peripheral heavy ion collisions at the LHC. Such proposal has already found interest within the ATLAS collaboration.

Further development of the software package Atom has progressed alongside its usage and is on track for its public release around the MC4BSM conference in May 2017. Further progress on Fastlim package was also performed with the inclusions of general neutralino and chargino production and decay. A new release of Fastlim is also expected in 2017.

On the model building end, S.Knapen continued the study of models of neutral naturalness and Twin-Higgs. In particular, he built and studied models where new vector-like quarks can be present. A connection between Dark Matter and neutral naturalness models was also performed, leading to the identification and investigation of specific signatures arising in gamma ray astronomy for this class of models.

On the topic of supersymmetry, Knapen performed a complete study of the current status of LHC searches for general gauge-mediated model (a continuation of the program started with the FY15 LDRD). He also built gauge mediated models giving rise to a hierarchical spectrum of superparticles known as “mini-split”.

On the front of the connections between particle physics and cosmology H.Yoo also continued the research on the behavior of the Standard Model Higgs during Inflation, further studying the implication of bubbles of negative vacuum energy in our past light cone and found that the existence of such bubbles would be incompatible with our current Universe, therefore strengthening the bounds on the inflationary scale in models where there is no BSM physics besides the inflaton.

Project Title Intent-based Networking for ESnet Network Operating System (ENOS)
Principal Investigator(s): Inder Monga

Project Description

The purpose of this project is to dramatically simplify the process of configuring network services by applications through specification of their high-level ‘intent’. Intent allows users and networks to communicate – specify network needs like *fast response time* or *service reliability*, share service state like *resource unavailable* or *recovering from fault*. These needs, expressed in *English*, are quantified into network variables, converted to network configurations and implemented in network. Science users or applications can submit their intent in descriptive language such as “For project1 transfer files between LBL and BNL”. Software translates these intents into network provisioning commands, using knowledge about the network like topology, end-points and so on, to set up links between data transfer nodes (DTN) at both locations and enable project1 transfer.

A tool called INDIRA (Intelligent Network Deployment Intent Renderer) was developed to showcase application intents instigating APIs for NSI (for network path provisioning) and Globus (for file transfers). The tool allows us to create multiple network requests for different applications, configure multiple network provisioning tools and collects information on user-application needs for further analysis of network usage.

To implement this tool, we developed a natural language processing technique using semantic ontologies and intent data dictionaries, which can requests to meet service needs. Having established this method, we will integrate with more network provisioning tools, enhancing network configurations and user experience, automating path provisioning and QoS optimization for science applications.

Accomplishments

Our most significant accomplishments are two – an innovative method of using natural language processing or ontologies to improve user specification of their needs expressed as network intent, and development of INDIRA to demonstrate this. Our method uses ontology engineering with minimal implementation of AI reasoning, to assess user-network needs, topology awareness, bandwidth permissions and profile checking. Successful demonstration with INDIRA showcased intents expressed in ‘English’ expressed as network API calls that provisioned network dynamically, leveraging existing tools such as NSI and Globus, to meet the desired intent. We are hopeful that this approach will start a new research direction in intent-based networking, which focuses on expression of end-user needs using simpler network abstractions. This method expresses intents as minimal command configuration process, as opposed to using multiple lines of code to configure networks, an approach still widely used by other intent networking projects.

With this new approach, applications can specify what they want, rather than understand details of how. In addition to rendering requests, we developed a feedback loop, communicating back to users the state of network and administrative policies, to refine their intent when it could not be met. This approach will drive the area of autonomic networking. We are in the process of enhancing INDIRA and publishing more papers on this approach to the network research community.

Publications List

AF-Ji LB16001 Development of a Compact Laser-driven Ion Beam Accelerator for Discovery Plasma Science Applications

Journal Publications

S. S. Bulanov, E. Esarey, C. B. Schroeder, S. V. Bulanov, T. Z. Esirkepov, M. Kando, F. Pegoraro, W. P. Leemans, “Radiation Pressure Acceleration: the factors limiting maximum attainable ion energy”, Phys. Plasmas 23, 056703 (2016)

Workshops, Conferences, and Presentations

Q. Ji, S. S. Bulanov, S. Steinke, T. Schenkel, E. H. Esarey, W. P. Leemans

“Design of a Compact Ion Beam Transport System for the BELLA Ion Accelerator”, Proceeding of 7th International Particle Accelerator Conference, Busan, Korea, May 8-13, 2016. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/thpmr004.pdf>

S. S. Bulanov, Q. Ji, S. Steinke, T. Schenkel, E. Esarey, and W. P. Leemans
“Advanced Acceleration Mechanisms for Laser Driven Ions by PW-lasers”, Proceeding of 7th International Particle Accelerator Conference, Busan, Korea, May 8-13, 2016. <http://accelconf.web.cern.ch/AccelConf/ipac2016/papers/weoab01.pdf>

Q. Ji, S. S. Bulanov, S. Steinke, T. Schenkel, D. Leitner, E. Esarey, and W. P. Leemans, “Ion Transport Beamlines for Laser Plasma Ion Accelerators”, 3th EliMED Workshop, Catania, Italy, September 7-9, 2016

S. S. Bulanov, “All-Optical Hadrontherapy”, 3th EliMED Workshop, Catania, Italy, September 7-9, 2016

S. Steinke, S. S. Bulanov, Q. Ji, T. Schenkel, E. Esarey, W. Leemans, “Ultra-intense Laser-matter Interactions with the BELLA-i PW Laser User Facility”, 3th EliMED Workshop, Catania, Italy, September 7-9, 2016

AF-Vay LB16002 High-Performance Advanced Particle Accelerator Simulator

Journal Publications

R. Lehe, M. Kirchen, B. B. Godfrey, A. R. Maier, J.-L. and Vay, “Elimination of Numerical Cherenkov Instability in Flowing-Plasma Particle-In-Cell Simulations by using Galilean Coordinates”, Phys. Rev. E 94, 053305 (2016), <https://doi.org/10.1103/PhysRevE.94.053305>

M. Kirchen, R. Lehe, B. B. Godfrey, I. Dornmair, S. Jalas, K. Peters, J.-L. Vay and A. R. Maier, “Stable Discrete Representation of Relativistically Drifting Plasmas”, Phys. Plasmas 23, 100704 (2016), <http://dx.doi.org/10.1063/1.4964770>

AF-Wilcox LB15001 A New Concept for High Average Power Ultrafast Lasers

Workshops, Conferences, and Presentations

R. Wilcox, D. Dahlen, T. Sano, “Femtosecond Beam Combination Using Diffractive Optic Pairs”, Conference on Lasers and Electro-Optics 2017, submitted

AL-Hexemer LB15002 T-ReXS - Tender Resonant X-Ray Scattering: A Spatio-Chemical Probe for Materials, Biology and Energy Sciences

Journal Publications

M. Segad et al, “Identifying Sulfur-microphase in Block Copolymer Membranes Using Tender Resonant X-ray Scattering”, in process

AL-Shapiro LB16005 High-Dimensional Ptychographic Imaging for Studying Nanoscale Dynamics, Chemistry and Morphology at the ALS and ALS-U

Journal Publications

- D. A. Shapiro, Y.-S. Yu, M. Farmand, T. Tyliszczak, J. Cabana, R. Celestre, A.L.D. Kilcoyne, S. Marchesini, T. Warwick and H. Padmore, "Ptychographic Imaging of Nano-Materials at the Advanced Light Source with the Nanosurveyor Instrument", Journal of Physics: Conference Series, accepted, 2016
- R. Celestre, K. Nowrouzi, D. A. Shapiro, P. Denes, J. M. Joseph, A. Schmid, H. A. Padmore, "Nanosurveyor 2: a compact instrument for nano-tomography at the advanced light source", Journal of Physics: Conference Series, accepted, 2016
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AL-Steier LB14003 Novel Accelerator Techniques for Diffraction Limited Light Sources

Workshops, Conferences, and Presentations

- C. Steier, et al., "Progress of the R&D towards a diffraction limited upgrade of the Advanced Light Source", Proceedings of International Particle Accelerator Conference 2015, Richmond, VA,
<http://accelconf.web.cern.ch/AccelConf/IPAC2015/papers/tupma001.pdf>
- J. Byrd, S. De Santis, T. Luo, C. Steier, "Phase Transients in the Higher-Harmonic RF Systems For the ALS-U Proposal", Proceedings of International Particle Accelerator Conference 2015, Richmond, VA,
<http://accelconf.web.cern.ch/AccelConf/IPAC2015/papers/wepty044.pdf>
- H. Nishimura, D. Robin, K. Song, C. Steier, C. Sun, W. Wan, "Development of Simple Tracking Libraries for ALS-U", Proceedings of International Particle Accelerator Conference 2015, Richmond, VA,
<http://accelconf.web.cern.ch/AccelConf/IPAC2015/papers/mopwi020.pdf>
- C. Steier, et al., "ALS Upgrade", Low Emittance Rings Workshop, Grenoble, France, 2015, <https://indico.cern.ch/event/395487/session/6/contribution/12>
- S. De Santis, et al., "On-axis injection and bunch length control in the ALS upgrade: studies for a stripline kicker and harmonic cavities", Low Emittance Rings Workshop, Grenoble, France, 2015,
<https://indico.cern.ch/event/395487/session/17/contribution/59>
- A. Anders, et al., "Exploring the Limits of Sputter-depositing Non-evaporative Getters (NEG) in Very Narrow Chambers", International Workshop on Functional Surface Coatings and Treatment for UHV/XHV Applications, Chester, UK, 2015,
https://eventbooking.stfc.ac.uk/uploads/functional_surface_coatings/14---a-anders-and-x-zhou---neg-in-very-narrow-chambers.pdf

A. Anders, et al., "Deposition of Non-Evaporative Getters (NEG) in Very Narrow Chambers", AVS 62nd International Symposium & Exhibition, San Jose, CA, 2015, http://www2.avs.org/symposium2015/Papers/Paper_VT-MoA6.html

BU-Hong LB16016 URBan Integrated System (URBIS): A Data and Computing Platform for Urban Systems

Journal Publications

M. Wetter, M. Bonvini, and T.S. Nouidui, "Equation-based languages - A new paradigm for building energy modeling, simulation and optimization", Energy and Buildings, 117:290–300, 2016,
<http://www.sciencedirect.com/science/article/pii/S0378778815303315>

R.Z. Pass, M. Wetter, and M.A. Piette, "A Thermodynamic Analysis of a Novel Bidirectional District Heating and Cooling Network", journal, 2016, under review

Workshops, Conferences, and Presentations

T. Hong, Y. Chen, S. Lee, and M.A. Piette, "CityBES: A Web-based Platform to Support City-Scale Building Energy Efficiency", The 5th International Workshop on Urban Computing, August 14, 2016,
<http://www2.cs.uic.edu/~urbcomp2013/urbcomp2016/papers/CityBES.pdf>

R.Z. Pass, M. Wetter, and M.A. Piette, "A Tale of Three District Energy Systems: Metrics and Future Opportunities", ACEEE Summer Study on Energy Efficiency in Buildings, August 24, 2016,
http://aceee.org/files/proceedings/2016/data/papers/10_135.pdf

CH-Hartwig LB14005 Design of Mesoscale Catalyst Networks

Journal Publications

Key, H. M.; Dydio, P.; Clark, D. S.; Hartwig, J. F. "Abiological catalysis by artificial haem proteins containing noble metals in place of iron" Nature 2016, 534, 534-537.

Dydio, P.; Key, H. M.; Nazarenko, A.; Rha, J. Y.-E.; Seyedkazemi, V.; Clark, D. S.; Hartwig, J. F. "An artificial metalloenzyme with the kinetics of native enzymes" Science 2016, 354, 102-106

Key, H. M.; Dydio, P.; Hayashi, H.; Clark, D. S.; Hartwig, J. F. "Chemoselective, Enzymatic C-H Bond Amination Catalyzed by a Cytochrome P450 Containing an Ir(Me)-PIX Cofactor" JACS accepted with minor revisions

CH-Houle LB14007 Computational-Experimental Studies of Aerosol Transformations from the Liquid to Glassy State

Journal Publications

A. A. Wiegel, M. J. Liu, W. D. Hinsberg, K. R. Wilson, and F. A. Houle, "Diffusive Confinement of Free Radical Intermediates in the OH Radical Oxidation of Semisolid Aerosol", submitted for publication

M. Liu, A. A. Wiegel, W. D. Hinsberg, K. R. Wilson, and F. A. Houle, "Concurrent free radical and acid-base oxidation of aqueous citric acid aerosol by OH radicals", in preparation

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- M. J. Liu, A. A. Wiegel, K. R. Wilson, F. Houle, B. Hinsberg, “Oxidative Aging of Citric Acid Aerosol by Heterogeneous Reactions with OH Radicals”, Berkeley Atmospheric Science Symposium, Berkeley, CA, February 18-19, 2016
- A. A. Wiegel, M. J. Liu,¹ K. R. Wilson, W. D. Hinsberg, and F. A. Houle, “Accelerated free radical chemistry in the heterogeneous oxidation of semisolid organic aerosol”, 251st ACS National Meeting & Exposition, San Diego, CA, March 13-17, 2016
- F. A. Houle (invited) “Stochastic simulations of liquid aerosol chemistry”, 251st ACS National Meeting & Exposition, San Diego, CA, March 13-17, 2016
- F. A. Houle (invited) “Stochastic simulations of organic aerosol ageing kinetics”, Towards a Molecular Understanding of Atmospheric Aerosols, Santa Cruz, CA, Aug 28 - Sep 2, 2016
- A. A. Wiegel, M. J. Liu, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, “Accelerated free radical chemistry in the heterogeneous oxidation of semisolid organic aerosol”, Towards a Molecular Understanding of Atmospheric Aerosols, Santa Cruz, CA, Aug 28 - Sep 2, 2016
- A. A. Wiegel, M. J. Liu, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, “Accelerated free radical chemistry in the heterogeneous oxidation of semisolid organic aerosol from diffusive confinement”, American Association for Aerosol Research 35th Annual Conference, Portland, OR, October 17-21, 2016
- M. Liu, A. A. Wiegel, W. D. Hinsberg, K. R. Wilson, and F. A. Houle, “The interplay between acid-base and free radical chemistry in the heterogeneous oxidation and fragmentation of citric acid in aqueous aerosol by OH radicals”, AGU Fall Meeting, San Francisco, CA, December 12-16, 2016
- A. A. Wiegel, M. Liu, W. D. Hinsberg, K. R. Wilson, and F. A. Houle, “Free radical confinement accelerates chemistry in the heterogeneous oxidation of semisolid organic aerosol”, AGU Fall Meeting, San Francisco, CA, December 12-16, 2016

CH-Toma LB16007 Spotlighting Catalysis: In situ and Operando Characterization of Photoelectrochemical Assemblies

Journal Publications

- F. M. Toma, J. K. Cooper, V. Kunzelmann, M. T. McDowell, Jie Yu, D. M. Larson N. J. Borys, C. Abelyan, J. W. Beeman, K. M. Yu, J. Yang, L. Chen, M. R. Shaner, J. Spurgeon, F. A. Houle, K. A. Persson, I. D. Sharp, “Mechanistic Insights into Chemical and Photochemical Transformations of Bismuth Vanadate Photoanodes”, Nat. Commun. 2016, 7, article number: 12012 [DOI]
- S. Y. Leblebici, L. Leppert, Y. Li, S. E. Reyes-Lillo, S. Wickenburg, E. Wong, J. Lee, M. Melli, D. Ziegler, D. K. Angell, D. F. Ogletree, P. D. Ashby, F. M. Toma, J. B. Neaton, I. D. Sharp, A. Weber-Bargioni, “Facet-dependent photovoltaic efficiency variations in single perovskite grains”, Nat. Energy 2016, 1, article number: 16093 [DOI]
- Ian D. Sharp, Jason K. Cooper, Francesca M. Toma, Raffaella Buonsanti, “Bismuth Vanadate as a Platform for Accelerating Discovery and Development of Complex Transition Metal Oxide Photoanodes”, ACS Energy Lett. 2017, 2, pp 139-150 [DOI]

- M. Favaro, C. Valero-Vidal, J. E. Eichhorn, F. M. Toma, P. N. Ross, J. Yano, Z. Liu, E. J. Crumlin, "Understanding the Oxygen Evolution Reaction Mechanism on Platinum by using Operando Ambient Pressure X-ray Photoelectron Spectroscopy", in preparation
- J. E. Eichhorn, J.K. Cooper, L.H. Hess, D. Ziegler, D.M. Larson, I.D. Sharp, F.M. Toma, Lawrence Berkeley Lab, USA "Nanoscale Imaging of Charge Carrier Transport in Monoclinic Bismuth Vanadate Photoanodes Via Atomic Force Microscopy", in preparation

CE-Ceja Navarro LB15016 The Soil Metazoan Microbiome: A Compartment of Importance to Soil Nutrient Cycling

Journal Publications

- Ceja-Navarro, J.A., Arellano, A., Kvietok, M. Arthropods are vessels of microbial diversity and biological transformations. In preparation. To be submitted to the Microbial Ecology Journal
- Ramanculova, Leila., Arellano, A. Ceja-Navarro, J. A. Environmental conditions drive the composition of the arthropod microbiome. In preparation. To be submitted to the Microbial Ecology Journal

CE-Jones LB16039 Ultra High Resolution Climate Projections to Support Climate Readiness in the San Francisco Bay Area

Journal Publications

- P. Vahmani, A. Jones, "Water Conservation Benefits of Urban Heat Mitigation", Nature Communications, in review

CE-Keenan LB16045 Predicting the Maximum Rate of Carbosylation Based on Optimal Leaf Resource Allocation

Journal Publications

- T.F. Keenan, I. C. Prentice, J. G. Canadell, C. A. Williams, H. Wang, M. Raupach, and G. J. Collatz. "Recent pause in the growth rate of atmospheric CO₂ due to enhanced terrestrial carbon uptake." NATURE COMMUNICATIONS 2016 7:13428
- T.F. Keenan, U. Niinemets. "Global leaf trait estimates biased due to plasticity in the shade." NATURE PLANTS 2017 (in press)
- T.F. Keenan, U. Niinemets. "The Canopy Trait Plasticity (CANTRIP) database V1.0.0." ZENODO. 2016 doi:10.5281/zenodo.164883
<https://github.com/trevorkeenan/traitPlasticity>
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CE-Tas Baas LB16024 Assessing Microbial Functions at Terrestrial-Aquatic Interfaces by Metagenome-Based Metabolic Flux Analysis

Journal Publications

- J. Voriskova, K.H. Williams and N. Tas, "Deciphering microbial functions at aquatic terrestrial interphases in East River, CO", in preparation

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CR-Calafiura LB16008 Kalman Filters on TrueNorth

Workshops, Conferences, and Presentations

R. Carney, K. Bouchard, P. Calafiura, D. Clark, D. Donofrio, M. Garcia-Sciveres, and J. Livezey, “Neuromorphic Kalman filter implementation in IBM’s TrueNorth”, Journal of Physics Conference Series (CHEP 2016 Proceedings), submitted

CR-Canning LB15005 Unconstrained Functionals for Massively Parallel Scaling of Conjugate Gradient Eigensolvers

Journal Publications

M. Del Ben, O. Marques and A. Canning, “Unconstrained Functionals for Massively Parallel Scaling of Conjugate Gradient Eigensolvers”, In draft form

CR-de Jong LB16011 Design of Quantum Chemistry Simulations for Superconducting Circuits

Journal Publications

JR. McClean, ME. Schwartz, J. Carter, WA. de Jong “Hybrid Quantum-Classical Hierarchy for Mitigation of Decoherence and Determination of Excited States” arXiv:1603.05681 (2016) <https://arxiv.org/pdf/1603.05681.pdf>

J. McClean, J. Romero, R. Babbush, A. Aspuru-Guzik “The theory of variational hybrid quantum-classical algorithms”, New Journal of Physics, 18 (2016), <http://iopscience.iop.org/article/10.1088/1367-2630/18/2/023023/meta>

NPD. Sawaya, M. Smelyanskiy, JR. McClean, A. Aspuru-Guzik, “Error Sensitivity to Environmental Noise in Quantum Circuits for Chemical State Preparation” Journal of Chemical Theory and Computation 12(7), 2097-3108 (2016) <http://pubs.acs.org/doi/abs/10.1021/acs.jctc.6b00220>

P. J. J. O’Malley, R. Babbush, I. D. Kivlichan, J. Romero, J. R. McClean, R. Barends, J. Kelly, P. Roushan, A. Tranter, N. Ding, B. Campbell, Y. Chen, Z. Chen, B. Chiaro, A. Dunsworth, A. G. Fowler, E. Jeffrey, E. Lucero, A. Megrant, J. Y. Mutus, M. Neeley, C. Neill, C. Quintana, D. Sank, A. Vainsencher, J. Wenner, T. C. White, P. V. Coveney, P. J. Love, H. Neven, A. Aspuru-Guzik, J. M. Martinis “Scalable Quantum Simulation of Molecular Energies” Physical Review X 6 (3), 031007 (2016) <http://journals.aps.org/prx/abstract/10.1103/PhysRevX.6.031007>

R. Santagati, J. Wang, AA. Gentile, S. Paesani, N. Wiebe, JR. McClean, SR. Short, PJ. Shadbolt, D. Bonneau, JW. Silverstone, DP. Tew, X. Zhou, JL. OBrien, MG. Thompson “Quantum simulation of Hamiltonian spectra on a silicon chip” arXiv:1611.03511 (2016) <https://arxiv.org/abs/1611.03511>

CR-Johansen LB16012 Modeling the Earth’s Hydrological Cycle from Watershed to Global Scales

Journal Publications

Rhoades, A.M., Johansen, H., Margulis, S., Ullrich, P.A., Xu, Z., Zarzycki, C.M., & Collins, W.D., “Truncation vs Transport – A Variable-Resolution CESM Case Study

of the Comparative Importance of Model Resolution and Microphysics in a Mountainous Region." In preparation for Journal of Hydrometeorology
Rhoades, A.M., Johansen, H., Margulis, S., Ullrich, P.A., Xu, Z., Zarzycki, C.M., & Collins W.D., "Ascending and Traversing the Uncertainty of Modeling Mountain Climate - A Case Study of the California Sierra Nevada Using Variable-Resolution CESM." In preparation

CR-Lin LB15007 Fast Numerical Methods for Green's Function in Mesoscale Simulation
Journal Publications

- X. Li, L. Lin, J. Lu, PEXSI-\Sigma: A Green's function embedding method for Kohn-Sham density functional theory, Ann. Math. Sci. Appl. in press 2016
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- L. Lin, Adaptively compressed exchange operator, J. Chem. Theory Comput. 12, 2242, 2016 <http://dx.doi.org/10.1021/acs.jctc.6b00092>
- L. Lin, J. Lu, Decay estimates of discretized Green's functions for Schrodinger type operators, Sci. China Math., 59, 1561, 2016 <http://dx.doi.org/10.1007/s11425-016-0311-4>
- L. Lin, "Localized spectrum slicing", Math. Comp., in press, 2016,
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CR-Moore LB15041 Solving Problems in Materials Theory via Quantum Networks
Journal Publications

- R. Vasseur and J.E. Moore, "Nonequilibrium Quantum Dynamics and Transport: from Integrability to Many-Body Localization", J. Stat. Mech. (2016) 064010
- M. Kolodrubetz, P. Mehta and A. Polkovnikov. "Geometry and non-adiabatic response in quantum and classical systems." arXiv:1602.01062 (invited for submission to Physics Reports)
- M. Kolodrubetz, B. M. Fregoso and J. Moore. "Nonadiabatic bulk-surface oscillations in driven topological insulators." Phys. Rev. B 94, 195124 (2016)
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- M. Bukov, M. Kolodrubetz and A. Polkovnikov. "Schrieffer-Wolff Transformation for Periodically Driven Systems: Strongly Correlated Systems with Artificial Gauge Fields." Phys. Rev. Lett. 116, 125301 (2016)
- T. Souza, M. Tomka, M. Kolodrubetz, S. Rosenberg and A. Polkovnikov. "Enabling adiabatic passages between disjoint regions in parameter space through topological transitions." Phys. Rev. B 94, 094106 (2016)

CR-Nugent LB15008 EXDAC: Extreme Data Analysis for Cosmology
Journal Publications

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W. Bhimji, D. Bard, M. Romanus, D. Paul, A. Ovsyannikov, B. Friesen, M. Bryson, J. Correa, G. K. Lockwood, V. Tsulaia, S. Byna, S. Farrell, D. Gursoy, C. Daley, V. Beckner, B. Van Straalen, N. J. Wright, K. Antypas, Prabhat, "Accelerating Science with the NERSC Burst Buffer Early User Program", Cray User Group, May 11, 2016, LBNL LBNL-1005736

CR-Siddiqi LB15038 Simulating Quantum Chemistry with Superconducting Circuits

Journal Publications

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- L. Martin, M. Sayrafi, and K. B. Whaley, "What is the fastest way to prepare an entangled state using measurement and feedback?", in preparation (2017)
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CR-Wu LB16014 Open Framework for High-Performance Streaming Analytics

Journal Publications

- Kim, T., et al., Predicting Baseline for Analysis of Electricity Pricing. Available at SSRN 2773991, 2016

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- Sim, A., D. Lee, and K.J. Wu, Implementation of Dynamic Extensible Adaptive Locally Exchangeable Measures (IDEALEM) v 0.1. 2016, Lawrence Berkeley National Laboratory (LBNL), Berkeley, CA (United States)
- Kim, T., et al. Extracting Baseline Electricity Usage Using Gradient Tree Boosting. in 2015 IEEE International Conference on Smart City/SocialCom/SustainCom (SmartCity). 2015. IEEE

CR-Yang LB16015 Neuromorphic Image Analysis and Pattern Recognition

Journal Publications

- D. Ushizima, C. Yang, S. Venkatakrishnan, F. Araujo, R. Silva, H. Tang, J. V. Mascarenhas, A. Hexemer, D. Parkinson, J. Sethian, "Convolutional Neural Network at the Interface of Physical and Digital Data", AIPR2016

Workshops, Conferences, and Presentations

J. V. Mascarenhas, C. Yang, D. Ushizima, "Quantization for Energy Efficient Convolutional Neural Networks", poster presented at the 2016 Supercomputing Conference, Salt Lake City. http://sc16.supercomputing.org/sc-archive/src_poster/poster_files/spost138s2-file2.pdf

EA-Gerke LB15011 IDEA - The International Database of Efficient Appliances: A New Tool for Optimizing Energy-Efficiency Policy

Journal Publications

- B. Gerke, M. McNeil, and T. Tu, "The International Database of Efficient Appliances (IDEA): A new tool to support appliance energy efficiency deployment", Draft journal article, to be submitted to Applied Energy
- S. Touzani, B. Gerke, T. Tu, and M. McNeil, "Machine learning approach for estimation of cost of conserved energy of efficient appliances", Draft journal article, to be submitted to Applied Energy

Workshops, Conferences, and Presentations

- B. Gerke, M. McNeil, T. Tu, and F. Xu, "The International Database of Efficient Appliances (IDEA): A New Resource for Global Efficiency Policy", In 2016 ACEEE Summer Study on Energy Efficiency in Buildings. Pacific Grove, Ca, 2016

EA-Gopal LB16042 Transportation System Science for Energy Savings

Journal Publications

- C. J. R. Sheppard, A. Harris, A. R. Gopal, "Cost-Effective Siting of Electric Vehicle Charging Infrastructure with Agent-Based Modeling", IEEE Transactions on Transportation Electrification (2016). doi: 10.1109/TTE.2016.2540663

EA-Todd LB15013 Behavior Analytics: Using Data Science to Draw Insights from Smart Meter Data

Journal Publications

- T. Kim, D. Lee, J. Choi, A. Spurlock, A. Sim, A. Todd, K. Wu, "Predicting Baseline for Analysis of Electricity Pricing," International Journal of Big Data Intelligence (Forthcoming 2017). Available at SSRN: <http://ssrn.com/abstract=2773991>
- S. Borgeson, D. Fredman, L. Jin, A. Spurlock, A. Todd, "Targeting and Predicting Outcomes of Utility Programs Using Smart Meter Data," Draft Manuscript
- L. Jin, S. Borgeson, D. Fredman, L. Hans, S. Patel, A. Spurlock, A. Todd, "Load Shape Clustering Using Residential Smart Meter Data," Draft Manuscript

Workshops, Conferences, and Presentations

- L. Jin, D. Lee, A. Sim, S. Borgeson, K. Wu, A. Spurlock, A. Todd, "Comparison of Clustering Techniques for Residential Energy Behavior using Smart Meter Data," Proceedings of the 2nd Association for the Advancement of Artificial Intelligence (AAAI) Workshop on Smart Grid and Smart Building (Forthcoming 2017)
- T. Kim, D. Lee, J. Choi, A. Sim, A. Spurlock, A. Todd, K. Wu, "Extracting Baseline Electricity Usage with Gradient Tree Boosting," Proceedings of 2015 International Conference on Big Data Intelligence and Computing (2015) <https://sdm.lbl.gov/perf/DataCom2015-91-final.pdf>.

GO-Arora LB16020 Multi-Scale Modeling of Geochemical Impacts on Fracture

Evolution

Journal Publications

D. Trebotich, S. Molins, B. Arora, and C.I. Steefel "Multiscale Model for Geochemical Evolution of Fractures", in preparation

Workshops, Conferences, and Presentations

D. Trebotich, S. Molins, C.I. Steefel, and H. Deng, "Adaptive Multiscale Modeling of Geochemical Impacts on Fracture Evolution (Invited)", AGU Fall Meeting (2016), H34D-02

GO-Christensen LB16022 Metal Isotope Fingerprint of Redox Reactions

Workshops, Conferences, and Presentations

S.T. Brown, A. Basu, J.N. Christensen, and D.J. DePaolo, "Uranium Isotope Fractionation: A Critical Review" Goldschmidt Conference p. 311 (2016)
<https://goldschmidt.info/2016/uploads/abstracts/finalPDFs/A-Z.pdf>

GO-Guglielmi LB16021 Advanced In-Situ Experiments for Understanding Induced Seismicity

Workshops, Conferences, and Presentations

TBD Y.Guglielmi, J.Birkholzer, J.Ruqvist, P.Jeanne, C.Nussbaum, "Can fault leakage occur before or without reactivation? Results from an in situ fault reactivation experiment at Mt Terri", Greenhouse Gas Control Technologies 13th International Conference (Lausanne, Switzerland, Nov. 14-18 2016), 2016, www.ghgt.info/

Y. Guglielmi, C.Nussbaum, L. de Barros, J. Birkholzer, and F. Cappa,"First results of aseismic fault slip and leakage preceding an earthquake induced during an in situ fault reactivation experiment in shales (Mont Terri FS experiment, Switzerland)", Geological Society of America annual meeting, Denver 2016, <http://www.global-events.list.elsevier.com/events/2016/09/the-geological-society-of-america-gsa-2016-annual-meeting>

P. Henry, Y. Guglielmi, A. Morereau, S. Seguy, R. Castilla, C. Nussbaum, P. Dick, J. Durand, D. Jaeggi, F. V. Donze and A. Tsopela, "T54B-04: Permeability - Fluid Pressure - Stress Relationship in Fault Zones in Shales", AGU Fall Meeting, San Francisco, CA, December, 2016, <https://fallmeeting.agu.org/>

C. Nussbaum and Y. Guglielmi, " MR41D-2720: Observations of fault zone heterogeneity effects on stress alteration and slip nucleation during a fault reactivation experiment in the Mont Terri rock laboratory, Switzerland", AGU Fall Meeting, San Francisco, CA, December, 2016, <https://fallmeeting.agu.org/>

A. Tsopela, Y. Guglielmi, F. V. Donze, L. D. Barros, P. Henry, R. Castilla and C. Gout, "S22B-08: Exploration of the role of permeability and effective stress transfer effects on Earthquakes Migration in a Fault Zone induced by a Fluid Injection in the nearby host rock: Experimental and Numerical Result", AGU Fall Meeting, San Francisco, CA, December, 2016, <https://fallmeeting.agu.org/>

GO-Lammers LB15033 Clay Interlayer Stratification: Deconstructing Drivers of Mass Transport in Shales

Journal Publications

L.R. Pestana, K. Kolluri, T. Head-Gordon, L.N. Lammers, "Direct Exchange Mechanism for Interlayer Ions in Non-Swelling Clays," Environmental Science & Technology, accepted

L.R. Pestana, T. Head-Gordon, L.N. Lammers, "Macroscopic Dynamics of Interlayer Ion Exchange in Illite," in preparation

Workshops, Conferences, and Presentations

L.N. Lammers, L.R. Pestana, K. Schaettle, T. Head-Gordon, "Dynamics of radiocesium exchange and interstratification in anhydrous clay interlayers: Bridging the atom and single crystal scales," Oral presentation, AGU Fall Meeting, (2016)

GO-Nakagawa LB15019 Frequency-Modulated Hydraulic Fracturing for Secure and Efficient Reservoir Permeability Enhancement

Workshops, Conferences, and Presentations

S. Nakagawa, "Laboratory Visualization of Hydraulic Fracture Propagation Induced by Variable-Rate Fluid Injection within Analogue Rock Samples Containing Preexisting Fractures", Abstract submitted to the 2017 American Rock Mechanics Association /US Rock Mechanics Symposium meeting

GO-Rutqvist LB15017 Dynamic Fracture Simulation of Geomaterials at Multiple Length Scales

Journal Publications

A.F. Queiruga and G. Moridis, "Numerical Experiments on the Convergence Properties of State-based Peridynamic Laws and Influence Functions in Two-Dimensional Problems." Computer Methods in Applied Mechanics and Engineering, 2016, in revision.

GO-Stringfellow LB16023 Characterizing the Environmental Impact of Chemical Compounds Used in Oil and Gas Development

Journal Publications

M. K. Camarillo, J. K. Domen, and W. T. Stringfellow. "Physical-chemical evaluation of hydraulic fracturing chemicals in the context of produced water treatment." J. Environ. Management 183: 164 – 174 (2016)

R. M. Tinnacher, D. Dwivedi, J. E. Houseworth, M. T. Reagan, W. T. Stringfellow, C. Varadharajan, and J. T. Birkholzer. "Chapter 4: Hydraulic Fracturing from the Groundwater Perspective." In: Groundwater Research on Exploration, Assessment, Modelling and Management of Groundwater Resources and Pollution, Taylor & Francis (2016). ISBN 9781498742849

Workshops, Conferences, and Presentations

S. B. C. Shonkoff, W. T. Stringfellow, and J. K. Domen. "Preliminary Hazard Assessment of Chemical Additives Used in Oil and Gas Fields that Reuse Their Produced Water for Agricultural Irrigation in The San Joaquin Valley of California." Technical Report. PSE Healthy Energy, Inc. Oakland, CA. (2016, September)

W. T. Stringfellow, S. B. C. Shonkoff, M. K. Camarillo, C. Varadharajan, P. Jordan, and J. Birkholzer. (Invited Presentation). "Implications of Oil Field Chemicals for Produced Water Beneficial Reuse." Presidential Symposium on Fracking:

- Economics vs. Environment. 252nd American Chemical Society National Meeting & Exposition, Philadelphia, PA August 21-24 (2016)
- W. T. Stringfellow, M. K. Camarillo, N. Spycher, and P. Nico. "Produced water from oil & gas fields as a potential source of irrigation water." Toward Sustainable Groundwater in Agriculture – An International Conference Linking Science and Policy, Burlingame / San Francisco, CA, June 28-30 (2016)
- W. T. Stringfellow. (Invited Presentation). "Reuse of industrial wastewater for irrigated agriculture & other beneficial uses." Annual Water Conference. E & J Gallo Winery, Modesto, CA. March 11 (2016)
- W. T. Stringfellow, M. K. Camarillo, J. K. Domen, W. Sandelin, C. Varadharajan, P. Jordan, M. Reagan, H. Cooley, M. Heberger, and J. Birkholzer. (Invited Presentation). "Quantitative Analysis Chemicals Used for Hydraulic Fracturing in California (USA)." Symposium on Environmental Aspects of Unconventional Oil and Gas Production and Hydraulic Fracturing, 251st American Chemical Society National Meeting & Exposition, San Diego, CA, March 13-17 (2016)
- M. K. Camarillo, W. T. Stringfellow, J. K. Domen, and W. L. Sandelin. "Screening treatment technologies for hydraulic fracturing wastes based on physical and chemical data." Symposium on Environmental Aspects of Unconventional Oil and Gas Production and Hydraulic Fracturing, 251st American Chemical Society National Meeting & Exposition, San Diego, CA, March 13-17 (2016)
- Shonkoff, S. B. C., J. Domen, M. K. Camarillo, and W. T. Stringfellow. (Invited Presentation). "From 'fracking' to oil and gas development: chemical constituents and potential implications for the beneficial reuse of produced water." Symposium on Environmental Aspects of Unconventional Oil and Gas Production and Hydraulic Fracturing, 251st American Chemical Society National Meeting & Exposition, San Diego, CA, March 13-17 (2016)

ED-Kostecki LB16040 Volumetric Absorption of Solar Radiation in Liquids and Gases by Tuning the Emissivity of Surfaces

Journal Publications

- J. P. Freedman, H. Wang, and R. S. Prasher, "Comparison of volumetric and surface-based heating of fluids for power generation and hot water production", in preparation

ED-Srinivasan LB16018 Accelerating Technology Development by Disruptive Scaling and Manufacturing Processes

Journal Publications

- Higa, H. Zhao, D. Y. Parkinson, H. Barnard, M. Ling, G. Liu, and V. Srinivasan, "Electrode slurry particle density mapping using X-ray radiography", Journal of the Electrochemical Society, submitted

ED-Stewart LB16019 Intelligent Distribution Grid Analytics: Distribution Phasor Measurement Unit and Operational Data Counseling For Resilience and Reliability Applications (ID-GRID)

Workshops, Conferences, and Presentations

- M. Sankur et al: Model Predictive Control of Flexible Demand for Voltage Support in Unbalanced Distribution Systems, IEEE PES General Meeting Conference, July 2017
- M Stadler et al: Optimal Sizing and Placement of Distributed Generation: MILP vs PSO Comparison in a Real Microgrid Application, IEEE PES General Meeting Conference, July 2017
- E. Stewart et al: A Data-Driven Analysis of Lightning-Initiated Contingencies at a Distribution Grid with a PV Farm Using Micro-PMU Data, IEEE PES General Meeting Conference, July 2017
- J. Opara et al: Real vs. Simulated Voltage Phasor Measurements, IEEE PES General Meeting Conference, July 2017
- E. Stewart et al: Controllability, Measurement and Analytic Nodes in Distribution for DER, International Conference on Electricity Distribution), June 2017
- D Arnold M Sankur et al: Data Driven Approach for Monitoring, Protection and Control of Distribution System Assets Using micro-PMU Technology, International Conference on Electricity Distribution), June 2017
- E. Stewart et al Improving Actionable Observeability of Large Distribution Networks for Transmission Operators to Support Improved System control, Fault detection & Mitigation, International Conference on Electricity Distribution), June 2017

EG-Denes LB14031 Neuro/Nano Technology for Brain Mapping

Journal Publications

- TBD E. S. Levy, C. Tajon, T. S. Bischof, A. F.-Bravo, D. J. Garfield, J. Iafrati, M. Chamanzar, V. Sohal, M. Maharbiz, P. J. Schuck, B. E. Cohen, E. M. Chan; "Energy-looping upconverting nanoparticles for non-resonant imaging in highly scattering media", ACS Nano 10, 8423-8433
- C. Tajon, A. Fernandez-Bravo, B. Tan, E.M. Chan, P.J Schuck, B.E. Cohen; "Stable and efficient upconverted energy transfer between lanthanide-doped nanocrystals and organic fluorescent biosensors", to be submitted
- Bouchard, K.E., Conant, D., Anumanchipalli, G., Dichter, B.; Johnson, K., Chang, E.F.; "High-resolution, non-invasive imaging of upper vocal tract articulators compatible with human brain recordings"; PLoS One. March, 2016
- Dichter, B., Bouchard, K.E., Chang, E.F.; "Dynamic structure of neural variability in the cortical representation of speech sounds"; J. Neuroscience, July, 2016
- Muller, L; Hamilton, L; Edwards, E; Bouchard, K; Chang, E.; "Spatial resolution dependence on spectral frequency in human electrocorticography"; J. Neural Engineering, Aug., 2016
- Bouchard, K.E., Brainard, M.S.; "Predictive neural dynamics in songbird sensory-motor circuitry reflects behavioral statistics"; PNAS, Aug., 2016
- Troyer, T.W., Brainard, M.S., Bouchard, K.E.; "Timing during transitions in Bengalese finch song: implications for motor sequencing"; Submitted to J. Neurophys
- Bouchard, K.E., Ledochowitsch, P., Yazdan-Shahmorad, A., Hasenstaub, A., Schriener, C.E., Sabes, P., Maharbiz, M.M., Chang, E.F.; "Functional response properties and laminar origin of different high-frequency components of field potential recorded from the cortical surface", Submitted to eLife

- Bouchard, K.E., et al., "High-Performance Computing in Neuroscience for Data-Driven Discovery, Integration, and Dissemination", *Neuron*, Oct. 2016
- Bouchard, K.E., Bujan, A.F., Roosta, F., Prabhat, Snijders, A., Mao, J-H., Chang, E.F., Mahoney, M., Bhattacharyya, S.; "The Union of Intersections Method for Interpretable Data Driven Discovery and Prediction", Under Review at PNAS/Statistics
- Rübel, O., Prabhat, Denes, P., Conant, D., Chang, E.F., Bouchard, K.E.; "BRAINformat: A Data Standardization Framework for Neuroscience Data", *Front. Neuralinformatics*, Nov., 2016

Workshops, Conferences, and Presentations

- M. Chamanzar, D.J. Garfield, J. Iafrati, V. Sohal, E. Chan, B.E. Cohen, P. J. Schuck, M. M. Maharbiz, "Deep tissue targeted near-infrared optogenetic stimulation using fully implantable upconverting light bulbs", Proceedings of the International Conference of the IEEE Engineering in Medicine and Biology Society 2016, 821
- Tang, H., Byna, S., Harenberg, S., Zou, X., Zhang, W., Wu, K., Dong, B., Rubel, O., Bouchard, K.E., Klasky, S., and Samatova, N.F., "Usage Pattern-Driven Dynamic Data Layout Reorganization", IEEE/ACM CCGrid, 2016
- Murugesan, S., Bouchard, K.E., Brown, J.A., Hamann, B., Seeley, W.W., Trujillo, A., Weber, G. H., "Brain Modulyzer: Interactive Visual Analysis of Functional Brain Connectivity", IEEE TCBB, May, 2016
- Murugesan, S., Bouchard, K. E., Chang, E. F., Dougherty, M., Hamann, B. and Weber, G. H., "Hierarchical spatio-temporal visual analysis of cluster evolution in electrocorticography data", Brain-KDD, Aug., 2016

EB-Bowen LB15039 High-Performance Chemical Identification for Hyperspectral Data Science

Journal Publications

- Fischer CR, Ruebel O, Bowen BP. "An accessible, scalable ecosystem for enabling and sharing diverse mass spectrometry imaging analyses". *Arch Biochem Biophys.* 2016;589:18–26. <http://dx.doi.org/10.1016/j.abb.2015.08.021>
- de Raad M, de Rond T, Ruebel, O, Keasling JD, Northen TR, Bowen BP. "OpenMSI Arrayed Analysis Toolkit: Analyzing spatially defined samples using mass spectrometry imaging." Submitted.
- Ruebel O, Bowen BP. "BASTet: Shareable and reproducible analysis and visualization of mass spectrometry imaging data via OpenMSI." Submitted
- Fischer CR, Ruebel O, Bowen BP. "Precomputed spectral trees for small-molecule structural elucidation via tandem mass spectrometry." Draft publication

EB-Brown LB14027 Reinventing Pre-clinical and Environmental Testing Paradigms

Journal Publications

- TBD Snijders AM, Langley SA, Kim YM, Brislaw CJ, Noecker C, Zink EM, Fansler SJ, Casey CP, Miller DR, Huang H, Karpen GH, Celiker SE, Brown JB, Borenstein E, Jansson JK, Metz TO, Mao JH. Influence of early life exposure, host genetics and diet on the mouse gut microbiome and metabolome. *Nat Microbiol.* 2016 Nov 28;2:16221. doi: 10.1038/nmicrobiol.2016.221

Zhang W, Mao JH, Zhu W, Jain AK, Liu K, Brown JB & Karpen GH. "Centromere and kinetochore gene misexpression predicts cancer patient survival and response to radiotherapy and chemotherapy". *Nature Communications*. 2016. In press. DOI: 10.1038/ncomms12619

Orsini L, Gilbert D, Podicheti R, Jansen M, Brown JB, Solari OS, et al. (2016). *Daphnia magna transcriptome by RNA-Seq across 12 environmental stressors*. *Scientific data*, 3. PMID: 27164179 PMCID: PMC4862326 DOI: 10.1038/sdata.2016.30

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Stoiber MH, Celniker SE, Cherbas L, Brown JB*, Cherbas P. "Diverse hormone response networks in 41 independent *Drosophila* cell lines". *G3 (Bethesda)*. 2016 Jan 15. pii: g3.115.023366

EB-Celniker LB15022 Microbiome Adaptation in Response to Environmental Challenges

Journal Publications

Snijders AM, Langley SA, Kim YM, Brislaw CJ, Noecker C, Zink EM, Fansler SJ, Casey CP, Miller DR, Huang Y, Karpen GH, Celniker SE, Brown JB, Borenstein E, Jansson JK, Metz TO, and Mao JH. Influence of early life exposure, host genetics and diet on the mouse gut microbiome and metabolome. *Nat Microbiol*. 2016 2:16221, <http://www.nature.com/articles/nmicrobiol2016221>

JG-Woyke LB15021 Tackling Microbial-Mediated Plant Carbon Decomposition Using Function-Driven Genomics

Journal Publications

D, Doud, T, Woyke, "Novel approaches in function-based single-cell genomics", *FEMS Microbiology Reviews*, 28 Oct 2016, In Review
T, Woyke, D, Doud, F, Schulz, "A trajectory of microbial single-cell sequencing", *Nature Methods*, 22 Dec 2016, In Review
D, Doud, Y, Yoshikuni, S, Deutsch, N, Ivanova, T, Woyke, "Function-based single-cell genomics of active environmental cellulose degraders", Dec 2016, In Preparation
D, Doud, T, Woyke, "Illuminating cellulose deconstruction in the Koala microbiome", Dec 2016, In Preparation

Workshops, Conferences, and Presentations

D, Doud, T, Woyke, "Function-based single-cell genomics of uncultivated environmental cellulose-degrading bacteria", *Lake Arrowhead Microbial Genomics*, Sept 2016, Poster

MS-Fadley LB14033 Hard X-Ray Photoemission for Materials Science

Journal Publications

Johannes Lischner, Slavomír Nemšák, Giuseppina Conti, Andrei Hloskovsky, Gunnar Karl Pálsson, Wolfgang Drube, Steven G. Louie, Charles S. Fadley, "Accurate determination of the valence band edge in hard x-ray photoemission spectra by means of GW theory", *J. Appl. Phys.* 119, 165703 (2016), April, 2016, <http://aip.scitation.org/doi/full/10.1063/1.4947594>

- D. Eiteneer, G. K. Pálsson, S. Nemšák, A. X. Gray, A. M. Kaiser, J. Son, J. LeBeau, G. Conti, A. Y. Saw, A. Rattanachata, A. Keqi, A. A. Greer, A. Bostwick, E. Rotenberg, E. M. Gullikson, S. Ueda, K. Kobayashi, A. Janotti, C. Van de Welle, A. Blanca-Romero, R. Pentcheva, S. Stemmer C. S. Fadley, "Depth-Resolved Electronic Structure of Buried Layers and Interfaces in a LaNiO₃/SrTiO₃ Superlattice from Soft X-ray Standing-Wave Angle-Resolved Photoemission", *J. Electron Spectrosc.* 211, 70-81 (2016), August, 2016, <http://www.sciencedirect.com/science/article/pii/S0368204816300536>
- S. Nemšák, G. Pálsson , A.X. Gray, D.Eiteneer, A.M. Kaiser, G. Conti, A.Y. Saw, A. Perona, A. Rattanachata, C. Conlon, A. Bostwick, V. Strocov, M. Kobayashi, W. Stolte, A. Gloskovskii, W. Drube , M.-C. Asencio, J. Avila, J. Son, P. Moetakef, C. Jackson, A. Janotti, C. G. Van de Walle , J. Minar, J. Braun, H. Ebert, J.B. Kortright, S. Stemmer, and C. S. Fadley, "Energetic, spatial, and momentum character of the electronic structure at a buried interface: The two-dimensional electron gas between two metal oxides", *Phys. Rev. B* 93, 245103 (2016), June, 2016, <http://journals.aps.org/prb/abstract/10.1103/PhysRevB.93.245103>
- B. A. Gray, S. Middey, G. Conti, A. X. Gray, C.-T. Kuo, A. M. Kaiser, S. Ueda, K. Kobayashi, D. Meyers, M. Kareev, I. C. Tung, Jian Liu, C. S. Fadley, J. Chakhalian & J. W. Freeland, "Interface driven superconductor to insulator transition in ultra-thin manganite-cuprate superlattices" S. Middey, *Scientific Reports* 6, Article number: 33184 (2016), September, 2016- <http://www.nature.com/articles/srep33184>
- C.S. Fadley, "Hard X-ray Photoemission: An Overview and Future Perspective", invited introductory chapter to appear in the book Hard X-ray Photoelectron Spectroscopy, J. C. Woicik, Editor, Springer (2015), review of 37 pages and 20 figures. Published 2016, <http://fadley.physics.ucdavis.edu/HAXPES.Book.Woicik.Fadley.reprint.final.pdf>
- Slavomir Nemšák, Alexander X. Gray, and Charles S. Fadley, "Standing-Wave and Resonant Soft- and Hard- X-Ray Photoelectron Spectroscopy of Oxide Interfaces", invited chapter for the book Spectroscopy of transition-metal oxide interfaces, Editors: C. Cancellieri and V.N. Strocov (Springer, in press), <http://fadley.physics.ucdavis.edu/Nemsak,%20Gray,%20Fadley.Oxide.Interface.Boo k.SW.XPS.&.ARPES.preprint.pdf>
- G. Conti, S.Nemšák, H. Fang, C. Conlon, G. K. Pálsson, C. Battaglia, A. Javey, C.S. Fadley, "Depth Profiling of Semiconductor InAs Stripes via Standing-Wave Hard X-ray Photoelectron Spectroscopy", in preparation
- Shih Chieh Lin, Cheng-Tai Kuo, Ryan B. Comes, Steve M. Heald, Steven R. Spurgeon, Despoina M. Kepartsoglou, Quentin M. Ramasse, Mark Engelhard, Julien Rault, Slavomir Nemsak, Charles S. Fadley, Peter V. Sushko, and Scott A. Chambers, "Interface composition and electronic structure of LaCrO₃/SrTiO₃ from standing wave- and resonant core- and valence- photoemission", in preparation
- C.-T. Kuo, S.-C. Lin, S.T. Pi, A.F. Santander-Syro, A. Bostwick, L. Moreschini, J. Garst, J. Rault, Warren Pickett, A. Taleb-Ibrahim, "Atomic-layer resolved electronic structure of the high-temperature superconductor Bi₂Sr₂CaCu₂O₈ from standing-wave soft x-ray angle-resolved photoemission", in preparation
- S. Nemšák, Sven Döring, Christof Schlueter, Markus Eschbach, Ewa Mlynaczak, Tien-Lin Lee, Lukasz Plucinski, Jan Minar, Juergen Braun, Hubert Ebert, Claus

Schneider, Charles Fadley, "Standing-wave hard x-ray angle-resolved photoemission: element- and momentum-resolved band structure for a dilute magnetic semiconductor", in preparation.

C.-T. Kuo , S.-C. Lin, G. Ghiringhelli, G. De Luca, N. Brookes, D. Di Castro, M. Huijben, Y. Y. Ping, L. Moreschini, A. Bostwick, J.B. Kortright, J. Meyer-Ilse, E. Gullikson, A. Taleb-Ibrahimi, J. Rault, S.-H. Yang, L. Braicovich, C.S. Fadley, "Depth-resolved resonant inelastic x-ray scattering near a high-TC/half-metallic ferromagnet interface from standing-wave photoemission", in preparation

MS-Martin LB16027 Exploring Strong Visible Light-Matter Interactions in Correlated Oxide Materials

Journal Publications

R. Gao, Y. Dong, H. Xu, H. Zhou, Y. Yuan, V. Gopalan, C. Gao, D. D. Fong, Z. Chen, Z. Luo, L. W. Martin, "Interfacial Octahedral Rotation Mismatch Control of the Symmetry and Properties of SrRuO₃", ACS Applied Materials and Interfaces 8, 14871-14878 (2016), <http://pubs.acs.org/doi/abs/10.1021/acsami.6b02864>, May 24, 2016

L. R. Dedon, S. Saremi, Z. Chen, A. R. Damodaran, B. A. Apgar, R. Gao, L. W. Martin, "Nonstoichiometry, Structure, and Properties of BiFeO₃ Films", Chemistry of Materials 28, 5952-5961 (2016), <http://pubs.acs.org/doi/abs/10.1021/acs.chemmater.6b02542>, July 25, 2016

Z. Chen, X. Wang, Y. Qi, S. Yang, J. A. N. T. Soares, B. A. Apgar, R. Gao, R. Xu, Y. Lee, X. Zhang, J. Yao, L. W. Martin, "Self-Assembled, Nanostructured, Tunable Metamaterials via Spinodal Decomposition", ACS Nano 10, 10237-10244 (2016), <http://pubs.acs.org/doi/abs/10.1021/acsnano.6b05736>, Nov. 9, 2016

MS-Minor LB16028 Defect Dynamics and Surface Structure Evolution of Tungsten Studied with Ultrafast Electron Diffraction

Journal Publications

D. Filippetto and H. Qian, "Design of a high-flux instrument for ultrafast electron diffraction and microscopy", Journal of Physics B: Atomic, Molecular and Optical Physics, 49, 10 (2016) <http://iopscience.iop.org/article/10.1088/0953-4075/49/10/104003/meta>

MS-Naulleau LB15025 Understanding Radiation-Induced Photo-Electron Chemistry in High-Cross Section Organometallic Resist Materials

Journal Publications

Closser, K. D.; Ogletree, D. F.; Naulleau, P.; Prendergast, D. The importance of inner-shell electronic structure for enhancing the EUV absorption of photoresist materials. J. Chem Phys. 2016, Submitted, 1–28

Workshops, Conferences, and Presentations

Deirdre Olynick, Patrick Naulleau, Musa Ahmed, Yi Liu, Paul Ashby, Frank Ogletree, David Prendergast, Kristi Closser, Oleg Kostko, Bo Xu, Andreas Schmid, Bill Hinsberg, Greg Wallraff, "Elements for EUV Electronic Resist Amplification," The Lithography Workshop 2016, Hapuna Beach, Big Island, Hawaii, Nov. 6-10, 2016

- O. Kostko, B. Xu, D.S. Slaughter, K.D. Closser, S. Bhattarai, D.L. Olynick, D.G. Prendergast, P.D. Ashby, D.F. Ogletree, Y. Liu, P. Naulleau, M. Ahmed, B. Hinsberg, G. Wallraff, "EUV radiation chemistry fundamentals: Gas-phase probing techniques," 2016 International Symposium on Extreme Ultraviolet Lithography, Hiroshima Japan, Oct. 24-26, 2016, proceedings available from LBNL Center for X-ray Optics, Berkeley, CA
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MS-Neaton LB15026 Computational Design of Smart Complex Oxides with Tunable Quantum Phases

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- R. Chen, H. Chun Po, J. B. Neaton, and A. Vishwanath, "Topological Materials Discovery using Electron Filling Constraints", submitted to *Nature Physics* (2016) (arXiv:1611.06860)
- M. Park, N. Kornienko, S. E. Reyes-Lillo, M. Lai1, J. B. Neaton, P. Yang, and R. A. Mathies, "Critical Role of Methylammonium Librational Motion in Methylammonium Lead Iodide (CH₃NH₃PbI₃) Perovskite Photochemistry", submitted to *Nano Lett* (2016)
- B. M. Wiers, S. C. Andrews, M. L. Aubrey, T. Sakurai, S. Hamed, C.-J. Yu, J. A. Mason, J.-O. Baeg, F. Grandjean, G. J. Long, S. Seki, J. B. Neaton, P. Yang, and J. R. Long, "Electron Mobility as a Function of Reduction in a Conductive Metal-Organic Framework", submitted to *Nature* (2016)
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MS-Rabani LB16029 A Stochastic Approach to Calculate Auger Recombination and Impact Excitation Rates: Application to Core-Shell Nanocrystals

Journal Publications

- A. D. Balan, H. Eshet, J. H. Olshansky, Y. V. Lee, E. Rabani and A. P. Alivisatos "Effect of Thermal Fluctuations on the Radiative Rate in Core/Shell Quantum Dots", submitted to *Nano Letters* (2016)

MS-Wang LB16030 Controlling Quantum Phenomena in Van der Waals Heterostructures: Excitons, Valleys, and Superconductivity

Journal Publications

- Chenhao Jin, Jonghwan Kim, Joonki Suh, Zhiwen Shi, Bin Chen, Xi Fan, Matthew Kam, Kenji Watanabe, Takashi Taniguchi, Sefaattin Tongay, Alex Zettl, Junqiao Wu, and Feng Wang, "Interlayer electron–phonon coupling in WSe₂/hBN heterostructures", *Nature Physics*, doi:10.1038/nphys3928 (2016)
<http://www.nature.com/nphys/journal/vaop/ncurrent/full/nphys3928.html>

MS-Yao LB15036 Optical and Electrical Characterization of 2-Dimensional Nanosheets

without Naturally Layered Structure

Journal Publications

Kyle Tom, Xi Wang, Yang Deng, Shuai Lou, Karen Bustillo, Frank Ogletree and Jie Yao, “Large scale solution based synthesis of van der Waals ZnO sheets”, in preparation

MB-Frei LB16035 Robust Synthetic Membranes for Microbial Electrocatalysis:
Separating Electron-Generating Organisms from the Catalytic Reaction Environment

Journal Publications

T. Fukushima, S. Gupta, B. Rad, J. A. Cornejo, C. Petzold, L-J. C. Chan, R. Mizrahi, M. Charrier, B. Peng, C. Ralston, C. M. Ajo-Franklin. “The electron transfer protein MtrF binds to its inorganic substrate through electrostatic interactions created by tertiary structure”, Submitted
H. Sheng, E. Edri, J. A. Cornejo, C. Ajo-Franklin, H. Frei. “Silica-embedded molecular wires with tuned electronic properties anchored on WO₃ and SnO₂ surfaces”, In preparation

MB-Hura LB15042 Life Science Applications of Xray Scattering at ALS Upgrade

Journal Publications

Hura G. L. et al, “Designing and defining dynamic protein cage nanoassemblies in solution”, Science Advances, Dec 2016
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NE-Wright LB14026 Codesigning Big Iron for Big Data

Workshops, Conferences, and Presentations

TBD C. S. Daley, D. Ghoshal, G. K. Lockwood, S. Dosanjh, L. Ramakrishnan, and N. J. Wright “Performance Characterization of Scientific Workflows for the Optimal Use of Burst Buffers”. Workflows in Support of Large-Scale Science (WORKS-2016) held in conjunction with the 28th IEEE/ACM International Conference for High Performance Computing, Networking, Storage and Analysis (SC16), November 2016

C. S. Daley, D. Ghoshal, G. K. Lockwood, S. Dosanjh, L. Ramakrishnan, and N. J. Wright. “Performance Characterization of Scientific Workflows for the Optimal Use of Burst Buffers”. Future Generation Computer Systems. Special Issue on Workflows for Data-Driven Research. Extended version of the WORKS2016 paper to be submitted

W. Bhimji, D. Bard, M. Romanus, D. Paul, A. Ovsyannikov, B. Friesen, M. Bryson, J. Correa, G. K. Lockwood, V. Tsulaia, S. Byna, S. Farrell, D. Gursoy, C. Daley, V. Beckner, B. V. Straalen, N. J. Wright, K. Antypas, and Prabhat. “Accelerating Science with the NERSC Burst Buffer,” Early User Program. Cray User Group (CUG), May 2016

W. Bhimji, C. Daley, D. Bard, J. Porter, K. Burleigh, L. Gerhardt, M. Fasel, P. Nugent, S. A. Farrell, and V. Tsulaia. “Extreme I/O on HPC for HEP using the Burst Buffer at NERSC”. The 22nd International Conference on Computing in High Energy and Nuclear Physics (CHEP 2016), October 2016. Write-up of oral presentation in preparation

NS-Crawford LB16032 Toward Next Generation Gamma-Ray Tracking Arrays:
Development of Inverted Coaxial Segmented HPGe Detector Technology

Journal Publications

M. Salathe, H. L. Crawford, R. J. Cooper, D. C. Radford, C. M. Campbell, R. M. Clark, M. Cromaz, P. Fallon, M. Jones and A. O. Macchiavelli, “Energy Reconstruction of a n-Type Inverted Coaxial Segmented HPGe Point Contact Detector”, in preparation for submission to Nucl. Instrum. and Methods in Phys. Res. A

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M. Salathe, H. L. Crawford, R. J. Cooper, and D. C. Radford, “Inverted Coaxial HPGe Segmented Point Contact Detector”, First AGATA-GRETINA Tracking Arrays Collaboration Meeting, 2016, <https://indico.in2p3.fr/event/13409/other-view?view=standard>

M. Salathe, H. L. Crawford, R. J. Cooper, and D. C. Radford, “Inverted Coaxial HPGe Segmented Point Contact Detector”, 2016 Fall Meeting of the APS Division of Nuclear Physics, 2016, <http://meetings.aps.org/Meeting/DNP16/Session/PD.2>

NS-Haxton LB15027 Computational Nuclear Physics Code Development for
Fundamental Interactions/Astrophysics

Journal Publications

E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P. Vranas, and A. Walker-Loud, “Two Nucleon Higher Partial-Wave Scattering from Lattice QCD,” Phys. Letts. B765 (2017) 285-292 (arXiv:1508.00886)

J. de Vries, E. Mereghetti, C.-Y. Seng, and A. Walker-Loud, “Lattice QCD Spectroscopy for Hadronic CP Violation,” arXiv:1612.01567

C. Bouchard, C.C. Chang, T. Kurth, K. Orginos and A. Walker-Loud, “On the Feynman-Hellmann Theorem in Quantum Field Theory and the Calculation of Matrix Elements,” arXiv:1612.06963

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A. Nicholson, E. Berkowitz, C. C. Chang, M. A. Clark, B. Joo, T. Kurth, E. Rinaldi, B. Tiburzi, P. Vranas, and A. Walker-Loud, “Neutrinoless Double Beta Decay from Lattice QCD,” to be published in the Proc. Int. Symp. On Lattice Field Theory (2016) (arXiv:1608.04793)

W. R. Hix, E. J. Lentz, S. W. Bruenn, A. Mezzacappa, O. E. B. Messer, E. Endeve, J. M. Blondin, J. A. Harris, P. Marronetti, K. N. Yakunin, “The Multidimensional Character of Core-collapse Supernovae,” Proceedings of the 34th Mazurian Lakes Conference on Physics (MLCP 2015), Piaski, Poland, September 6–13, 2015. Acta Physica Polonica B, 47, 645 (2016), doi:10.5506/APhysPolB.47.645

NS-Mei LB16033 Topmetal Charge Readout Plane for Neutrinoless Double Beta Decay Searches

Journal Publications

- TBD M. An et. al., “A low-noise CMOS pixel direct charge sensor, Topmetal-II-”, Nucl. Instr. and Meth. A 810, 144-150 (2016), 10.1016/j.nima.2015.11.153
M. An et. al., “Detailed study of the column-based priority logic readout of Topmetal-II- CMOS pixel direct charge sensor”, arXiv:1608.06399 [physics.ins-det]

NS-Orebi Gann LB15035 Next-Generation Neutrino and Rare-Event Detection

Journal Publications

- J. Caravaca, F.B. Descamps, B.J. Land, J. Wallig, M. Yeh, and G.D. Orebi Gann, “An Experiment to Demonstrate Cherenkov / Scintillation Signal Separation”, arXiv:1610.02029 [physics.ins-det], <https://arxiv.org/abs/1610.02029>, submitted to Phys. Rev. C (2016)
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NS-Vetter LB15028 Multi-disciplinary Research to Enhance Understanding of Transport, Risks, and Mitigation of Radioisotopes for Improved Radiological Resilience

Journal Publications

- A. Haefner, R. Barnowski, P. Luke, M. Amman, L. Mihailescu, K. Vetter. “Handheld Real-time Volumetric 3-D Gamma-ray Imaging”, accepted for publication in Nucl. Instr. Meth. A
A. Haefner, R. Barnowski, R. Pavlovsky, K. Vetter. “A gamma camera for three-dimensional gamma-ray vision”, in preparation for Nature Communications
S. Costes, D. Sridharan, S. Gauny, D. An, A.-C. Heuskin, A. Bertho, R. Pavlovsky, K. Vetter, R. Abergel, "Discriminating radiation damage from chemical toxicity using 53BP1 profiles in mammalian carcinoma cells exposed to various isotopes of cesium and external radiations." In preparation
T.A. Choi, S.V. Costes, R.J. Abergel, Understanding the Health Impacts and Risks of Exposure to Radiation. 2014 In Reflections on the Fukushima Daiichi Nuclear Accident, Springer, J. Ahn et al. (eds.), DOI 10.1007/978-3-319-12090-4_13
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C. Suzuki, T. Yaita, S. Suzuki, J. Pacold, A. B. Altman, S. G. Minasian, T. Tyliszczak, D. K. Shuh, and H. Yoshida, "Electronic State of Cs Halides and Cs-Adsorbed Clay Minerals Based on NEXAFS Analysis and Interpretation Using DFT Calculations," submitted to Phys. Rev. B, (2016)
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- E.R. Siirila-Woodburn, C.I. Steefel, K.H. Williams, A. Kitamura, J.T. Birkholzer, “Using Hydrologic Modeling to Evaluate Forest Remediation Strategies in the Fukushima Prefecture”, Second International Symposium for Resilient Communities, April 14-15, 2016
- E.R. Siirila-Woodburn, C.I. Steefel, K.H. Williams, “JAEA Annual Report: Multi-Scale Catchment to Watershed Characterization and Modeling”, September 27, 2016
- E.R. Siirila-Woodburn, L.N. Lammers, C.I. Steefel, K. Williams, I.C. Bourg, G. Sposito, J.T. Birkholzer, “JAEA Annual Report: Repository Geoscience and PA Technology Development Task C: Contribute to the Compilation of Knowledgebase of Repository Science and Technology”, May 16, 2016
- R. Abergel, S. Costes, K. Vetter, "Monitoring and Predicting the Impact of Exposure to Cs-137 in the Aftermath of Fukushima." 2015 Annual Meeting of the Radiation Research Society

PH-Hinchliffe LB15030 Searches for the Supersymmetric Particles at the LHC in Run-2 and Beyond

Journal Publications

- Morad Aaboud (Oujda U.) et al; “Search for heavy long-lived charged R-hadrons with the ATLAS detector in 3.2 fb^{-1} of proton- $\bar{\text{p}}$ collision data at $s^{\sqrt{}}=13 \text{ TeV}$ ”, Published in Phys.Lett. B760 (2016) 647-665
- Morad Aaboud (Oujda U.) et al , “Search for supersymmetry in a final state containing two photons and missing transverse momentum in $s^{\sqrt{}}=13 \text{ TeV}$ pp collisions at the LHC using the ATLAS detector”, Published in Eur.Phys.J. C76 (2016) no.9, 517 CERN-EP-2016-146
- Georges Aad (Marseille, CPPM) et al, “Search for supersymmetry at $s^{\sqrt{}}=13 \text{ TeV}$ in final states with jets and two same-sign leptons or three leptons with the ATLAS detector”, Published in Eur.Phys.J. C76 (2016) no.5, 259

PH-Kusaka LB16037 Enabling Technologies for Next Generation Receivers to Measure the Polarization of Cosmic Microwave Background

Workshops, Conferences, and Presentations

- Charles A. Hill, Shawn Beckman, Yuji Chinone, Neil Goeckner-Wald, Masashi Hazumi, Brian Keating, Akito Kusaka, Adrian T. Lee, Frederick Matsuda, Richard Plambeck, Aritoki Suzuki, Satoru Takakura, “Design and development of an ambient-temperature continuously-rotating achromatic half-wave plate for CMB polarization modulation on the POLARBEAR-2 experiment,” Proc. SPIE 9914, Millimeter, Submillimeter, and Far-Infrared Detectors and Instrumentation for Astronomy VIII, 99142U (2016); doi:10.1117/12.2232280, <https://doi.org/10.1117/12.2232280>

PH-Lee LB14024 Next Generation Cosmic Microwave Background Detector Arrays: Enabling a Factor 10-100 Increase in Array Size

Journal Publications

- A. Suzuki et al., “Commercialization of micro-fabrication of antenna coupled Transition Edge Sensor bolometer detector for studies of the Cosmic Microwave Background”, In preparation

PH-Papucci LB15031 Confronting Beyond the Standard Model Theories with New LHC and Astrophysical Data

Journal Publications

- TBD S.Knapen, T.Lin, H.K.Lou and T.Melia, "Searching for axion-like particles with ultra-peripheral heavy-ion collisions", <http://arxiv.org/abs/arXiv:1607.06083>
- W.E.East, J.Kearney, B.Shakya, H.Yoo and K.M.Zurek, "Spacetime Dynamics of a Higgs Vacuum Instability During Inflation", Phys. Rev. D 95, 023526 (2017), <http://arxiv.org/abs/arXiv:1607.00381>
- S.Knapen and D.Redigolo, "Gauge Mediation at LHC: status and prospects", JHEP 1701, 135 (2017) <http://arxiv.org/abs/arXiv:1606.07501>
- K.Howe, S.Knapen and D.J.Robinson, "Diphotons from electroweak triplet-singlet mixing", Phys. Rev. D 94, no. 3, 035021 (2016) <http://arxiv.org/abs/arXiv:1603.08932>
- M.Freytsis, S.Knapen, D.J.Robinson and Y.Tsai, "Gamma-rays from Dark Showers with Twin Higgs Models", JHEP 1605, 018 (2016) <http://arxiv.org/abs/arXiv:1601.07556>
- N.Craig, S.Knapen, P.Longhi and M.Strassler, "The Vector-like Twin Higgs", JHEP 1607, 002 (2016) <http://arxiv.org/abs/arXiv:1601.07181>
- T.Cohen, N.Craig and S.Knapen, "Gauge Mediated Mini-Split", JHEP 1603, 103 (2016) <http://arxiv.org/abs/arXiv:1512.06128>
- S.Knapen, T.Melia, M.Papucci and K.Zurek, "Rays of light from the LHC", Phys. Rev. D 93, no. 7, 075020 (2016) <http://arxiv.org/abs/arXiv:1512.04928>

SN-Monga LB15032 ESnet Operating System

Workshops, Conferences, and Presentations

- M Kiran, E Pouyoul, A Mercian, B Tierney, C Guok, I Monga, "Enabling Intent to Configure Scientific Networks for High Performance Demands", 3nd International Workshop on Innovating the Network for Data Intensive Science (INDIS) 2016, November 2016.
- https://scinet.supercomputing.org/workshop/sites/default/files/INDIS16_paper05.pdf

