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Laboratory Directed Research and Development Program FY 2015

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Report on
Ernest Orlando Lawrence
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Laboratory Directed Research and Development Program

FY 2015

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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) 2015 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 FY2015* 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 413.2B Admin Chg 1 (dated January 31, 2011). 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 FY2015, Berkeley Lab was authorized by DOE to establish a funding ceiling for the LDRD program of $25M including General & Administrative (G&A) overhead, which equated to ~3.4% of Berkeley Lab's FY2015 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 $24.8M was expended for operating expenses.

In FY2015, scientists submitted 172 proposals, requesting about $41.7M in funding prior to assessing laboratory overhead. Eighty six projects were funded, with awards ranging from $14K to $1.15M.

Towards the Development of a Fiber Based Laser Plasma Accelerator (LPA) and Assessment of its Utility for Potential Biomedical Applications

Principal Investigator(s): Wim Leemans

Project Description

The purpose of this project is to develop the technology necessary for a fiber based laser plasma accelerator (LPA) to be used for electronic brachytherapy treatment of prostate cancer. Such a device would deliver MeV electrons suitable for medical applications in a small form factor machine. The laser pulse is transported through a hollow core fiber optic that terminates at an embedded gas target where ionization and acceleration occurs. LPAs operate with energy gradients 1000 times larger than conventional accelerators allowing for the energy gain to occur within a millimeter of the treatment area, increasing the therapeutic dose to the tumor site while minimizing collateral irradiance of adjacent healthy tissue.

This research will target several milestones that will ultimately culminate in a prototype device. These milestones include, design of a gas jet capable of providing 1-10 MeV electrons, development of a hollow core fiber suitable for transporting the necessary laser energy, and establishing a program to evaluate the efficacy of LPA produced electrons as a radiation source. Initial efforts will focus on developing a gas jet target. The target will utilize a tailored gas profile featuring a sharp density transition reducing the level of laser energy needed for electron injection. Laser plasma simulations will be conducted to establish the gas parameters and physical dimensions necessary to produce MeV electrons. This will be followed by design and fabrication of a gas jet able to deliver the requisite profile.

Accomplishments

Improved simulations since last year's effort accurately capture the ionization and pulse propagation physics. The simulations have identified that the laser pulse intensity plays an integral roll in the injection of electrons. The laser properties found to be necessary for therapeutic electrons at energies of 1-10 MeV are 10 mJ of 800 nm at a pulse compressed down to ~10 fs. In order to achieve this, state of the art, hollow-core, photonic crystal fiber optics have been obtained through a collaboration instigated through the current effort with the University of Limoges. These fibers allow for further pulse compression and have demonstrated transport of 2.6 mJ of 800 nm laser with a theoretical limit much higher than the requisite 10 mJ. An experimental setup to test these limits has recently been established at LBNL.

Gas jet development has rapidly advanced through several iterations in the past year. The jet design from the previous year has been replaced with a new "shock-injector". This new concept greatly simplifies the fabrication while still delivering the sharp density gradient needed for injection. The length of the density transition has been verified through Direct Simulation Monte Carlo (DSMC) done at LBNL. Additionally, the jet length scales are sub-mm which is required for the final medical device. They have been incorporated into the 10 TW laser system and achieved the targeted 1-10 MeV electrons albeit at 200 mJ of laser energy at 45 fs. The ultimate goal of 10 mJ will only be possible with further pulse compression through the hollow-core fiber system. The jets successfully run with continuous flow making >1kHz operation possible and will ultimately reduce treatment times when incorporated into a therapy device.

Probing Point Defect Dynamics in Solids with Short Ion Beam Pulses

Principal investigator: T. Schenkel, Accelerator Technology & Applied Physics Division
Co-PI: Andrew Minor, Materials Science Division and UC Berkeley

Project Description:

Many properties of solids depend on the presence of defects. Defects can be engineered to tune desired properties, or defects can lead to materials failure. The understanding of defects dynamics in solids has to date been limited largely to "static" studies, where defects are first formed and the resulting changes in materials properties are probed much later. Simulations aim at capturing defect dynamics, but they are severely hampered by the lack of direct experimental validation. We have a unique short pulse (nanoseconds), intense ion beam capability available at LBNL and in this third and final year of this LDRD we used it to gain access to the dynamics of radiation induced defects in solids on a ~1 to 100 ns time scale. Advances in our fundamental understanding of defect dynamics will enable advanced materials development, e. g. for radiation tolerant high performance structural components in reactors and for materials with tailored defect properties e. g. for applications in energy conversion.

Accomplishments:

In the third year of this LDRD we have routinely used pulses of lithium and helium ions (~1 MeV) with tunable pulse lengths of (2-600 ns), and with up to 10^{11} ions/pulse/mm^2 to implant samples. We have increased lateral focusing of the ions 100 fold to 1 mm^2 beam spots and also compressed the pulse duration though neutralized drift compression from ~20 ns to ~2 ns. The resulting peak current densities are now about 1 A/mm^2 and the energy fluence is equivalent to ~1 J/cm^2. We have added the capability to created helium ions. It is of broad fundamental interest and of great technological importance to understand radiation damage form helium ions, as it pertains directly to natural processes such as alpha decay and to materials in high radiation environments, such as structural materials in reactors and also detectors, etc.

At these high ion dose rates, we can now see effects of the dynamics of radiation induced defects in situ. We show an example with optical diagnostics in Figure 1, where we plot the time evolution of light emission from a scintillator (YAP) following a single pulse (2 ns long) of lithium ions using streaked optical spectrometry.

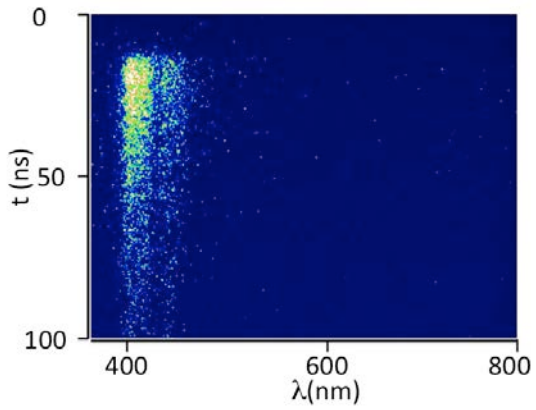


Fig. 1: Streaked optical spectrometry of light emission form a YAP scintillator (as a model sample) following a single pulse of lithium ions (2 ns pulse, 10^{11} ions/mm^2). Detection of the intensity and wavelength of emitted light is one sensitive way to track the sample lattice evolution during intense ion pulses. With data like these we can elucidate for the first time the formation and recombination dynamics of lattice defects on a ps to μs time scale.

High-Accuracy Scalable Solvers for Modeling of Future Ultrafast Photon Sources

Principal Investigator(s): Jean-Luc Vay, Leroy Drummond, Brendan Godfrey, Alice Koniges, Rémi Lehe

Project Description

This proposal is laying the groundwork for the development of computer codes that will be ultimately capable of virtual prototyping and virtual computer experiments on the next generation of supercomputers. The advanced design of future particle accelerators requires consideration of a variety of physical processes that are not appropriately modeled with current techniques and computational power. We are pursuing the development of a new, highly accurate and scalable solver combining the accuracy of spectral methods with the scalability of finite-difference methods.

We propose a crucial change to the scalable algorithm, namely changing the solver portion from FDTD to PSATD solver, to mitigate significant unphysical effects from discretization errors. Traditionally, such a move would compromise the scalability of the PIC method and render the calculation intractable for the required accuracy and spatial resolution. Key to our approach is the design and high-performance implementation of a new solver to take advantage of multilevel parallelism in emerging systems by naturally subdividing the computational domain and workload in a way that is optimally assigned to the heterogeneous computational resources. Our algorithmic research will provide high numerical accuracy and stability.

Accomplishments

Our most significant accomplishment in this time period has been the development of a spectral, quasi-cylindrical and dispersion-free Particle-In-Cell algorithm [1]. The new algorithm is based on the combination of Hankel transforms in the transverse direction and Fourier transforms in the longitudinal direction. For physical problems that have close-to-cylindrical symmetry, this algorithm can be much faster than full 3D PIC algorithms. In addition, unlike standard finite-difference PIC codes, the proposed algorithm is free of a number of numerical artifacts, including for instance spurious numerical dispersion. Importantly, this spectral algorithm is now already used in production, to simulate the experiments that are carried out in the ATAP division. In some of these simulations, standard finite-difference PIC code introduce artificial effects, that may look physical to the untrained eye (e.g. artificial direct laser acceleration), while our spectral code is entirely free of these artificial effects and can accurately model the experiments. Finally, this algorithm has been implemented for multi-CPU as well as multi-GPU architectures, and scaling tests will be performed in the near future.

Another significant achievement was the development of an improved method for the suppression of the numerical Cherenkov instability in the Generalized Pseudo-Spectral Time-Domain algorithm that we had introduce during the preceding year [2]. The new method offers an approach that completely eliminates the fundamental mode of the numerical Cherenkov instability while minimizing the transverse field corrections. Comparisons with simulations using the code Warp were conducted. In some instances, there are no numerical instabilities whatsoever when using the new method, at least in the linear regime.

We also extended the theoretical and numerical analysis of the coefficient of reflection of Perfectly Matched Layers to solvers of any order of accuracy. Results show that the PML efficiency is preserved at any order, including at the infinite order limit that is attained by the pseudo-spectral formulation [3].

A New Concept for High Average Power Ultrafast Lasers

Principal Investigator: Russell Wilcox

Project Description

A method for extracting high pulse energies from a laser is proposed using solitary or cascaded Gires-Tournois type resonator cavities. Such cavities will allow coherent time-domain stacking of multiple optical pulses to reach high energies. This would allow a significant (by orders of magnitude) reduction of pulse peak powers in an optical amplifier, and significantly increase extractable pulse energies well beyond what is currently achievable by using only a standard chirped pulse amplification (CPA) technique. When used with coherently combined laser arrays, this approach could enable a new generation of laser driven accelerators operating at 10^3 - 10^4 times higher repetition rates than is possible with the existing laser technology. If successfully applied to the case of fiber lasers, the combination of high average power and high wall plug efficiency would be feasible.

Our experiment will use a mode-locked Nd:YAG oscillator producing short pulses (as short as 10 ps) at 400 MHz repetition rate with pulse energy of ~250pJ. This oscillator will be followed by amplitude and phase modulators to produce pulse burst with phase and amplitude characteristics required for achieving pulse stacking, and a low power fiber amplifier. This will be followed by several GTI stages, multiplexed in series, and arranged in two different cascades. The first cascade will consist of 4 GTI resonators each with the cavity length corresponding to 2.5ns round-trip time. This cascade should achieve pulse stacking/energy enhancement factors of up to x9 times. The second cascade will consist of 2 GTI stages each with 22.5ns round-trip time. The resulting enhancement from the two cascades should reach up to x36 times.

Accomplishments

We have built the pulse burst source using a YAG laser and electro-optic modulators. To increase optical signal levels, we designed a polarization-maintaining fiber amplifier which was custom built and installed after the modulators. The amplified pulse burst is delivered to four, concatenated GTI cavities using a simple triangular design. We have also built two longer cavities using a compact, multi-pass optical design. The modulators are driven by an FPGA-based, digital control system which reads pulse amplitudes from sensors in the GTI array. Using this system, we automatically stabilize the amplitude modulator bias point. The amplitude and phase modulators and their electronics have also been characterized, allowing us to compensate amplitude and time-dependent distortions of the pulse burst.

To analyze the optical system, we have developed a frequency domain, Z-transform model of the GTI cavity array, which runs faster compared to time domain models. Using this code, we have showed that analysis of the pulse patterns from each cavity can be used to tune the cavity phases in a deterministic way. Single-cavity experiments with special probe pulse bursts show that output pulse trains indicate cavity phase. Control of this phase is by piezoelectric actuators. We have measured the frequency-resolved temporal response of several actuated mirrors using an interferometer, allowing us to optimize control bandwidth. Analysis of the longer, multi-pass cavity has resulted in a new theoretical framework, using optical Fourier transforms, which reveals more information more elegantly than previous methods. We have used this to design highly stable, compact cavities now used by us and our collaborators.

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 of 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 first six months of this LDRD project, we have characterized and developed our special adaptation of a crystal monochromator and order suppressor, which allows access to the extreme Bragg angles needed to access the tender energies. A Helium environment sample chamber was designed and manufactured for SAXS/GISAXS. A new Pilatus 1M has been commissioned for data acquisition.

We have collected promising data for Li-S thin films showing tender resonance. From the collected data, it is obvious that tender S K-edge X-ray scattering can distinguish signals from polysulfides contained in block-copolymer electrolytes. A Li-S pouch battery cell was prepared for new experiments investigating polysulfide formation during the next ALS cycle. Our attention has shifted towards new collaborations with groups at UC Berkeley, Michigan University, and Penn State University. This will open new opportunity to build up a new pouch battery and to investigate a highly demand biological systems as well. Also, we are pursuing collaborations with resonant scattering groups at BESSY-II (Berlin) and PF (Japan) to promote the use of this new scattering technique, TReXS.

Ultra-high resolution microscopy of nano-materials by scanning x-ray diffraction microscopy
Principal investigator: David Shapiro

Project Description

Scanning x-ray diffraction microscopy (x-ray ptychography) is a robust diffraction imaging method that can take full advantage of the high brightness of the ALS and future ultra-high brightness synchrotron light sources. The purpose of this project is to apply the method to difficult problems in the materials sciences. Soft x-ray ptychography achieves a spatial resolution that is superior to conventional microscopies and has unprecedented sensitivity to chemical, magnetic and morphological states of matter. Therefore, we have applied the technique to material science problems which require high spatial resolution and chemical or magnetic sensitivity. The ALS has developed the instrumentation for ptychographic imaging as part of an aggressive research and development program in preparation for the very high brightness of the ALS-U storage ring upgrade. This project used such instruments on a dedicated diffraction imaging beamline with an energy range and resolution suitable for studying a wide range of materials. In particular, we aimed to study correlations between the chemical phase transformation in LiFePO4 nanoparticles and morphological defects, the nano-porous structure in cement and sintered yttria stabilized zirconia and the domain wall structure in magnetic thin films.

Accomplishments

This project has made possible several landmark achievements in the field of x-ray microscopy. First, we demonstrated chemical composition mapping at a spatial resolution unachievable with conventional imaging systems using complex valued reference spectra which are only available via x-ray ptychography. We showed that such spectra provide enhanced chemical specificity which made it possible to elucidate chemical composition within structural cracks in nano-particles of a LiFePO4 battery electrode. Such cracks are partly responsible for the deterioration of battery performance and we made the first measurements of chemical composition within their interior which verified that the cracks are only on the surface of the cathode particles. Furthering this line of research, we made the first measurements of complex valued reference spectra, of pure materials, using x-ray ptychography and showed that they could be used to precisely quantify chemical composition in heterogenous materials. Our new method of complex spectral analysis provides chemical maps with higher fidelity than maps calculated from only the x-ray absorption spectra. Finally, we have taken these types of measurements into extra dimensions with chemical state tomography. By recording tomograms at multiple x-ray energies, chemical composition can be assessed in three dimensions (3D). We have achieved the highest resolution x-ray tomography ever, 11 nm resolution in 3D, and used that capability to quantify the state of charge in a many particle agglomerate from a partially delithiated LiFePO4 cathode. Our data allows for the visualization of interior chemical states as well as statistical analysis across many individual particles. The tomograms clearly show a lack of correlation between chemical phase boundaries and crystallographic axes which is counter to the theoretical prediction for particles of this size. We have also used ptychographic tomography to quantify the pore structure in sintered zirconia at 20 nm spatial resolution and have investigated correlations between impurities and domain wall pinning sites in a thin film of SmCO5.

Novel Accelerator Techniques for Diffraction Limited Light Sources
Principal Investigator: Christoph Steier

Project Description

Recent developments in accelerator technology and lattice design open the door for very large increases in brightness – more than 100 times, particularly by reducing the horizontal emittance. This can greatly enhance the capability of light sources for imaging and spectroscopy. The fundamental driver in a soft x-ray diffraction limited light source is that the highest possible brightness requires large field gradients, and this requires crucially important R&D to eliminate risk in multiple areas. The goal of this project was to investigate, demonstrate and improve critical technologies necessary for diffraction limited storage ring light sources and carry out tests with some of those new systems using beams in existing light sources.

Accomplishments

Our high level goals were to document a detailed, optimized design of a soft x-ray diffraction limited storage ring, well matched to the science case and user needs, to evaluate strategies for installation and commissioning, including staging, as well as to demonstrate necessary key technologies at the component and/or subsystem level. Excellent progress was made in all of these areas. Specific achievements include:

1. Built and started testing of a full prototype pulser suitable for swap-out injection.
2. Non Evaporative Getter (NEG) coated 6 mm diameter vacuum chamber, a world record.
3. Demonstrated required bunch lengthening factors >4 with realistic fill patterns.
4. Finished pre-conceptual magnet designs with fully three dimensional pole shapes.
5. Developed lattices with improved momentum aperture and photon phase space matching.
6. Started analysis of coherence preserving photon optics including advanced cooling.

Some successful results of the accelerator technology R+D are shown in Figure 1. They included coating of extremely small diameter vacuum chambers, construction and tests of a pulser for the fast injection magnets, and bunch lengthening studies at very large lengthening factors.

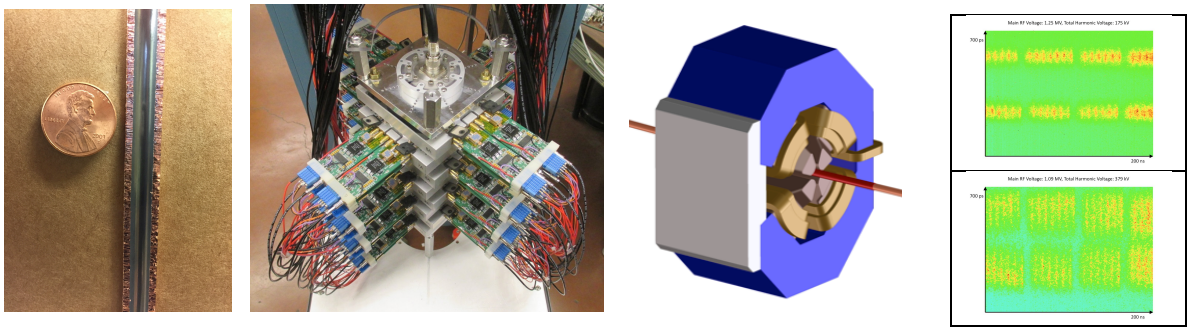


Figure 1: Examples of successful results: Record small NEG coated chamber; fully assembled inductive adder; optimized 3d magnet designs; demonstration of required bunch lengthening factors with realistic fill patterns.

High Efficiency Soft x-ray *In-situ* Spectroscopy (*HESIS*) for ALS-II Energy Sciences

Principal Investigator(s): Wanli Yang, Jinghua Guo, Yi-de Chuang, Zahid Hussain, Tom Devereaux

Project Description

The purpose of this project is to commission a unique in-situ soft x-ray absorption (XAS), emission (XES) and resonant inelastic x-ray scattering (RIXS) system with much improved resolution and efficiency at Beamline 8.0.1 of the Advanced Light Source (ALS). The new system will enable unprecedented experiments in the broad field of energy science for both fundamental understanding and practical applications. Moreover, this project will bring together experimentalists and theoreticians to develop new scientific cases of energy material studies with the new experiment setup. It will also increase both the capacity and capability for handling user proposals at the ALS, and reclaim the uniqueness of the techniques based on soft x-ray spectroscopy (SXS) in US.

We will develop this high efficiency soft x-ray in-situ spectroscopy (HESIS) system that will replace the current soft x-ray fluorescence (SXF) endstation at Beamline 8.0 that has been in use for twenty years. The HESIS system will feature the sample manipulator that can accommodate in-situ cells with the variable temperature control of 25K-800K and the high efficiency spectrograph based on planar variable line spacing (VLS) gratings that covers the photon energy range 80-2600eV. The detection efficiency will be 10^2 times higher than present. The new system will be installed during the ALS shutdown period, November 2015 – January 2016. After the photon beam is brought back, we will work on specific in-situ cells and materials for both commissioning and scientific demonstrations.

Accomplishments

Our most significant accomplishment has been to build the four critical subsystems of the HESIS system, which includes a new home-designed bendable soft x-ray mirror, the main sample characterization chamber equipped with various detectors, and two slitless VLS spectrographs focusing on high efficiency and moderate resolution. We are in the process of installing the whole new system at the beamline. We will start commissioning the new system when the photon beam is resumed in Juanuary 2016.

We have also succeeded in exploring more scientific cases, and provided more demonstrations to the field of energy materials by using soft x-ray spectroscopy. Our studies provide the first experimental probe of atypical Nickel valences in battery compounds, and cover a wide range of functional components in electrochemical energy storage systems. These scientific studies will be further enhanced and explored following the HESIS commissioning.

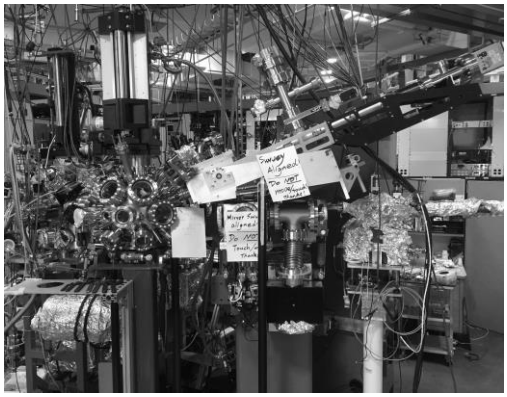


Figure: Commissioning status of HESIS system as of December 15, 2015.

Project Title: PROBING DYNAMICS WITH MULT-COLOR, MULTI-PULSE LASER AND SYNCHROTRON PHOTONS

Principal Investigators: Musa Ahmed, Dan Slaughter

Project Description

The aims of the project are to develop multi-color laser and synchrotron spectroscopic techniques to achieve unprecedented combinations of femtosecond time resolution with electronic-state and site-specific molecular interrogation of gas phase systems. These are potentially offered by bringing femtosecond laser electronic excitation schemes and high energy-resolution synchrotron VUV and soft x-ray spectroscopic probes together, while exploiting the unique capabilities of the Advanced Light Source.

Accomplishments

A portable tabletop transient absorption experimental apparatus, developed in the first year of the project, was used to perform analysis of ultraviolet laser excitation schemes in a variety of gaseous systems at the Advanced Light Source, where we measured absorption cross sections in a series of model chromophores.

A new in-vacuum soft x-ray transient absorption gas cell was developed in this phase of the project, designed to exploit the soft x-ray characteristics of Beamline 6.0.2 and the typical laser excitation requirements. The cell consisted of two aluminium foils, opaque to soft x-rays, aligned mutually parallel with adjustable separation from 0.5 – 1.5 mm. A 30 μm aperture was micro-machined through each foil using a laser mill to allow a fraction (typically 10%) of the x-ray focal volume (70 μm x 370μm) to propagate through the cell to a fast avalanche photodiode x-ray detector. This geometry restricted the x-ray focus to be well-overlapped with the laser focal volume, which was 20 μm (full width at half maximum) x 6.5 mm Raleigh length. Spatial and temporal alignment were performed with an alignment tool, consisting of a fast avalanche photodiode detector (sensitive to both UV and soft x-rays) and a 30 μm pinhole mask. Time-gating of the detector acquisition system allowed specific soft x-ray bunches to be selected at the laser repetition rate of 2 kHz.

Soft x-rays near the carbon, nitrogen or oxygen K-edges were transmitted through the cell and soft x-ray absorption (NEXAFS) spectra were measured. The laser was configured in a split and delay setup such that one ultrafast (150 fs) laser pulse at wavelength of 263nm excited o-nitrophenol while a second identical pulse, at a tunable delay, shifted the excited state population. NEXAFS datasets were recorded for the model chromophores o-nitrophenol, acetonitrile, t-butylnitrite, nitroethane and acetaldehyde. NEXAFS spectra were then recorded with 2-color experiments with 15μJ and 30 μJ UV laser pulses. The analysis of these datasets is ongoing. The experimental tools developed and the preliminary data collected at the ALS during this LDRD project have enabled new photochemistry experiments in the Chemical Sciences Division.

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 are conducting 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. In this work, we have sought 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. Artificial metalloenzymes containing noble metals in place of native metals in cofactors of natural metalloproteins have the potential to catalyze abiological reactions within an unperturbed substrate-binding site. Such enzymes could work in tandem with natural enzymes or chemical catalysts in multistep processes that would mimic natural biosynthetic pathways. However, this class of artificial metalloenzyme has been elusive. We discovered and have a paper provisionally accepted to *Nature* on the formal replacement of iron in the porphyrin IX (PIX) of heme proteins with a series of abiological, noble metals. In this work we demonstrate that the resulting enzymes catalyze reactions that are not catalyzed by native Fe-enzymes. In particular, we prepared variants of myoglobin containing an Ir(Me) site, and the resulting enzymes are the first known to functionalize C-H bonds by carbene insertion and to add carbenes to both b-substituted vinylarenes and unactivated aliphatic α-olefins. Directed evolution of the Ir(Me)-myoglobin generates mutants that form either enantiomer of the products of C-H insertion and that catalyze the enantio- and diastereoselective cyclopropanantion of unactivated olefins. These discoveries were enabled by developing an efficient method to prepare PIX-proteins containing abiological metal-porphyrins. This strategy sets the stage to generate artificial enzymes from innumerable combinations of PIX-protein scaffolds and unnatural metal cofactors that catalyze a wide range of abiological transformations.

2) Hydroaminomethylation. In a second aspect of this program, we developed a dual catalyst system to convert *alpha*-olefins to tertiary 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 earlier progress reports, we disclosed a system in which the reductive amination occurs in the aqueous phase of the reaction medium and is catalyzed by the combination of $Cp^*Ir(H_2O)_3$ and a water-soluble diphosphine ligand. However, it proved difficult to run these reactions on preparative scale in a two-phase reaction system, presumably due to inefficient mixing of the organic and aqueous phases. Thus, we sought a suitable transfer hydrogenation catalyst that is soluble in the organic phase and identified Xiao's catalyst as suitable for this application. This catalyst is not inhibited by the CO atmosphere and selectively reduces iminium substrates in the presence of aldehydes. The amine product is cleanly produced in high yield and very high (>50:1) linear/branched selectivity. Thus, we have developed a preparatively useful system involving two catalysts, and two sequential steps in a single system that gives high yields of product, in part, by eliminating the accumulation of an unstable aldehyde intermediate.

New Algorithms for Performing and Analyzing Large Scale Electronic Structure Calculations

Principal Investigator(s): Head-Gordon, Martin

Project Description

There are two synergistic purposes to this project. The first objective is to improve our ability to understand the physical factors that are responsible for intermolecular interactions. Electronic structure calculations are nowadays capable of calculating intermolecular interactions nearly as accurately as they can be measured. However such calculations by themselves do not provide any understanding of why the interactions have the magnitudes that they do. Methods for this purpose are called energy decomposition analyses (EDA). It is an important open challenge to design improved EDA's, a problem that is best attacked by deepening our understanding of the factors controlling intermolecular interactions.

The second objective of the project is to develop new, more efficient numerical methods for solving the equations of electronic structure theory for molecular clusters (i.e. the same systems for which we are seeking new EDA's). There should be natural connections between new EDA tools, and the problem of computing those interactions more efficiently than has been hitherto possible. We believe the combination of improved EDA's for analysis together with lower-scaling (i.e. more computationally efficient) algorithms for calculating the interactions will be a potentially significant step forwards in quantum chemistry.

Accomplishments

Our major activity has been exploring new ways of using the natural separation of energy scales between intra-molecular and intermolecular interactions to improve the efficiency of electronic structure theory calculations. Specifically, we have explored whether coupled cluster calculations (CCC) can be approximated starting from a CCC performed on only the intra-molecular excitations (linear model) or intra-molecular + dispersive intermolecular excitations (quadratic model). The remaining (quartic) contributions are then evaluated approximately by perturbation theory (PT). Can this approach can improve the often-questionable accuracy of PT, without the prohibitive computational cost of a full CCC on a molecular cluster. Our results indicate that PT based on the linear model does not significantly improve upon direct use of PT, while the quadratic model does yield significant gains in accuracy.

Building on these results, we then began to investigate methods that might permit very large clusters and potentially molecular liquids to be treated using similar ideas. The key issue is that large atomic orbital basis sets are required for high accuracy, but involve very high computational cost. We can potentially greatly reduce the cost of such calculations by making the basis set adaptive to the molecular and intermolecular environment. We have shown that one can employ a remarkably small adaptive basis that is no larger than twice the number of electrons. Half of these functions are monomer-localized, coming either from the molecular orbitals of isolated monomers. The other half of the functions describe remaining charge-transfer effects and are derived from a singular value decomposition of the perturbation amplitudes at the end of the zero-order calculation. For molecular clusters and potentially liquids as well, this is a very promising low-cost alternative to conventional calculations in large basis sets, which achieves the same accuracy. Efficient implementation remains a challenge for future work, with the results we have obtained offering strong proof of principle.

Designing Fluctuations and Dynamics of Enzyme Catalytic Networks

Principal Investigator: Teresa Head-Gordon

Project Description

The purpose of this project is to develop a powerful theoretical framework capable of discovering general design rules based on nanoscale properties of molecule shape and size, charge distributions, ionic strength, and concentration to influence the mechanism, percolation, morphology, and rates of assembly over mesoscale time and lengthscales. The ability to control for structure and dynamics of the assembly process is a fundamental problem that, if solved, will broadly impact basic energy science efforts in nanoscale patterning over mesoscale assemblies of block copolymer materials, polyelectrolyte organization at solid or liquid interfaces, forces governing multiphasic soft colloids, and growth of quantum dots in polydisperse colloidal medium. Fundamental design rules applied to complex and heterogeneous materials are important to DOE mission science that will enable next generation fuel cells, photovoltaics, and light emitting device technologies.

At present our ability to design and control complex catalytic activity by coupling simpler modular systems into a network that executes novel reactive outcomes is an unsolved problem. And yet, highly complex catalytic processes in nature are organized as networks of proteins or nucleic acids that optimize spatial proximity, feedback loops, and dynamical congruence of reaction events to optimize and fine tune targeted biochemical functions. The primary intellectual activity of biomimetic scaffolding – the design of spatial organizations of modular biocatalysts – is to restore their catalytic power in these new chemical organizations after they have lost their catalytic functions optimized in a separate biological context. That is our goal.

Accomplishments

Over 2015/2016 we have the following accomplishments

- PB-AM (analytical model) has been released in the APBS code (collaboration with Nathan Baker at PNNL in 2015)
- Nucleated new direction in simulated THz spectroscopy for water and enzyme catalysis (with Dominik Marx, Bochum-Ruhr in 2015)
- New effort (1 postdoc, Luis Ruiz) to exploit altered bulk properties of metastable water under confinement between mesoscale surfaces to control chemical reactivity. [1]
- Applied for ALCC grant with Tom Markland (Stanford) to characterize new meta-GGA functionals with nuclear quantum effects for water
- New analysis tools for back-calculating radial distribution functions from experiment [2]
- Working with Laura Lammers on understanding ion interactions with clays
- Enzyme catalysis work has resulted in predictive methods that are capable of replacing laboratory directed evolution [3,4,5]
- SAXS and theory on star polymers (with IBM Almaden) [6,7]

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 second year of this LDRD we have extended the multi-generational mechanism for OH oxidation of nanoscale aerosols developed in the first year to include fully coupled reaction-diffusion. By incorporating the chemical mechanism into a model that includes diffusion, the interplay between viscosity and reactivity can be characterized. We have examined two cases involving similar chemistry but different physical states by comparing the oxidation of aerosols composed of two alkane isomers, squalane (liquid) and triacontane (semisolid). While the liquid aerosol transforms uniformly, the semisolid aerosol forms a core (unreacted)-shell (oxidized) geometry despite very high driving forces for diffusional mixing. This finding provides an explanation for recent optical studies that indicate aged particles have a core-shell structure, in contrast to the general assumption that even viscous particles are well-mixed in the atmosphere. Through this work, important gaps have been revealed in the scientific understanding of key processes in atmospheric aerosol chemistry, in particular how heterogeneous oxidation influences the volatility of the aerosol components and thus how the aerosol size varies with time. A new complementary model is being developed for citric acid in order to investigate oxidative processes in a single chemical system exposed to water vapor, where humidity affects viscosity over a wide dynamic range. These accomplishments have required the addition of significant capabilities to the computational code and the development of a rheometry technique to determine diffusion coefficients in organic materials with varying degrees of humidification. Papers describing these accomplishments are in preparation.

High Performance Geometric Multigrid: A New Computer Architecture Benchmark
Principal Investigator(s): Mark, Adams

Project Description

The purpose of this project is to develop a benchmark to measure, and rank, supercomputers and provide compact application relevant code for computer architects to use to drive their design process. This code, HPGMG (hpgmg.org), is compact and stand alone and is intended to be a potential replacement for HPL as the Top500 metric. It is also a vehicle for understanding the computer performance by providing a small code that encapsulates many of the challenging aspects, though certainly not all, of hardware that inhibit application performance on high performance computer platforms and emerging architectures. It is thus intended to be more relevant than a micro-benchmark like STRAMS and more tractable than a full proxy application that might be used, for instance, in procurement. This project funded the development of this code its dissemination to the community.

We will develop the HPGMG benchmark code, disseminate it with a public *git* repository on bitbucket.org, support its use, public releases, instructions for ranking submissions on a email forum and a web page: hpgmg.org.

Accomplishments

We developed a new 4th order accurate version of the finite volume version of the benchmark – HPGMG-FV. This version stresses the machine more evenly, relative to our experience with application sensitivities. We succeeded in convincing Intel and Nvidia to create optimized versions of HPGMG-FV for their respective emerging architectures. We also funded a collaborator from the Stuttgart computing center's modeling group to visit LBNL for a month and analyze HPGMG-FV and compare it with two other benchmarks of its class: HPCG and HPL. The figure shows the current ranking of the 4th order version. The releases of the code, managing the list and optimizing it for Titan were funded by this project. This project also sponsored our Birds-of-a-feather meeting at SC14 and SC15.

System			HPGMG DOF/s			Parallelization			DOF per	Top500
Rank	Name	Site	h	2h	4h	MPI	OMP	ACC	Process	Rank
1	Mira	ALCF	5.00e11	3.13e11	1.07e11	49152	64		36M	5
			3.95e11	2.86e11	1.07e11	49152	64		36M	
2	Edison	NERSC	2.96e11	2.46e11	1.27e11	10648	12		128M	34
3	Titan (CPU-only)	OLCF	1.61e11	8.25e10	2.37e10	36864	8		48M	2
4	Hopper	NERSC	7.26e10	5.45e10	2.74e10	21952	6		16M	62
5	SuperMUC (22%)	LRZ	7.25e10	5.25e10	2.80e10	4096	8		54M	20
6	Hazel Hen (7%)	HLRS	1.82e10	8.73e09	2.02e09	1024	12		16M	-
7	SX-ACE (vector)	HLRS	3.24e09	1.77e09	7.51e08	256	1		32M	-
8	Babbage (MIC-only)	NERSC	7.62e08	3.16e08	9.93e07	256	45		8M	-

Specific activities supported by this LDRD (not by leveraged programs like co-design):

- We developed a scalable, high-performance, low latency, distributed memory V-cycle.
- We created a high-performance, performance-portable implementation for MPI, MPI+OMP2, and MPI+OMP3 based computing systems.
- We developed a 4th order accurate implementation ... (co-deign was moving this direction, but only for the residuals, not the smoothers, interpolation, or FMG)
- We ported NVIDIA's 2nd order HPGMG implementation to Titan, resolved all kernel panics, crashes, garbage data creeping into UVM, correctness issues, and run on the full 18K GPUs.

Surrogate Model Algorithms for Computationally Expensive Black-box Optimization Problems
Principal Investigators: John Bell, Juliane Mueller

Project description

With increasing computational power, simulation models are becoming increasingly complex and computation time demanding. Hence, scientists in many application areas such as global climate modeling, transportation network design, and environmental engineering are facing computationally expensive optimization problems that arise when tuning parameters with the objective of minimizing the error between simulation model outputs and observations. Our goal is to develop efficient optimization algorithms for these types of computationally expensive black-box problems. In order to alleviate the computational cost, we use surrogate models to approximate the computationally expensive objective functions. Throughout the optimization algorithm, we use the objective function value predictions from the surrogate model to guide the search for promising parameter values at which we evaluate the expensive objective.

So far, surrogate model algorithms have mainly been developed for problems with continuous variables and box-constraints. Optimization problems are often reformulated and simplified in order to apply an off-the-shelf surrogate model algorithm. Optimization application problems have, however, a large variety of characteristics and we need algorithms that can directly address them in order to obtain meaningful results. Our goal is to develop new surrogate model algorithms that are able to address problems with integer, mixed-integer, and binary variables, problems with computationally expensive objective functions and/or constraints, problems for which the evaluation of the expensive simulation model may crash and hence no function values can be obtained, and problems with multiple conflicting objectives.

Accomplishments

We finished a project that was started at Cornell University in which we tuned the parameters of the methane module in CLM4.5bgc in order to decrease the error between the simulation model predictions and actual observations.

We developed an algorithm for optimization problems with binary variables, a computationally expensive objective function, and a computationally cheap constraint. This work was motivated by a transportation network design problem. We showed that our algorithm finds the global optimum within significantly fewer function evaluations than other algorithms commonly used in the transportation literature.

We also developed a surrogate model algorithm framework for mixed-integer problems. We are in the process of publishing a MATLAB toolbox that allows the user to choose between different types of surrogate models, initial experimental designs, and sampling strategies. We used the algorithm to solve application problems arising in structural optimization and reliability-redundancy optimization.

Lastly, we devised an algorithm for optimization problems whose objective function is computationally cheap and that have computationally expensive black-box constraints. These problems are often encountered in environmental engineering. We used the algorithm to solve a groundwater cleanup problem and a watershed management problem.

Graph-based analysis and visualization of multimodal multi-resolution large-scale neuroimaging data

Principal Investigator: Aydın Buluç

Project Description

We aim to massively accelerate multimodal data analysis to enable real time data explorations in order to speed the discovery and hypothesis generation process in neurosciences. We plan to precisely quantify changes in network structure, especially those that lead to neurodegenerative diseases. Our collaborative research project promises to significantly improve the fidelity and scope of neuroimaging analysis using high-performance computing methodologies via state-of-the-art graph analysis, image processing, and visualization techniques. The research developed for these techniques will be applicable to a variety of evolving big data domains of interest to the DOE. Overall, our work will address the 3V (variety, volume and velocity) components for big data neuroscience problems. Performance improvements in the segmentation of structural MRI and high speed computation of adjacency matrices will allow the end user to process more data (volume) in a shorter time, with expectations to view and analyze data in real time to speed the discovery and hypothesis generation process (velocity). By enabling researchers to integrate and interrogate data from multiple data modalities at the same time, we address the issue of variety. Additionally the volume problem is also addressed via the significant acceleration of comparative data analysis from multiple measurements for the same or multiple patients.

Accomplishments

We developed a data driven method for functional parcellations of brain regions as well as an adaptive hierarchical community detection method to fine tune parcels. This is a very challenging problem with more than 100K dimensions and relatively smaller sample size. The data is also very noisy due to fMRI measuring indirect blood oxygen levels as opposed to direct neural activity. Consequently, using global correlations is known to give unsatisfactory results because many nearby “voxels” have very similar time series data.

CONCORD is the first method with provable global convergence properties (when the dimensionality is larger than the number of samples) that performs sparse inverse covariance estimation. The accelerated version of this algorithm, CONCORD-ISTA, uses block sparse linear algebra instead of coordinate-wise updates. What is needed is the partial correlation between voxels, i.e. the correlation of pairs of voxels after removing for the effects of all other voxels. We apply CONCORD-ISTA to our problem as it provides the best theoretical guarantees for estimating partial correlations between voxels. The bottleneck in the efficient execution of CONCORD-ISTA in parallel is the multiplication of a sparse matrix (the structure we are trying to estimate) and a dense matrix. We developed a communication-avoiding parallel algorithm to provide a scalable solution for the sparse matrix - dense matrix product.

We also developed a method for interactive visual exploration of functional magnetic resonance imaging (fMRI) data to analyze the correlation between activities in different human brain regions when resting or when performing mental tasks. Our visualization tool improves visual data exploration by generating multiple coordinated views, supporting the brushing-and-linking concept, and integrating community detection. Our tool provides neuroscientists with a powerful means to comprehend such complex data more effectively and efficiently.

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

To date we have tested and implemented different unconstrained functional forms in the PARATEC materials science code and carried out performance comparisons (convergence, parallel scaling) for different benchmark systems between the different functional forms. We determined that the simpler functional form based on a first order expansion of the overlap matrix has the best overall performance in terms of cost and parallel scaling. We then performed large simulations on large core counts (10,000s of CPUs) to compare the unconstrained method to the conventional constrained conjugate gradient methods to determine the parallel scaling regime where they outperform the standard methods. The unconstrained method was also implemented in the widely used publicly available materials/chemistry code CP2K so that we would also have an evaluation of the code for materials/chemistry codes that use a Gaussian basis as well as the plane wave basis method used in PARATEC. Plane wave basis and Gaussian basis account for most of the first-principle simulations performed in materials and chemistry codes. We found for the CP2K code that in the regime of about 2,000 atoms and larger running on greater than ~5000 cores the unconstrained method outperforms the existing method and also exhibits much better parallel scaling to even higher core counts. In the case of the PARATEC code we found that for more than 1000 atoms on more than ~2000 cores the unconstrained algorithm can outperform the standard algorithms particularly for systems with a small band gap.

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

ADVANCED COMPUTATIONAL CHEMISTRY AND SEMANTIC DATA TOOLS FOR MESOSCALE SCIENCE

Principal Investigator(s): Wibe Albert de Jong

Project Description

Mesoscale is DOE's next frontier in their effort to develop to control chemical and physical processes that lead to new or more efficient renewable energy resources and approaches to reduce the carbon footprint. Modeling the emergent mesoscale phenomena utilizing computational chemistry methodologies requires the exploration of essential collective variables and order parameters in systems of sufficient size and disorder and with sufficient statistical sampling using accurate and scalable computational chemistry methods. We will improve the performance of key *ab initio* methodologies utilizing tools developed by the SciDAC Institutes, and by developing new and advanced algorithms for two-electron integrals and planewave FFT for the Intel Xeon Phi. We will develop computational chemistry tools that integrate a Kinetic Monte-Carlo methodology with scalable high accuracy *ab initio* and Car-Parrinello methodologies available in NWChem.

To enable major scientific discoveries of mesoscale phenomena, computational models need to be integrated with a broad range of complex spectroscopic imaging experiments. To enable integration of mesoscale modeling efforts with complementary experimental work, we will develop the semantics and tools for needed to analyze and enable knowledge discovery in scientific data generated from mesoscale experiments and simulations.

Accomplishments

Additional work was performed to make the Global Arrays/GASNet Interface called GAGA more robust and production ready. This work was done in collaboration with members of the DEGAS project.

The compute intensive triples term of the coupled cluster algorithm was optimized to run efficiently on the Intel Xeon Phi using a hybrid MPI-OpenMP approach with a performance improvement of 65x over a single thread on the card. In addition to optimizing the most expensive six-fold loop we demonstrate significant performance improvements in the data sorting routines and others that become a secondary bottleneck in parallel performance. Key algorithms for the plane wave capability in NWChem were analyzed on the Intel Xeon Phi. In collaboration with PNNL OpenMP capability was introduced int the most extensive components, such as the Lagrangian. Significant performance improvements have been obtained, but work is ongoing through the Intel Parallel Computing Center funding that was obtained.

The NWChem software was modified to generate semantic output based on an extensive dictionary with terminology for computational chemical sciences that was developed as a standard for computational chemical data. NWChem can now write JSON or CML style semantic data. Going forward the JSON format will be the sematic data format of choice in the continued collaboration with Kitware. An early demonstration of linking computational and experimental data in a semantically rich framework was build and is hosted at NERSC. A SBIR Phase-II proposal expanding on this framework led by Kitware has been submitted.

Computational Approaches to Understanding Ultrafast Science

Principal Investigator(s): Alexander Kemper

Project Description

During the past few decades, great advances have been made in the field of experimental time domain spectroscopy. New experiments carried out at the Advanced Light Source, and the Linac Coherent Light Source (LCLS) have already been completed on some of these systems and more are likely to come in the near future as x-ray science moves into the ultrafast regime, particularly at LCLS and future world-wide x-ray free electron lasers due to come online in the next few years. We have already taken important steps both in developing the non-equilibrium algorithms and codes and in solving fundamental problems that now set the stage for our advanced studies. Based on these results, we are now making inroads into self-consistently described ordered states; including superconductivity and complex charge density waves that emerge out of systems with interacting degrees of freedom. We study how light affects the ordered state, what can be learned about the equilibrium ordered state from pump-probe spectroscopy, and in what ways the pumped system is fundamentally different. Finally, we are now considering the feedback of the electronic degrees of freedom on the lattice.

Accomplishments

Our most significant accomplishment has been extending the code to allow for matrix-valued Green's functions. This opens up many new fields of study in non-equilibrium physics; in particular, we can now self-consistently treat broken symmetry states. We can now melt ordered phases, and fully observe the melting and reformation. Our first efforts in this direction were focused on s-wave superconductivity, where we observed the presence of Higgs, or amplitude mode oscillations. The Higgs mode is a fundamental concept in broken symmetry states, yet has been elusive. In a superconductor, the Higgs mode does not couple directly to external fields, making it difficult to observe. By going to pump-probe experiments, one can perturb the superconductivity in such a way that the Higgs mode arises naturally. This is only possible in non-equilibrium, making it one of the first physical phenomena that are uniquely accessible by pump-probe experiments. We have gone on to address certain aspects of light-enhanced superconductivity, where ultrafast laser pulses are used to modify the electronic properties that produce superconductivity. Furthermore, we are extending our efforts to ordered states with d-wave symmetry – a key property relevant to the high-Tc cuprates.

Secondly, we have investigated the complex process of energy transfer between various subsystems after pumping. This process is extremely important to understand fully, as it dominates the experimental observations. We have succeeded in addressing the feedback loop between the electrons and the lattice, and are now beginning our scientific investigations.

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 enable 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 will 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 discrete formulation of the DtN map for quantum-classical interface fully at the numerical linear algebra level. We demonstrate that consistent boundary conditions can be formulated using full space Green's function instead of the exterior Green's functions, commonly used in Schur complement based construction. This is particularly attractive for 2D and 3D systems where the exterior problem requires the solution of a large vacancy problem that is as difficult as the original problem. We are currently in progress implementing this methodology in the DFTB+ package, a community software package for *ab initio* calculations based on density functional tight binding theory, for the study of dislocation dipoles in graphene sheets.

We have developed a new method called localized spectrum slicing (LSS) method for compressing the dimensionality of a sparse Hermitian matrix within a localized region of the spectrum. The LSS representation can be useful for reducing the dimensionality of the Kohn-Sham Hamiltonian matrix without losing accuracy, a key feature required for the efficient application of the PEXSI method. We develop a divide-and-conquer strategy with controllable error to construct the LSS basis set. This is a purely algebraic process, and can also be applied to general sparse Hermitian matrices.

The LSS method is related to the decay properties of Green's functions, and in general smooth matrix functions. For discretized Schrodinger type operators, recently we analyzed its discretized Green's functions under finite difference as well as pseudo-spectral type representation. We provide the first sharp off-diagonal decay estimate of the discretized Green's functions, and the estimate is sharp with respect to the resolution parameter. Such estimate is particularly important for understanding the near-sightedness properties when high resolution discretization, such as planewaves and finite difference methods.

Solving Problems in Materials Theory via Quantum Networks

Principal Investigator: Joel E. Moore

Project Description

Considerable attention has been focused on the ability of a quantum computer to speed up exponentially the solution of certain problems in computer science. However, the number of qubits required is large and the demands on error rates are stringent, and furthermore it is unclear how useful a quantum computer of this type would be for general-purpose computing. The present LDRD is motivated by the observation that the most accessible problems where a quantum computer has a dramatic edge over classical computation may well be drawn from quantum chemistry and materials.

The most important class of computationally difficult problems in quantum chemistry and materials involve strong correlations, and the most common approach to such problems is to devise a simplified Hubbard/PPP model capturing the essential orbital(s) on each atom, then diagonalize the Hamiltonian matrix whose dimension is exponential in system size. A quantum network essentially builds this Hamiltonian matrix with synthetic qubits and interactions.

The PI is an expert in correlated electronic materials and has considerable experience in studying standard many-body models such as the Hubbard model and antiferromagnetic spin chains/lattices. He will work with the experimental groups of the CoQuNAC proposal, especially Prof. Irfan Siddiqi, to design and implement test "benchmark" networks and understand how they behave. Two thrusts are to understand how to model the environmental interactions that eventually destroy quantum coherence in superconducting qubits, and to work toward a systematic procedure to extract effective models for real materials.

Accomplishments

Six weeks of funding were brought forward to this fiscal year to enable a postdoc, Dr. Michael Kolodrubetz, to begin work early. Given the limited period of work, there are not yet publishable outcomes, but Dr. Kolodrubetz has developed theoretical methods for analysis of slow variations in an oscillatory quantum system that are currently being applied to some of the problems mentioned above.

EXDAC – EXtreme Data Analysis for Cosmology

Peter Nugent

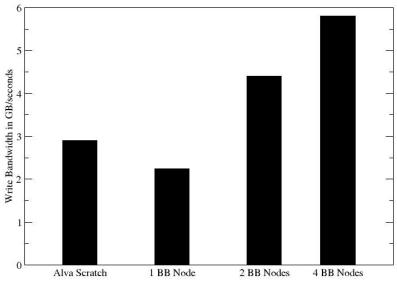
Project Description

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 interface with the NERSC-Cori NRE effort and determine the scale and scope of the project as Cori Phase I would came online in late 2015. We carried out this research on the BurstBuffer testbed system "Alva". Here we created a demo of a typical astrophysics analysis workflow, which we presented at SuperComputing 2014, and created a framework for processing a given N-body/hydro simulation for validating the approximate mock-catalog effort – key to constraining systematics in next-generation cosmological surveys. In addition we generated a test dataset for MANTISSA effort that we then ran on both the Lustre and BurstBuffer filesystem.



We were able to debug many issues, including discovering one with the use of FITS files, a standard astronomical file format for imaging data, which were exacerbated on the Lustre filesystem, but hidden on the BurstBuffer system due to its sheer speed (see figure). Here the speed-up achieved on just 4 BurstBuffer Nodes was 2X over the Lustre filesystem.

High-Performance Parallel Graph-Analysis for Key Genomics Computations

Principal Investigator: Leonid Oliker

Project Description

The goal of this project is to develop new clustering and data reduction algorithms for large-scale data analysis, leveraging structural properties of the data that can be inferred using domain knowledge. Our primary application focus has been genomic data analysis, specifically on large-scale, fine-resolution genetic map construction. Genetic maps are powerful tools for linkage pattern analysis, with diverse applications. For example, a high-resolution map of the human genome can help researchers locate disease-causing genes. Other genetic mapping applications include problems in agriculture and the study of biodiversity. The primary obstacle in analyzing genetic mapping data, as has been noted in many other fields suffering from the "big data" epidemic, is simply the scale of the dataset, which cannot be efficiently analyzed by algorithms requiring more than linear- or near-linear-time. We have been developing efficient algorithms to cluster and reduce large-scale data, focusing on applications to genetic map construction.

Currently, our focus is on exploiting underlying structure in input data in order to quickly cluster data points. Just as dimensionality reduction methods assume that high-dimensional input data lie close to a low-dimensional linear subspace, we design methods that make assumptions on local linearity and cluster structure in high-dimensional spaces. We use these assumptions to accelerate the clustering process. In genetic mapping, we assumed a roughly linear shape of linkage groups, enabling us to quickly cluster the input data into these groups while avoiding all pairwise similarity comparisons between input data points. Furthermore, by taking into account the fundamental resolution of a particular genetic map, we have devised a data reduction method that clusters together all input points with sufficient evidence of belonging to the same map location. Such a clustering aids in error elimination and the estimation of missing data values. We believe that this clustering approach is not limited to genetic mapping data, and we are experimenting with other data sets, such as those from the domain of recommender systems, which we believe to have an underlying structure that can be exploited by our methods.

Accomplishments

Building on our previous work on scalable clustering methods for the linkage-group-finding phase of genetic mapping, our most notable accomplishment has been a novel data reduction method for genetic map construction. We use a coarse-to-fine clustering approach to reduce a large-scale, noisy, and sparse set of input data to a small-scale, much more complete and accurate set of genetic map locations. Experimental results on synthetic data reveal nearly linear running time, a significant accomplishment for previously intractable input data. Our method can thus enable the quick generation of a genetic map, requiring only an ordering phase as the post-processing step on the reduced data to produce a complete map. Results on real data from the wheat and barley genomes reveal promisingly accurate estimations of error rates in the data, as well as the number of estimated map locations. We have released our code for genetic map data reduction to the public.

We are now expanding our work to more diverse data sets, as the clustering approach we have developed can be potentially impact large-scale, sparse, high-dimensional data that exhibits low-dimensional structures. Preliminary results on recommender system data reveals that our method can be effective even in the presence of high missing data rates and errors in large-scale data sets.

High-Order Implicit Interface Methods for Complex Fluid Flow and Multiple Interface Dynamics

Principal Investigator(s): Robert Saye

Project Description

The aim of this project is to develop advanced, high-order accurate numerical methods for the computation of multi-physics processes involving moving interfaces. Example applications include surface tension driven flow, e.g., in the study of foam dynamics and droplet formation; fluid-structure interaction, e.g., in wind turbine dynamics and submersed vessel locomotion; and free surface flow, e.g., in ocean wave dynamics. In these applications, the motion of the interface is strongly coupled to the fluid dynamics: subtle changes in interface geometry can affect fluid flow far away from the interface, and at the same time, small boundary layers in the fluid nearby the interface can drastically affect its evolution. There are a multitude of existing numerical methods for the computational simulation of these applications, however these are typically only low-order accurate – our goal is to develop high-order accurate algorithms that can successfully capture fine-scaled details for challenging fluid flow problems. We expect that the resulting methods will be of use in a wide variety of computational physics problems, including complex-geometry fluid flow problems such as incompressible fluid flow in porous structures, multiphase foam dynamics, cellular transport in a network of vessels, and surface-tension-driven interface dynamics.

Accomplishments

We have developed a new computational framework for complex fluid flow problems based on an implicit mesh discontinuous Galerkin method. The framework capitalizes on mathematical and computational advantages provided by implicitly-defined geometry. In tandem with developing this framework, we have also developed a new set of techniques for computational fluid flow with moving interfaces, called “interfacial gauge methods.” These methods reformulate and extend the now well-known “projection methods” pioneered by Chorin, and provide a high-order accurate framework for studying multi-scale fluid dynamics. Analysis and test applications of these frameworks show that they successfully capture the effect of small scale features (such as boundary layers) on global dynamics – effects that would not be captured by existing lower-order methods. These frameworks consist of several parts:

New high-order dG methods for implicitly-defined geometry, capturing curved interface geometry with high accuracy, including new multigrid methods for solving elliptic partial differential equations with prescribed jump conditions on multiple interconnected interfaces in curved domains.

New high-order quadrature methods for implicitly-defined surfaces and volumes, yielding efficient numerical quadrature schemes with demonstrated orders of accuracy as high as 20.

New high-order accurate methods for computing distances to and closest points on implicitly-defined surfaces: C++ code implementing these algorithms have been made available.

Our results demonstrate the usefulness of these methods with applications to surface tension dynamics that reveal unexpected fine-scale flow features, and in a free surface flow problem exhibiting a certain type of Plateau-Rayleigh instability, which, as far as we know, has not been examined before in a computational setting.

Coherent Information Propagation in Superconducting Qubit Trimer
Principal Investigator: Irfan Siddiqi

Project Description

Simulations of quantum chemistry via classical algorithms are designed in a tradespace of scalability, speed, and accuracy. The computational resources required for an exact solution scale exponentially with the size of the system studied, making the simulation of complicated molecules classically intractable. Quantum chemistry is therefore a highly attractive target for quantum computation and simulation, which may enable scalable, efficient simulation of complex quantum mechanical systems. Our project aims to develop and demonstrate a multi-quantum bit (qubit) architecture, including hardware and software, for the purpose of performing advanced quantum chemistry calculations.

The computational infrastructure we are building is based on the Quantum Variational Eigensolver (QVE) algorithm. This hybrid classical-quantum algorithm optimally divides computational tasks between classical software and quantum hardware. Classical code is used to efficiently map the configuration space of atomic nuclei onto a fermionic spin-1/2 system encoded in the qubits. A multivariable parametrization of the (generally unknown) total quantum state is controlled by a classical minimization algorithm. By preparing a test state and making a series of correlation measurements amongst the individual qubits, the energy associated with the test state is extracted and can be efficiently minimized, thus bypassing the classically onerous task of calculating these correlations *a priori*. Our first implementation of the QVE will be in the simulation of the hydrogen molecule (H_2) using superconducting quantum circuits. This classically tractable problem, which requires two qubits to simulate, provides a benchmark for our device as we develop the architecture.

Accomplishments

The initial task under LDRD was the development of a control architecture for the simultaneous manipulation and readout of many qubits. This substantial software development will enable real-time control of the complex set of operations required to implement the QVE, including event synchronization, trigger programming, pulse modulation generation, and data visualization. This software was developed as qnl_ctrl, an open-source experimental management solution that is specialized for our quantum information architecture. It relies upon a central Configuration, which stores all parameters used in a given experiment in order to ensure traceability and reproducibility of experiments; an Orchestrator, which coordinates and synchronizes the behavior of parallel timelines; and Compilers, device-specific programs responsible for converting pulse and sequence instructions into formats that can be read and performed by the target hardware. This software package will enable rapid scaling of the experiment to accommodate multiplexed qubit architectures.

Simultaneously, a first implementation of the QVE for the purposes of modeling the hydrogen molecule (H_2) is underway. Qubit designs were completed using high-frequency electromagnetic simulations, and fabrication of the superconducting qubits used for this device was begun. We expect to complete a first demonstration of the QVE algorithm in FY2016.

SPOT SUITE – TOWARDS AN END-TO-END SOLUTION FOR LIGHT SOURCE DATA

Craig E. Tull [1], Jack Deslippe [2], Alexander Hexemer [3], David Prendergast [5], Brian Tierney [4] (1- CRD, 2- NERSC, 3- ALS, 4- ESNet, 5- MSD)

Project Description

We propose a systematic investigation and design of the light source analysis environment that can provide an end-to-end solution for data access, management, and analysis; will seamlessly integrate with simulation codes; and will present easy-to-use web interfaces. The result of the LDRD will be a functional prototype end-to-end solution for current ALS data that will enable R&D in the critical areas of data intensive computing that need to be addressed to enable large-scale photon science at the ALS, other BES national facilities, and eventually the ALS-U.

Accomplishments

SPOT Suite (https://spot.nersc.gov) has been in constant operation at ALS micro-tomography Beamline 8.3.2 since March 2013, delivering 24/7, automated, near real-time reconstruction and visualization and at ALS beamline scattering (SAXS/WAXS/GISAXS) 7.3.3 since February 2014. As of October 1, 2015 SPOT has processed more than 244,000 datasets (>1.7 PB of data) and launched more than 3.5 million jobs on NERSC resources in realtime (d10x wrt FY 2013). We have also transferred in real-time over 290 TB of data from LCLS to NERSC for processing and visualizing on NERSC resources using SPOT and psana. The combination of pseudo-production 24/7 running and data demos illustrate the capabilities of the Superfacility and give us confidence that this is, indeed the next, necessary evolution of BES national user facilities.

In FY 2015, we have studied techniques for running real-time analysis in a queue-based system which facilities like NERSC and OLCF typically provide. We developed a novel approach using a message queue-based system implemented on Rabbit-MQ (https://www.rabbitmq.com/). This new technique reduced the average queue-wait time penalty from 80% of overall feedback latency to 30%. And further analysis of our performance data indicate that we can reduce to below 20% with the ability to dynamically allocate additional resources.

Remote visualization capabilities were improved by developing the capacity to allocate resources on Edison and launch VisIt on demand for any micro-tomographic reconstruction dataset in SPOT. NERSC's real-time queues are critically needed for both remote visualization and dynamic resource allocation for our worker jobs.

We conducted 2 demos to show a prototype implementation of ScienceDMZ-as-a-Service using ExoGENI racks (ExoGENI is part of NSF GENI federation of testbeds) deployed at StarLight facility in Chicago and at NERSC. The virtual ScienceDMZs deployed on-demand in these racks use the SPOT software suite developed at LBNL to connect to a data source at Argonne National Lab and a compute cluster at NERSC to provide seamless end-to-end high-speed data transfers of data acquired from Argonne's Advanced Photon Source (APS) to be processed at NERSC. The ExoGENI racks dynamically instantiate necessary compute virtual resources for ScienceDMZ functions and connect to each other on-demand using ESnet's OSCARS and Internet2's AL2S system.

Finally, in preparation for the decommissioning of NERSC systems and the move of NERSC from OSF to CRT, we have investigated using Shifter images for virtualization of SPOT.

ANALYZING THE MICROBIAL RESPONSE OF NUTRIENT LOADING IN THE MAUMEE RIVER AGRICULTURAL WATERSHED TOWARDS THE FORMATION OF ALGAL BLOOMS

Principal Investigator: Gary L. Andersen

Project Description

The objective of this study is to develop an experimental framework to identify causes and mitigate the impacts of algal blooms in Lake Erie. Existing studies on this issue of national importance concentrate on measuring levels of reactive phosphorus that enter the watershed without regard for source of nutrients or the microbial interactions that lead to the creation of a toxic algal bloom. It is our hypothesis that nutrient input drives aquatic ecosystem productivity and influences the composition and ecology of bacterial communities. Accessibility of readily available nutrients is thought to promote change in species richness and composition due to the increased energy available to support the coexistence of multiple species and trophic levels.

Changes in the precipitation patterns are linked to increased mobility of soil phosphorus that is fueling summer algal blooms. Poorly drained soils are pervasive in this region, and heavy rainfall quickly causes soil saturation and flooding. The trend of more frequent and extensive periods of soil saturation can promote low redox microbial processes, namely ferric iron reduction, that can mobilize mineral bound phosphorus that is considered immobile in soil. Episodic but widespread soil iron reduction by microorganisms may release substantial phosphorous into runoff discharge but is not currently considered in models of watershed phosphorus cycling.

As a first step towards the understanding of microbial responses to nutrient loading that lead to the formation of toxic levels of algae in Lake Erie, we will need to identify and partner with individuals in Ohio that are currently sampling water throughout the Maumee River watershed. With knowledge of the optimum locations over a spatially distributed network for future water sampling we will develop an experimental framework for a detailed study over multiple time points to understand each area's overall contribution to the nutrient contamination.

Accomplishments

Our most significant accomplishment was to set up a partnership with multiple stakeholders in Ohio, including Dr. Jim Hoorman and Dr. Steve Culman at Ohio State University, School of Environment and Natural Resources. We developed an experimental plan to study iron-redox cycling and phosphorus under field conditions, and conduct simulated rainfall experiments in the lab to quantify P speciation and leaching potential under variable iron-redox conditions. We selected field sites managed by Ohio State in NE Ohio that include six different land use conditions including forest, grassland, tilled cropland (high and low soil P) and no-till cropland (high and low soil P). Sample collection will happen in Spring 2016 and the preliminary experiment will demonstrate the potential for Fe-reduction and resulting changes in P speciation and mobilization under different treatments.

In 2015 Lake Erie experienced one of its worst algal blooms on record, and current management efforts are failing to address the problem because there is an inadequate understanding of phosphorus dynamics. The research proposal that we have developed will create improved watershed scale models and develop an improved understanding of how extreme climactic events are altering terrestrial biogeochemistry.

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

We have made some significant advances this year, we established our 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 μXRF at the Advanced Light Source demonstrated that hotspots of P in soil were organic. Bacterial growth media based on plant root exudate sugars and these insoluble P containing substrates yielded >400 bacterial and > 200 fungal isolates. Screens were developed for P solubilization activity by organic acid production, enzyme secretion and siderophore production and effective solubilizers were identified and DNA sequenced. A large majority of these bacterial isolates belong to a single bacterial genus (*Burkholderia*). We have conducted a field survey to determine their distribution across the nutrient limitation observatory. We are currently determining the molecular mechanisms of P solubilization by these bacteria and their growth promoting effect on plants (*Arabidopsis*, *Brachypodium* and Switchgrass). Work to characterize the fungal P solubilizers is ongoing. Some of the concepts and approaches developed in this LDRD directly contributed to a component of a university led DOE-BER award to study microbial roles in the sustainability of switchgrass feedstock production systems.

The Soil Metazoan Microbiome: A Key Functional Compartment of Importance to Plant Health and root C Stabilization

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

Project Description

Typically, when studying the biological processes involved in the cycling of soil nutrients and the potential stored in soils for the improvement of those processes, studies focus on free-living soil associated microorganisms or soil microorganisms as a bulk. In nature, microbial communities and their functions are compartmentalized in different environments that provide the conditions for the microbes' activity. In soil the compartmentalization of microbiomes and their processes is mostly being studied in the soil rhizosphere and soil aggregates, leaving aside the contribution of metazoan-associated microorganisms to nutrient cycling. 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 will study the diversity of arthropods in the soils of the Ecological Staircase in Mendocino, CA as well as the makeup of the microbial communities associated with them. For this, we plan to develop a strategy for the large-scale isolation of DNA from single arthropod specimens that usually have a size of 100 um to 5 mm. Once this strategy is completely developed, we will use the obtained DNA for the characterization of the symbiotic microbial populations associated with the soil animals and their potential for nitrogen fixation. We will also isolate 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. also isolate 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.

Accomplishments

We have optimized the protocol for DNA extraction from a small amount of starting material – little animals for a body size of 100 um. We also performed the first samplings at the Ecological Staircase in Mendocino and collected 100 arthropod specimens that were categorized based on morphology. 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. Our results demonstrated that each specimen contained a distinct set of associated prokaryotic populations, a result that may also indicate their different role in soil environmental processes. The obtained DNA was also used for the screening of nitrogenase genes as a proxy to determine the potential for nitrogen fixation stored in the arthropods. Thirty of the 100 tested arthropods yielded positive amplification of a nitrogenase. These results are in the process of being confirmed using molecular cloning and phylogenetic analyses.

We are in the process of isolating plant polymer degrading and nitrogen-fixing microorganisms from four groups of soil metazoans.

Fracture Characterization During and After Multistage Hydraulic Fracturing in Unconventional Gas Reservoirs Using Temperature Data

Principal Investigator(s): Barry Freifeld

Project Description

One of the challenges in the development of unconventional oil and gas reservoirs is assessing the efficacy of hydraulic stimulation techniques in generating new conductive fractures. Evaluation of hydraulic stimulation effectiveness is typically done by examining overall production along with performing occasional logging runs using tools such as a PLT(production logging tool). The downside of performing periodic logging operations is that it interferes with production and the costs are significant given the mobilization and demobilization of highly specialized tools and operators.

Permanently deployed fiber-optic distributed temperature sensing (DTS) technology provides the opportunity to continuously collect data that can be used as a proxy for fluid flow to image fracture networks. The challenge our project sought to address is developing an analytical framework for assessing thermal profile data. While our project was in progress we had the opportunity to work with field data acquired at a hydraulic stimulation project occurring at the Raft River Geothermal Field. This enabled us to test our analytical tools using real world fracture flow data.

Accomplishments

Using the TOUGH2 numerical simulator we developed a framework for using DTS profiles to assess flow based on 2D axisymmetric heat and mass transport models. We discretized our wellbore using a grid that honors the size and geometry of tubing, casing and annular space. Coupling this with the iTOUGH2 code we performed sensitivity studies to examine levels of minimum detectability for changes in flow regimes associated with hydraulic fracturing operations. In particular we looked at minimum detectabilities for flow along a casing and determined a rate of 0.1 kg/s is appropriate when accounting for uncertainty in model parameters.

To exercise our code we used DTS profiles collected during the creation of a fracture at the Raft River geothermal field during a hydraulic stimulation activity at well RRG-9. We collected time series data at 15 minute intervals for over a year of monitoring. During a hydraulic stimulation activity we recorded data revealing the creation of a fracture and the ensuing thermal disturbance. Throughout the hydraulic stimulation we also collected flow rate and pressure data. Performing a joint inversion process on all the disparate data collected allowed us to calibrate the model we created and perform a data worth evaluation of the addition of DTS profiles to our collected data set.

While it is clear that our research showed DTS can be used to image fluid flow and the creation of fractures during hydraulic stimulation, there remain engineering and economic challenges for the widespread adoption of the monitoring technology.

Using Experiments and Numerical Models to Examine Ecosystem and Land Management Interactions with Atmosphere and Climate

Principal Investigator: Lara M. Kueppers

Project Description

The purpose of this LDRD was to build capacity and expertise in linking dynamic global vegetation models (DGVMs) with field experimental results to improve understanding and prediction of climate-ecosystem feedbacks. The goals of the project were to, (1) determine the sensitivity of Western U.S. forest dynamics to parameterizations of forest regeneration and migration processes in DGVMs, and (2) evaluate model performance relative to field climate change experiments. Demographic processes, such as forest regeneration, are critical to accurate simulation of forest change. Decadal to century scale changes in the distribution and structure of forests can have large leverage on the climate system. Current large uncertainties in Earth system model climate projections are due, in part, to uncertain biogeochemical and biogeophysical feedbacks from forest ecosystems. The proposed research is an important foundation for a new SFA in the area of Dynamic Vegetation, currently under development.

We proposed to run dynamic vegetation models for Western U.S. forests, examining model sensitivity to parameterization of tree regeneration and migration processes. We proposed to conduct model simulations using the Community Land Model (CLM(ED)) and a new forest demography model (ED2) that track tree cohorts, thus more explicitly modeling temporal dynamics of forest change through time, as it is sensitive to environmental conditions. We proposed to compare model output to data synthesized from a set of field experiments at Niwot Ridge in Colorado, established to determine the sensitivity of tree regeneration and migration to climate change, and to tree demographic rates synthesized from the literature. A final aim was to determine whether population matrix models, are a potentially useful benchmark for DGVMs.

Accomplishments

Key accomplishments in FY15 were analysis of tree regeneration data from a climate warming experiment in Colorado, and synthesis of data from long-term demography plots and the literature for use in demographic models. We also developed population matrix models for two subalpine tree species that are widespread in western North America and compared population responses to scenarios of climate change at a single site using the experimental and observational data. The modeling results, which suggest long lags between forest decline at low elevations and forest expansion above treeline with warming, were presented at two international meetings and the all results are in revision for publication.

Another key accomplishment in FY15 was the recruitment of a postdoc who is skilled in demographic modeling of forest ecosystems using the Ecosystem Demography (ED2) dynamic vegetation model. Although he started late in the LDRD period, he was able to get a version of ED2 running at LBL that better represents tree responses to drought, and he will be conducting modeling sensitivity studies and data synthesis consistent with the aims of this LDRD as part of NGEE Tropics, which was fully funded in July 2015. We also conducted data analysis to examine seedling growth sensitivity to climate warming using experimental data, and are developing a publication on the results.

I gave a presentation to BER program managers (Jan 2015) with Nate McDowell (LANL), and Margaret Torn regarding the need for an expanded, coordinated focus on dynamic vegetation responses to climate change and helped to organize a DOE/BER workshop on dynamic trait-based vegetation modeling (held in November 2015). I am continuing to coordinate a Divisional initiative to advance empirical and modeling capabilities related to dynamic vegetation.

Clay Interlayer Stratification: Implications for Ion Exchange and the Mobility of Neutral Molecules in Shales

Principal Investigator(s): Laura Nielsen Lammers

Project Description

The main objective of this project is to understand the physiochemical mechanisms governing ion exchange and mass transport in anhydrous clay minerals (illites), which are dominant phases in shales and other clay-rich sedimentary reservoir rocks. Shales serve several key functions in energy production and emissions mitigation as reservoirs for natural gas, as caprocks limiting the subsurface migration of geologically sequestered CO_2, and as impermeable barriers for nuclear waste storage. Clay minerals mediate the transport of ions and neutral molecules through clay-rich rocks, but no prior studies have investigated the kinetics of mass transport through anhydrous clays at a molecular level. In addition, ion exchange in illites has been shown to cause layered (stratified) structures that cannot be described or predicted by existing models for clay ion exchange reactions.

Accomplishments

The key accomplishments of this project in FY2015 were (1) to determine the magnitude of and controls on the kinetics of ion migration in illite interlayers, and (2) to investigate the impact of interlayer ion substitution (Cs^+ for K^+) on subsequent exchange kinetics. In the course of the research, we developed a methodology to map activation energy barriers for single ion migration events in clay interlayers and a general method to evaluate the optimal distribution of interlayer ions. The following paragraphs provide a brief synopsis of our findings.

Our first key accomplishment was to determine the migration kinetics of interlayer K^+ ions in illite. Clay layers are composed of stacks of sheets, with corresponding interlayer regions occupied by ionic species that compensate the negative structural charge of the material, which arises due to isomorphic substitutions (*i.e.*, Al^{3+} for Si^{4+}) in the clay lattice. Illite contains anhydrous and strongly bound interlayer cations, typically K^+, and is therefore a very strong adsorbent material. We calculated activation energy barriers for migration of K^+ ions to their adjacent sites to be in the range 2.2–3.5 eV using atomistic simulations and the Nudged Elastic Band (NEB) method. Remarkably, the migration path and barrier of an event are not affected by K^+ neighbors. However, the barrier varied significantly due to a wide range of cohesive energies of K^+. Using stochastic sampling techniques, we developed a method to obtain an optimal distribution of ions in clay interlayers. Our results demonstrate that interlayer ion distribution is likely controlled by the positions of isomorphic substitutions, providing for the first time a quantitative basis for the long held view that charge distribution impacts ion distribution and exchange.

Our second significant accomplishment was to demonstrate the role of layer spacing on migration barriers. By varying the interlayer spacing from the fully K^+ substituted end-member, to the larger Cs^+ substituted end-member, we found that the migration barrier was dramatically reduced. This finding implies that as Cs^+ substitutes for K^+ near clay edges, the kinetics of subsequent exchange events are accelerated, causing a positive feedback mechanism that promotes Cs^+ exchange. Our results give a mechanistic explanation for the observed interstratification effect and will be used as a basis to develop macroscopic models of ion exchange in anhydrous clays.

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

Principal Investigator(s): Seiji Nakagawa, Valeri Korneev, 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, the extent and orientation of hydraulic fracture propagation can be manipulated. Laboratory hydraulic fracturing experiments are conducted, using small rock and transparent, soda-lime glass blocks containing an analogue borehole. The geometry of the fractures as they propagate will be imaged either visually (for transparent samples) or by using X-ray CT (for opaque samples) under true-triaxial stresses. 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

In the laboratory, we developed an optical hydraulic fracturing visualization system which was designed to apply dynamic pressure shock and controlled pulses while elevated pressure is applied to an analogue borehole within a transparent sample block. The functionality of an manual, shock system was confirmed. However, in spite of the original prediction of the pressure magnitude for the controlled source consisting of a piezoelectric actuator and a hydraulic piston directly attached to the sample, the actual amplitudes of the controlled pressure pulses were too small to have an impact on hydraulic fracturing. The cause of this problem is currently being investigated. Also, preliminary fracturing experiments using fast and slow fluid injection indicated that, contrary to our original hypothesis, slow (considered low frequency) injection resulted in more dispersed fracturing in a heterogeneous sample containing numerous preexisting fractures than fast (high frequency) injection. The pressure history in these cases, however, are not "dynamic" (i.e., lacks actual frequency modulation by cyclic pulsing), and the effect of the modulation has yet to be tested.

For the numerical modeling, we built a fluid-filled fracture network model using a finite element code (COMSOL Multi Physics), and conducted preliminary investigation on the effect of pressure pulse frequency on the propagation of fluid pressure along the fracture network. The results demonstrated propagation of the pulses along the branches of the fractures, which diminished by both viscous dissipation and elastic scattering of the energy. Varying levels of stress concentration at the ends of the fractures was confirmed, which would result in further extension of the fractures. However, this effect also includes the stress induced by the propagation of seismic waves in the solid part of the model, and its impact needs to be delineated from the observed results.

Quantifying the Dynamics of Natural Organic Matter Conformation and Reactivity

Principal Investigator(s): (Peter S. Nico, Benjamin Gilbert)

Project Description

The purpose of this project is to observe—in situ, and over a range of length- and timescales—how changes in chemical conditions affect the conformation and reactivity of natural organic matter (NOM) relevant to both soil and shale systems. Natural organic matter is a complex mixture of organic molecules and associated metals and is ubiquitous in the near earth surface environment. In the form of soil organic matter and dissolved organic matter, NOM chemistry impacts practically every meaningful ecological process in soils, sediments, ground waters, surface waters, and marine systems. As kerogens in sedimentary rocks, NOM chemistry plays a key role in energy production capacity, efficiency and associated environmental impacts.

A core approach in this project is the application of recent technical developments from the Schuck group in surface-enhanced (SERS) and tip-enhanced Raman scattering (TERS) for nanoscale analysis. We will also plan to take advantage of the technique of nano-FTIR spectroscopy and X-ray ptychography (both being developed at Berkeley Lab's Advanced Light Source (ALS)) to explore the nano-scale structure of organic matter in natural shales.

Accomplishments

Our FY15 accomplishments pertain to the second part of the project proposal, specifically the use of novel spectroscopic techniques to analyze micro and nano-scale structure of shale and its' organic inclusions. We accomplished three complimentary measurements of a shale sample, specifically ptychographic imaging, nano-FTIR, and Ge hemisphere micro-ATR-FTIR. Preliminary ptychographic data showed differences between the overall intensity images and the phase data which is one of the distinct advantages of this approach. In addition, we utilized a laser milling technique as part of a new sample preparation procedure that allowed us to acquire higher quality ptychographic. In addition, using both nano-FTIR and Ge hemisphere micro-ATR we were able to show the nano scale distribution of what appear to be CO_2 inclusion/sorption within the shale as well as the distribution organic materials on a micron scale. All three measurements advance our ability to image small scale structure of shales which is important for understanding their bulk scale behavior. They also helped to further develop three synchrotron based measurement approaches based at the Advanced Light Source, thereby making these techniques more available to future ALS users. Finally the data obtained and the approaches developed by this LDRD contributed to the formation of the Digital Rock Dynamics Laboratory Initiative (DRDL) which is currently under discussion with DOE-BES program. The DRDL will integrate key Berkeley Lab competencies including 1) currently available and developing investigative tools, 2) Scientific Engineering, 3) Multi-modal Multi-scale Dynamic Imaging of Rock-Fluid Processes, 4) Pore-scale and Molecular Simulation, 5) Data Analysis and Integration, and 6) Smart Upscaling Strategies. Ultimately, the DRDL will provide reservoir rock analysis that we anticipate will become vitally useful for many DOE projects at Berkeley and in the US, particularly the growing complement of field observatories for many subsurface energy systems

Dynamic Fracture Simulation in Geomaterials at Multiple Length Scales

Principal Investigator(s): Jonny Rutqvist (FY16) and John Edminson (FY15)

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 will be 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 will be performed based on available analytical solutions from the literature. We will also choose well characterized experimental results from a purely mechanical problem with records of crack propagation and geometry. The final deliverable will represent an improvement over currently existing methods in being capable of large computation as well as other advantageous features for explicit demonstration of crack propagation.

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, a new code framework of 3D dynamic simulation program has been established. Modern programming features are implemented in Fortran 90, which will provide better computational efficiency and future code management. Also, the calculation of the inertial tensor of an arbitrary polyhedron is included in the code. The Voronoi polyhedra are the most fundamental elements for modeling, so it is crucial to obtain their geometrical information for establishing and solving mechanics ODEs. The solution phase is implemented using explicit time integration algorithms (e.g., velocity Verlet scheme), which will ease converting the code to a parallelized version.

For the peridynamics approach, we have focused on the simultaneous development of a parallel capable code, in addition to proposing solutions to unanswered questions regarding the use of peridynamics with pressurized cracks, which had not been demonstrated at the start of the grant period. This code has been developed in C++ to rapidly deploy the merits of open source libraries for time integration, such as PETSc and SUNDIALS. Parallelization was emphasized from the very beginning, therefore a generic framework for transmitting data between different simulation types using different grid resolutions (via interpolation functions) has been developed, including requirements for space partitioning and MPI capable data structures.

The verification of the numerical methods has been conducted through a mutual comparison of the simulation results for the same test example. We considered a purely mechanical behavior with a pre-cracked sheet material pulled in tension. Both of the numerical methods could accurately simulate a particular crack branching phenomenon in a rapid crack propagation.

Nanoparticles-Stabilized Supercritical CO_2 Foams: Developing Novel Material for CO_2-Enhanced Oil Recovery

Principal Investigator: Jiamin Wan

Project Description

The primary limitation in using CO_2 as the injection fluid for enhanced oil recovery (EOR) has been the low viscosity and high mobility of CO_2 that causes the injected CO_2 bypassing oil and resulting limited displacement efficiency. After decades of extensive research and practice on ways to reduce CO_2 mobility, the CO_2-bearing foam approach seems more promising. The major barriers limiting industrial applications of CO_2 foam-EOR include the high costs of surfactants, compare to the price of oil. Concerns over environment impacts also exist for some of these surfactants. If a CO_2-compatible surfactant that overcomes these limitations can be identified, such a discovery will benefit oil recovery, while at the same time increase the incentive to implement carbon capture and increase the capacity of geologic carbon sequestration in depleted oil reservoirs. The overall objective of this project is to develop a new and unconventional material, which is less expensive, non-toxic and highly effective as a substitute of conventional synthetic surfactants, for increasing CO_2 viscosity and control its mobility in EOR. The Earth's near-surface sediments contain deposits of natural organic matter produced primarily from degradation of plants. We hypothesize that these organic deposits contain a large fraction of surfactant-like material. This material can be extracted, and dispersed in the form of nano-particulates when re-dissolved in water. These nano-particulates can stabilize supercritical CO_2-brine foams, and are more cost-effective and environmentally friendly than synthetic surfactants currently used in CO_2 foam-EOR.

Accomplishments

We have identified the sources of NSS, which is abundant and inexpensive. We tested samples from 5 different geographic regions for NSS extraction. We have developed a method (proprietary) to produce the NBS. The NBS is capable of generating and stabilizing dense $scCO_2$-in-water foams containing CO_2 with controllable effective viscosities, three orders of magnitude higher than that of pure CO_2 at the same pressure and temperature.

We measured interfacial tension of NSS liquid solutions paired with N_2, and paired with $scCO_2$ as function of NSS solution concentrations. The NBS performs as an effective surfactant, significantly reducing interfacial tensions between the N_2-water and the supercritical (sc) CO_2-water interfaces. We have also just built a modified high pressure and high temerature foam-generator and successfully tested foam-stability vs. temperature. The NSS is a N_2- and CO_2-compatible and high quality surfactant.

We are in the process of optimizing NSS extraction method, estimating extraction costs, and optimizing laboratory CO2-EOR tests in cores.

Novel Magnetic Field Mapping Technology For Small And Closed Aperture Undulators
Principal Investigator: Arnaud Madur

Project Description:

The objective of this project is to develop a magnetic measurement technique that will enable the characterization of novel undulator geometries (small gap, ultra compact, closed aperture) dedicated to Diffraction Limited Storage Rings (ALS-U). Technological developments involving novel ultra-compact, virtually non-invasive optical methods are required to map magnetic fields accurately on a straight path in closed aperture devices Presently, none of the LBNL magnetic field mapping benches has this capability.

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 position feedback system, and 4) a new magnetic sensor transport mechanism concept. The scope for the FY15 LDRD was concentrated on both the position acquisition system and the transverse position feedback system (items 2 and 3 above).

The common key issue to the four areas described above that has to be dealt with is the miniaturization of the novel apparatus components. A laser system with its associated optical components must be developed since no other technology has the potential to track the sensor position without interfering with the small diameter vacuum chamber. Then for the feedback system effort must be put into identifying both the actuator and developing the software that will manage both the signal from the laser and the actual position of the novel sensor through the new actuator. This new magnetic measurement capability must be developed to support the development of a new generation of undulators custom designed to realize the full potential of a synchrotron radiation source from a diffraction limited light source. It is critical that this technology is in hand to properly produce optimized insertion devices for ALS-U.

Accomplishments:

First, a laser system was put together. It consists in a 6 mm diameter laser source, a set of optical components and a CCD camera. With this set-up, we managed to develop and test a transverse position acquisition software. Then a retro-reflector and a beam splitter were added into the optical system so that we could test the position acquisition system. We identified a retro-reflector technology that matches our requirements (small, non magnetic and non metallic): solid glass retro-reflector was chosen. After the successful test, we worked on reducing the size of the retro-reflector. As no manufacturers were able to provide what we needed, we machined an existing 1” diameter retro-reflector to get a 2 mm diameter one. This capability has been developed in house as no manufacturer could provide retro-reflectors that fit our needs. After careful polishing of the reflector surface, we were able to successfully test this new set-up i.e. to track the position of the retro-reflector attached to a manual stage to mimic position change of a magnetic sensor. Then we procured sets of MEMs to implement the position fine-tuning mechanism. A test set-up was put together and it will be used to further develop the position acquisition software and then to verify the MEMs tuning performance with the in-house retro-reflector attached to it.

Mesoscale Structuring of Surfaces for Energy and Water Applications

Principal Investigator: Andre Anders

Project Description

The main goal of this proposal is to develop mesoscaled surfaces by novel, scalable, low cost surface structuring approaches for renewable energy and water harvesting applications. Structuring of surfaces is highly desirable for many applications, and here we focussed on mesoscaled surfaces that could be the key to efficiently extract water from moist air, a little explored approach to mitigate water shortages in drought areas. We aimed to combine traditional methods of structuring, like chemical etching, imprinting, masked deposition, and de-wetting, with novel physical treatments of surface using plasmas. In particular, there is evidence that materials treated with low to medium energy helium ions develop mesoscaled structures, the details of which depend on the material, its temperature, and the energy and dose of incident ions.

Accomplishments

A high current plasma source was built based on a thermionic electron emitter that could produce a relatively dense helium plasma (10^{11} cm^{-3}). The plasma was confined by a magnetic field, generated by a coil, in which the to-be-treated samples could be placed. The samples were mounted on a holder with a heater and thermocouple. For conducting substrates, a bias voltage was directly applied, and for insulating substrates we used a capacitive coupling method with a frequency of up to 350 kHz to produce a desired negative surface potential relative to the plasma potential. With this setup, a number of materials have been processed to alter their surface structure. The modified surfaces were characterized before and after helium plasma treatment by microscopy, but most importantly by Fourier transform infrared spectrometry to determine their spectrally selective emissivity, and by contact angle measurements to evaluate their hydrophilic / hydrophobic properties. The combination of these properties is most important to achieve radiative cooling while also to promote condensation of water vapor and collection of water droplets once droplets have reached sufficient size to roll off the collecting surface. A critical point was the removal of latent heat, which represents an interesting coupling of water and energy issues.

We found that the formation of mesostructures required not just a high helium ion flux but also high substrate temperature. Contrary to earlier assumptions, mesoscopic patterns form only in a relative narrow, material-dependent process window of ion energy and substrate temperature, with substrate temperatures generally higher than what is practicable or permissible from a cost perspective. This factor, combined with the realization that the volume of water to be collected is much smaller than what is economically relevant, let to the conclusion of this project after only one year (the original plan was two years). This work has contributed to understanding of material and energy balance conditions used for other proposals, and a patent disclosure was developed with Prof. Philip Marcus of UC Berkeley.

A Hybrid MRS-TEM System for Mapping Shallow Aquifers

Principal Investigator(s): Shashi Buluswar, H. Frank Morrison, Erika Gasperikova, Alessandro Ratti

Project Description

The purpose of this project is to design and build a novel lightweight system for mapping the depth of shallow aquifers, and for determining the salinity of the water, using a combination of magnetic resonance sounding (MRS) and conventional ground resistivity mapping using a transient EM method (TEM). MRS is a variant of Nuclear Magnetic Resonance (NMR). For this application MRS detects total water content of soils and rocks by exciting protons in the water molecules with an externally applied magnetic field of the Larmor frequency, which is set by the local value of the Earth's static magnetic field. After excitation these precessing magnetic moments produce a secondary magnetic field that decays with time, and the decay rate is a function of the degree to which water molecules are bound to the mineral surfaces in the formation. Aquifers containing significant clay and silt have small pore spaces and rapid signal decays whereas sands and gravels with large pore sizes have very long time constants although both formations may have the same water content. The amplitude of the Larmor secondary field at the instant of cessation of the inducing field is directly proportional to the water content in the volume of the subsurface influenced by the primary inducing field. A fundamental limitation of the method is that it cannot directly respond to the salinity of the aquifer and thus is not directly useful for estimating water quality. An independent measurement of the resistivity distribution in the ground can remove this ambiguity. Electrical and EM methods measure the distribution of electrical resistivity in the ground. The resistivity of soil or rock depends on the porosity, salinity of the pore fluid, water saturation (the degree to which the pore space is filled with water), and on the clay content. The fact that the resistivity of a given region of the subsurface depends on so many factors means that working backwards from resistivity measurements to the identification of a good freshwater aquifer is highly problematic. The combination of MRS and resistivity mapping removes the ambiguities that are inherent in each method; particularly by identifying the salinity of an aquifer detected by MRS. This will be the first field system that combines both techniques in a common package using common transmitters and receivers.

Accomplishments

In the first phase of the project we developed and tested the MRS component of the dual MRS-TEM system. We collected data sets that demonstrated that the prototype MRS system is performing according to design. The innovative pulse generation system worked as planned and clearly demonstrated that signals could be measured much closer to the shutoff of the MRS excitation pulse than in existing systems, and that it easily converts to the generation of single pulse waveforms required for TEM operation. The receiver system demonstrated the sensitivity and noise levels needed to detect the very small MRS signals and the ability to recover quickly from the very large primary or exciting field. Three different approaches were explored to analyze the data. For high-quality data sets the results were consistent among these approaches. For noisier data sets one method performed better than the other. Despite of a limited amount of data and variable data quality, it is reassuring that all three methods produced similar results. The field test was done at a challenging site because of a high clay content that causes a fast decay of the MRS signal. However, even in these conditions useful data were recorded, which hasn't been possible with existing MRS systems.

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

Our most significant accomplishment has been to complete a functioning prototype of the IDEA application, which is collecting data from multiple different markets, processing it, and delivering it to researchers in an analysis-ready format. To accomplish this, we have built a software module allowing us to store data from arbitrary countries and economic regions, in a common format including arbitrary currency conversion. We have also developed data-collection software to gather data from retail and government websites in Mexico, India, China, Indonesia, and South Africa.

Using the data collected, we have also demonstrated key capabilities for IDEA in the areas of market characterization and market surveillance. In particular, using the data for refrigerators and air conditioners in India and China, we performed initial market characterization analyses and cross-market comparisons. For instance, we were able to determine that, although China has more stringent efficiency standards for air conditioners, there is greater room for efficiency improvement within the Indian market today. We also found some evidence for fraudulent efficiency label advertising within the Indian market. Results of this preliminary work were presented at the International Energy Program Evaluation Conference.

IDEA data gathered in Indonesia and South Africa are also currently being used to inform the evaluation and development of new energy efficiency programs in those countries, under the auspices of the Super-Efficient Appliance Deployment (SEAD) initiative of the Clean Energy Ministerial.

Application of Virtual Grid-Integration Laboratory (VirGIL)

Principal Investigator(s): Sila Kiliccote (now Emma Stewart)

Project Description

The purpose of this project was to develop a modular simulation framework that would facilitate the simulation of future power systems. These future 'smart' grids are set to dwarf the historical grid in terms of complexity. The traditional separation of generation and load is expected to become increasingly blurred with the emergence of technologies such as storage, electrical vehicles, and demand response, which are capable of rapidly traversing these traditional generation/load modes dependent on control strategies. A complex two-way communication network is required to be embedded into the physical grid in order to facilitate the transition of the historical grid towards a 'smarter' grid.

Traditional specialized power system simulation software packages are unsuitable for understanding these complex system interdependencies and determining the necessary control strategy for optimal power system operation. This project adopted the co-simulation approach, where mature and reliable simulation tools, specialized in their respective fields, are connected via a common co-simulation platform in order to study the interdependencies between systems and identify the appropriate control strategies in order to ensure system security and optimal operation of the grid.

VirGIL's master algorithm co-ordinates all its modules through the Functional Mockup Interface (FMI). This is a tool independent standard that provides a modular structure for exchange and testing of different co-simulation tools such as an EV simulator.

One of the primary motivations for this project was to understand the impact that demand response strategies have on the network and determine the optimal manner in which to utilize these flexible loads for power system operation.

Accomplishments

Our most significant accomplishment in this project was the successful coupling of a commercial power system simulator with advanced modeling tools for buildings and communication networks through the Functional Mock-Up interface, and demonstration of a partner utility network dispatch of Demand Response. The building FMU was successfully created via calibrating a simplified RC model in order to replicate the results of a more detailed EnergyPlus model. This ensures scalability while retaining accuracy, as a complete EnergyPlus model is too detailed to simulate each individual house in a distribution network.

The case study centered on two applications involving a building on the LBNL network. The first application of the platform studied was the interaction of loads during a high penetration of distributed energy resources, whereby a PV plant and battery connected. A DR control strategy was successfully implemented to reduce loading on the infeed cable serving the building.

The second application focused on Volt/Var control to control the voltage at the buildings terminals. In this case the reactive power infeed from the battery was adjusted so that the local voltage would track a reference voltage. Both use cases demonstrated the capabilities of VirGIL to accurately model and simulate the interactions between buildings, communication and power systems.

Characterization of Electrochemical Devices Using Differential Electrochemical Mass Spectrometry (DEMS)

Bryan D. McCloskey, EETD

Project Description

The goal of of this 2-year LDRD was to construct a mass spectrometer that will allow quantitative analysis of gas consumption and gas evolution from electrochemical or chemical systems. This spectrometer has become a critical component of a comprehensive and systematic approach designed to understand fundamental reactions occurring in metal-air batteries, Li-ion batteries, CO_2 reduction catalysis, oxygen reduction catalysis, and other systems where gas evolution occurs.

The differential electrochemical mass spectrometer (DEMS) was constructed over the first 9 months of FY2014 and was used to study electrochemical systems listed above in FY2015. The DEMS was custom-built to provide many unique features that allow *in-situ*, real-time quantitative analysis of gas consumption/evolution in electrochemical cells, which can then be related to Coulometry to more clearly understand electrochemical processes. This technique is extraordinarily powerful and sensitive and provides the capability to assign electrochemical currents to specific reactions. By combining this information with that provided by other spectroscopic and classic electrochemical characterization techniques, complex electrochemical processes can be clearly understood and more readily controlled.

Accomplishments

Construction and calibration of the DEMS was completed in June 2014, allowing it to have all of the useful features necessary to quantify gas consumption and evolution from electrochemical systems. We are currently exploring four avenues of research with this capability: new electrolyte systems for Li-air batteries (a BATT/OVT proposal was funded in part because of the DEMS capability in our laboratory), outgassing of Li-ion battery materials at high voltages, magnesium corrosion in aqueous electrolyte systems to understand limitations of aqueous Mg-air batteries, and oxygen and carbon dioxide CO_2 reduction electrocatalysis. PI McCloskey been integrated into JCAP II as an affiliate to provide product analysis support using DEMS for photoelectrocatalysis of CO_2 reduction. Proposals have been submitted to the NSF and ACS Petroleum Research Fund in an attempt to secure further funding for aqueous electrocatalysis research (which the DEMS would be ideally suited to study).

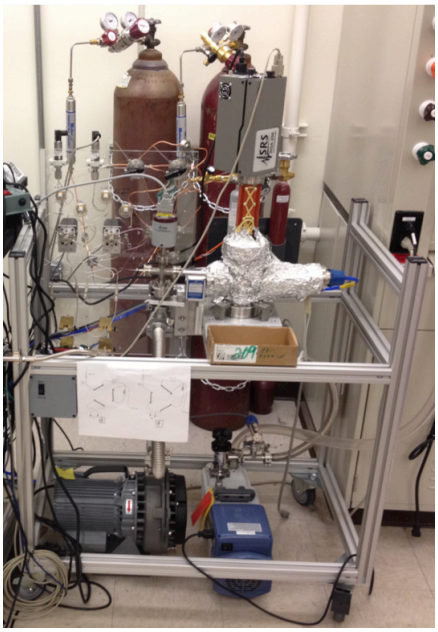


Figure 1: Differential Electrochemical Mass Spectrometer in operation in the McCloskey Lab.

To date, 2 articles (in *PNAS* and *ChemComm*) supported by this work have been published, with no less than 4 additional articles currently in preparation (see References for list of these articles). Among the interesting scientific outcomes of our endeavors, we have identified that oxygen outgassing of high voltage non-stoichiometric, Li(NiMnCo) Li-ion battery cathode materials occurs above 4.6 V and continuously occurs if the electrode is held above that potential, implying that O_2 evolution is a parasitic process that should be avoided. Furthermore, CO_2 evolution at potentials much lower than 4.6V occurs in this system, implying that the electrode catalyzes an unwanted side reaction. We have also quantified H_2 evolution from Mg electrodes immersed in various aqueous electrolytes as a function of anodic and cathodic currents, providing useful insight into the currently poorly understood Mg-corrosion reaction.

TRANSFORMING THE ELECTRICITY & AUTOMOTIVE MARKETS WITH THE LBNL VEHICLE-TO-GRID SIMULATOR (V2G-SIM)

Principal Investigator: Samveg Saxena

Project Description

Vehicle-grid integration (VGI) can simultaneously transform the electricity market and the automotive market. For the automotive market, VGI can: 1) allow vehicles to meet all corporate average fuel economy (CAFE) requirements and increasingly stringent emissions regulations, 2) move harmful vehicle emissions away from densely populated areas, and 3) provide revenue to offset the capital cost of vehicle electrification. For the electricity market, VGI can: 4) provide a distributed and growing source of grid energy storage, 5) provide better renewables integration, 6) provide a rapidly ramping resource for many electricity markets, and 7) encourage consumers to more closely scrutinize their home electricity bills just like with gasoline or diesel fuel prices. Despite these benefits, the widespread deployment of VGI faces many uncertainties and barriers within both the electricity market and the automotive market. This LDRD project has created the Vehicle-to-Grid Simulator (V2G-Sim) to provide systematic quantitative methods to develop solutions to the electricity market and automotive market barriers to VGI.

Additionally, as an unexpected breakthrough that was an 'off-shoot' of V2G-Sim, this project led to the creation of MyGreenCar. MyGreenCar is a phone app that provides car buyers with personalized fuel economy (e.g. my own MPG) comparisons for any car they are considering. It also eliminates EV range anxiety for buyers interested in an EV by showing them whether they would even come close to running out of charge on their trips. Essentially, it provides car buyers with a virtual test drive to take the uncertainty out of buying a clean car.

V2G-Sim Accomplishments:

1. V2G-Sim was selected as a 2015 R&D100 award recipient.
2. Finalized a release-ready version of the V2G-Sim code and established process for licensing V2G-Sim to users throughout the R&D community.
3. Published several high impact papers on EVs and vehicle grid integration, including publications that were featured in major international news media
4. Established LBNL as a part of US DOE's multi-lab EV Smart Grid Working Group.
5. Established collaborations with the California multi-agency VGI working group (CPUC, CEC, CARB, CAISO) that was convened by the Governor's Office.
6. Secured major research awards that will continue to build upon V2G-Sim, including $6.5M in primed proposals, and an additional $1.3M through sub-awards on proposals.

MyGreenCar Accomplishments:

1. Developed MyGreenCar and launched to beta users.
2. Created ~5,000 vehicle models, and tested on >30,000 mi of real-world travel.
3. Secured partnership with US EPA to deploy MyGreenCar as the tool for the next generation of fuel economy labeling for all car buyers in the United States.
4. Accepted to the inaugural class of EERE's LabCorps tech-to-market program. Identified product-market fit through >100 customer interviews. Accepted to several prestigious accelerators and offered venture capital funding to commercialize MyGreenCar (however chose to prioritize deployment in partnership with the federal government).
5. Secured $150k of external research awards to continue development of MyGreenCar.

Advanced Combustion Technology for Transportation Refrigeration Units

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

Project Description

The purpose of this two-year project is to develop a cost-effective, low emission, small-scale engine. The engine will dramatically reduce NO_x and particulate matter emissions via a novel mode of combustion, Homogeneous Charge Compression Ignition (HCCI). This new engine can be use for a wide range of applications including an existing market that can make immediate use of this technology once commercialized by an equipment manufacturer. This engine can be used in the installed and portable power generation market with applications such as military deployments, portable cooling, construction, grid resiliency, micro-grid generation, and emergency backup generation. In response to newly implemented California and US national regulations, a known market for this new engine is for Transportation Refrigeration Units (TRUs). TRUs are used on long haul and intercity trucks to provide cooling for perishable cargo.

The foundation for retrofit engine development will be established by studying the combustion principles of engines used in TRUs, measuring baseline emissions from a TRU surrogate engine, and identifying the engineering and scientific advancements needed to develop the retrofit engine. Year one objectives for this project include refurbishing and installing a 10hp diesel engine in a small-scale engine research and development facility. This facility will measure pollutant emissions including NO_x, CO, and particulate matter in addition to engine efficiency, fuel consumption, and power. With these data we will develop a strategy to rapidly develop a proof-of-concept TRU retrofit engine for consideration of TRU manufacturers in the second year of this project.

Accomplishments

The project has resulted in first of its kind small-scale diesel engine pollutant data, most notably particulate mater, which is absent from current literature. Additionally, we confirmed operation of the small-scale engine research and development facility and can facilitate the engine development efforts set out to accomplish in year 2.

We also completed a literature search of diesel engine NO_x and particulate matter emissions. Together with the new engine data we have established benchmarks against which our year 2 development efforts will be measured.

With the aim of having the year 2 engine development efforts fast tracked for commercialization, we established and built relationships with the two US based TRU manufactures which control over 90% of the domestic market, Carrier Transicold and ThermoKing – a UTRC company. Both Carrier Transicold and ThermKing visited our facilities at LBNL and have made promises to supply current state of the art and typical in field TRU engines for us to assess and work with, at no cost, in our year 2 development efforts.

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

We are currently working on four research papers, which are at various stages of completion. Only one project has been completed to the point of publication; 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.

We are currently in the process of completing drafts of three additional projects. The first is entitled "Whipping Load Data Into Shapes: Behavior Insights from Load Shape Clustering in the Context of Program Targeting," and outlines the innovations we've made in developing a methodology for applying clustering analysis to high frequency residential consumption data to isolate meaningful patterns of discretionary energy usage, improving significantly on other work in the literature. The next two projects currently being drafted have been accepted as alternates for the 2016 ACEEE Summer Study on Energy Efficiency in Buildings. The first of these is entitled "This American Life (style Group): Defining and Interpreting Energy Lifestyles Using Smart Meter Data." This works builds off of our work with clustering, and additionally employs C-tree and random forest models to identify drivers of pricing program uptake and response based on sophisticated metrics of energy consumption patterns. The second of these two project being drafted for intended presentation at ACEEE is entitled "Which Households Respond? Exploring Heterogeneity in Response to Experimental Pricing Programs Using Pre-treatment Smart Meter Data." The project uses instrumental variable regression analysis to explore drivers of pricing program response.

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 develop bacterial strains that can convert existing phosphorus sources in the soil to soluble forms available for plant uptake. In this proposal we will use functional genomics approaches to identify novel genes and pathways underlying the abilities of some soil bacteria to solubilize phosphate, and use synthetic biology approaches to demonstrate the stable transfer of these genes and functions to a novel plant associated bacterial host. We will first utilize available transposon mutant populations of phosphate-solubilizing bacteria with diverse substrate specificities, and use growth on limiting phosphate sources to identify novel genes required for phosphate solubilization. We will then take these novel sequences, along with candidate phosphate solubilizing genes from the literature, and refactor them *in silico* for optimal expression in *Pseudomonas.* We will synthesize the refactored genes, and integrate them into the genome of a known plant-root associating *Pseudomonas* strain. We will use growth assays to validate novel phosphate solubilization capabilities of these strains in liquid culture. Finally, we will test the engineered phosphate solubilizing strains for their ability to colonize and promote growth of the model biofuel plant *Brachypodium distachyon*.

Accomplishments

We identified four bacterial strains capable of solubilizing inorganic and organic phosphate sources, and with available transposon mutant libraries. We applied two approaches to screen these transposon mutant populations for mutants that have lost the ability to solubilize phosphorus, and recovered a gene previously shown to be important in P-solubilization, along with a small number of candidate novel P-solubilizing genes. We have developed a culture assay for quantification of P-solubilization by these strains. We will synthesize these genes for overexpression in the bacterium *Pseudomonas fluorescens.*

In parallel, we computationally identified 100 phylogenetically diverse phytase genes. These enzymes liberate phosphorous from phytic acid, the most abundant organic source of phosphorus in soil. Sequences were refactored for optimal expression in *P. fluorescens* and synthesized by the JGI DNA synthesis group. Sixteen genes have now been cloned in *E. coli* and will be transferred to *P. fluorescens* in the coming year.

In preparation for generating new phosphate solubilizing strains, we have we obtained a modified strain of *P. fluorescens* from the Yoshikuni lab (JGI) with a genomic landing pad for genomic integration and overexpression of candidate genes. In preparation for testing the impact of these strains on plants, we demonstrated that *P. fluorescens* is able to colonize the plants *Arabidopsis* and *Brachypodium.*

Modification of the Genetic Code to Construct a Safe Industrial Microbe for Synthetic Biology
Principal Investigator(s): Jan-Fang Cheng

Project Description

This project aims to develop a universal genome editing tool to facilitate the engineering of novel applications not only in *E. coli*, but in underexploited industrial producers such as *Streptomyces coelicolor* and *Corynebacterium glutamicum.* Following our initial demonstration of genome editing in *E. coli*, Cas9-based genome editing has been reported in a number of bacteria including *Lactobacillus reuteri*, *Tatumella citrea*, several *Streptomyces* species, and two *Clostridium* species. It has become apparent that high rates of transformation and recombination dictate the success or failure of the genome editing in a particular bacteria. Without high rates of transformation and recombination, the background mutation rate of the crisprRNA and Cas9 would account for most of the surviving transformants. We have been developing a universal approach to efficiently deliver all components of the Cas9 editing machinery into a wide range of bacterial hosts. Coupling with a tightly controlled inducible system to turn on the crisprRNA and Cas9 at the right time, we may be able to alleviate the transformation barrier.

One recent finding of using the mutated Cas9 protein that nicks the target without creating a double-stranded break (DSB) may circumvent the challenge of searching for a universal recombination system to drive high rates of homologous recombination in most bacteria. It was shown that the nicking Cas9 improves genome editing efficiencies to up to 95% in *Clostridium cellulolyticum* by reducing the lethality of targeting, whereas the wild-type Cas9 produces no colonies. Although the mechanism of repair/editing after nicking is not fully understood, it provides an example that in the absence of recombineering genes, creating targeted DNA nicks may be sufficient to drive intrinsic DNA repair/editing in bacteria that are poorly equipped to repair DSB.

Accomplishments

Our most significant accomplishment has been to develop a wide host range toolset and protocol to allow efficient delivery of large pathway size DNA from *E. coli* to many bacterial hosts. This work was performed in collaboration with Dr. Yasuo Yoshikuni's group. Our method utilizes transposon to mobilize and insert a Cre-LoxP cassette into the targeted host genome. With this cassette we can efficiently introduce all components of the Cas9 editing machinery into a wide range of bacteria. We are hopeful that this method will be generally applicable to non-*E. coli* hosts, which will greatly aid our future goal of modifying genetic codes of industrial microbes.

We have also succeeded in developing a designer yeast strain for isoprenoid production using the CRISPR-Cas9 editing tool. In a couple of month time we have scarlessly replaced all the promoters for the genes involved in the mevalonate pathway (also known as the isoprenoid biosynthesis pathway) to a strong constitutive promoter in an industrial host, Sacchromyces cerevisiae CEN.PK2-1c. This designer yeast will be used for several demonstration projects including the Terpenoid Atlas project and the Energy Flux Rewiring for Efficient Biofuel Production project at JGI.

As we had predicted, this approach provides a significantly faster turnaround time to modify genetic codes than any available tools. We will continue to improve this approach so that it can be applied to many other bacteria or yeast hosts.

Sequencing-Based Functional Genomic *in vivo* Characterization of Plant Promoters

Principal Investigator: Axel Visel

Project Description

Plants are photoautotrophic systems that convert sunlight into biochemical energy and represent attractive targets for precision engineering of traits desired for bioenergy and bioindustrial purposes. Significant progress has been made in understanding transcriptomic responses of plants to abiotic (e.g. drought) or biotic (e.g. colonization by plant-associated microbes) stimuli, but there is a lack of similarly deep knowledge of the regulatory sequences driving these responses.

We proposed the development of scalable screening methods to enable the interrogation of a large number of endogenous plant promoters using high-throughput sequencing. Our aims included the establishment of methods for high-throughput transformation of plant promoters driving expression of randomly barcoded transcripts in the model plant, *Arabidopsis thaliana*. These methods could be coupled with a multi-tissue pooling strategy involving thousands of independent transformants harboring many distinct promoter elements. In DNA and RNA extracted from each pool, the abundance of each barcoded transcript could be quantified based on RNA-seq data and normalized to each barcode's abundance determined from PCR-amplified genomic DNA.

Eventual application of this method at full scale is expected to enable a quantitative and tissue-specific readout of promoter activity across large numbers of promoters. The experimental design facilitates multiple independent tests of promoters in a single experiment. In contrast to lower-throughput, reporter-based methods for *Arabidopsis* promoter characterization, the proposed approach has significant scaling potential for generation of a curated promoter collection for plant engineering. In addition to enabling plant promoter studies, the proposal is expected to establish methods, capabilities, and expertise for experimental plant studies that will inspire and accelerate additional mission-critical areas of the DOE Joint Genome Institute (JGI), including plant-microbe interactions.

Accomplishments

We successfully implemented a medium-scale cultivation system for *Arabidopsis thaliana* plants for both soil-based and sterile experimental studies. For *in vitro* work, we also established an environmentally controlled growth chamber for growing seedlings on agar plates. To enable promoter screens, we obtained optimized vectors for *Agrobacterium tumefaciens*-mediated transformation of *Arabidopsis* plants, suitable for Gateway-compatible cloning and expression in plant hosts. These vectors were modified to accept a randomly barcoded YFP protein via Gateway cloning. We also successfully performed *Agrobacterium*-mediated transformation of this vector system into *Arabidopsis*, establishing plant-based capabilities for screens of cloned and synthetic promoters at the JGI.

In alignment with the strategic directions of the JGI toward the areas of plant functional genomics and plant-microbe interactions, we also leveraged the infrastructure and capabilities established through this project for co-cultivation of *Arabidopsis* with select microorganisms. In particular, we implemented a barcoding-based strategy similar to the one proposed for promoter studies to perform genome-wide functional assays to identify and characterize microbial genes necessary for plant association in root-colonizing microbes. These capabilities are currently wielded as part of a continued JGI project to perform larger-scale screens aimed at better understanding of the poorly annotated genomes of beneficial plant-associated microorganisms.

Developing Epigenomic Technologies to Interrogate Genome Functions Relevant for Environment and Bioenergy
Principle Investigator: Chia-Lin Wei

PROJECT DESCRIPTION

To aid the understanding of the genetic components crucial for the biofuel biosynthesis and carbon cycling, we proposed to develop an array of whole genome sequencing based epigenomic technologies to systematic interrogate the functional elements from the genomes important for JGI's science and DOE mission. These approaches include ChIP-Seq mapping of core histone modifications and variants, Methyl-Seq mapping of DNA methylation, FAIRE (formaldehyde assisted isolation of regulatory elements) mapping chromatin accessibility and ChIA-PET (chromatin interaction analysis through pair-end ditag) mapping of three dimensional (3D) chromatin architectures. The proposed plan also includes setting up data processing pipeline to provide users with the data and tools ready for biological interpretation and validation.

Accomplishments

We have successfully applied the epigenetic approaches to characterize the chromatin signatures associated with lipid production in green algae and identified lipid master regulators. The results were summarized and published in the high profiled journal ***Nature Plants*, 1: 15107 (2015)**. Epigenetic technologies developed under this LDRD funding support were further expanded in Brachypodium and Sorghum grass species to study drought responses and tissue specific gene expression regulation. A manuscript entitled "*DNA Methylation and Gene Expression Regulation Associated with Vascularization in Sorghum bicolor*" describing the methylation patterns and their association with tissue specific expression in Sorghum was submitted and reviewed in ***Plant Physiology***. Within this project scope, we pioneered the detection of a novel DNA modification mark 6methyl-adenine using the single molecule sequencing PacBio platform across multiple developmental lineages. The results were summarized and submitted to ***Nature*** for in-depth review. Lastly, the results and knowledge gained from this LDRD funding have resulted into two successful projects funded under DOE and NIH. Under DOE Funding Opportunity Number: DE-FOA-0001207 Systems Biology Research to Advance Sustainable Bioenergy Crop Development, A 5-year multi-PI proposal "Epigenetic Control of Drought Response in Sorghum (EPICON)" was awarded for total ~ $12 million (JGI was awarded for close to ~ $2 million). Applying the microfluidics based ChIA-PET analysis; a proposal for "High-resolution and haplotype-specific mapping technology of 3D genome organization" was awarded by NIH 4D nucleomics program https://commonfund.nih.gov/4dnucleome/overview for total of $ 311,229.

Tackling Microbial-Mediated Plant Carbon Decomposition using 'Function-Driven' Genomics

Principal Investigator(s): Tanja, Woyke; Natalia, Ivanova; Steven, Singer

Project Description

The principle goal of this proposed research is to advance our understanding of the role of microbial communities in carbon (C) cycling by developing a "function-driven" genomics approach. This approach will allow us to experimentally capture, prior to sequencing, particular microorganisms that catalyze a function of interest. Specifically, we will develop a pipeline for single-cell and mini-metagenome sequencing of uncultivated organisms involved in the decomposition of cellulose and apply it to the complex soil and rhizosphere ecosystem.

Hypothesizing that distinct soil taxa specialize in the decomposition of specific plant C substrates, we will apply novel approaches to experimentally capture bacteria that degrade plant-derived cellulose for sequence-based characterization. We will couple the use of fluorescently labeled substrates with single-cell sorting to obtain (i) substrate-enriched soil microbiomes for marker gene profiling and shotgun metagenomics and (ii) single-cell genomics. The approach will be developed and tested in the laboratory setting using cultivated bacterial isolates, then adopted for environmental samples and finally applied to study plant C decomposition in native grassland soil and rhizosphere.

Accomplishments

We selected microcrystalline cellulose as our first substrate for developing the substrate-based single-cell genomics isolation method. Multiple fluorophore labeling protocols were tested to determine the optimum procedure for creating labeled cellulose with a unique fluorescent signature that enabled conclusive identification of the substrate population by flow cytometry, while still maintaining native substrate binding properties to cellulolytic organisms. Binding of the labeled cellulose was tested with pure cultures of both cellulolytic and non-cellulolytic model organisms under aerobic and anaerobic conditions. All experiments and controls performed validate that the native interactions between the substrate and viable cellulolytic organisms are maintained and that no artificial binding events occur between the modified substrate and non-cellulolytic, or heat inactivated cellulolytic organisms.

Increasing mock community complexity beyond pure and binary cultures, we have created a defined synthetic community consisting of 7 bacterial members for use in quantifying the substrate-based approach for its ability to enrich our model cellulolytic organism. Ongoing results indicate that using the flow cytometer to isolate labeled cellulose bound by bacteria can enrich our target cellulolytic organism from an initial relative abundance of <1% to a final abundance ≥80%. Following sorting, cells isolated via the fluorescent substrate method are compatible with all high throughput downstream processes including the multiple displacement amplification required for single-cell genomics. In addition, unbound particles of labeled cellulose sorted from the culture do not carry non-specific free DNA and thus we expect a high degree of purity for recovered genomes. Currently we are using the optimized method to isolate cellulose-degrading organisms from characterized enrichment cultures that provide an increased level of community complexity similar to those environments we hope to ultimately use this method for recovery of novel cellulose degraders.

Development of a Cas9 Based Resource for Genome Engineering

Principal Investigator(s): Yiwen Zhu, Jennifer Doudna, Len Pennacchio

Project Description

Prior to the discovery of the CRISPR/Cas9 technology, precise genome editing of model organisms used in research was impractical or impossible. The simplicity of the CRISPR/Cas9 system offers the possibility of a universally applicable genome editing technology, and, indeed, it has been successfully used for genome modification in a variety of organisms. However, there remain some limitations to its use, and its use has not been previously demonstrated in many of the research organisms used at Lawrence Berkeley National Laboratory. The goals of this project are to establish the CRISPR/Cas9 editing technology at LBNL and to develop CRISPR/Cas9-based tools that can be used for genome editing in a wider variety of prokaryotic and eukaryotic organisms. Additionally, we aim to identify and characterize Cas9 proteins from a diversity of bacterial species in an effort to overcome the current limitations of the technology, namely the genome sequence specificity requirements and the difficulty in delivering the large *S.pyogenes* Cas9 protein to many cell types.

Accomplishments

Our most significant accomplishment has been in using Cas9 to make precise mutations in the mouse genome. In our hands, Cas9 can be used to delete, alter, or replace mouse loci with high efficiency. We now routinely use this technology to alter noncoding regulatory sequences in mice and mouse cell lines to assess their role in development and disease. Using preliminary data produced as part of this LDRD, we have succeeded in obtaining follow-on funding from the National Institute of Health to continue these efforts, including a $2.8M grant already awarded. We are also currently applying for funding of approximately $5.4M from the NIH's ENCODE program to continue to apply these CRISPR/Cas9 editing techniques to further understand the function of the mammalian genome. Additionally, we have successfully used Cas9 to modify the *E.coli* genome and have performed this as a user service to researchers at the Joint BioEnergy Institute. Cas9 editing was tested in algae and other bacterial species.

To address some of the current limitations of Cas9 editing, we have mined microbial and metagenomic sequence databases and identified hundreds of unique Cas9 sequences present in a phylogenetically diverse sample of bacterial organisms. Future efforts to identify Cas9 proteins that have different target specificities from that of *S.pyogenes* will rely on computational mining of CRISPR spacer sequences against a newly created viral DNA sequence database developed by the DOE-JGI.

Neuro/Nano Technoogy 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

To dramatically increase the channel count of electrical recordings, we have fabricated and are now testing a very high density (10,000 electrode/cm^2 x many cm^2) 2D electrocorticography neural amplification and data acquisition system. We will be performing in vivo experiments with this device in the coming months. 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, (b) developed a scalable algorithm for statistical inference of model parameters from data that gives more accurate and interpretable results than the state-of-the-art algorithms in machine learning, and applied it to neuroscience data, (c) applied deep neural networks to 'classify' produced speech from human electrocorticography data, achieving state-of-the-art results, (d) utilized FPGA's to process the neural data collected by the high density system in real-time, and capitalized upon a data visualization application to permit on-line examination of brain activity. Current efforts are focused on HPC implementations of data analysis methods on NERSC, and scaling–up the real-time processing capacity/interfacing with the high density system.

As optical probes, we have expanded our family of fluorescent probes for sodium developed in FY14 with a new palette of sensors that are selectively responsive to potassium. The reagents match well with standard microscopy laser lines and filter sets and poise us to monitor uptake and efflux of the central ions involved in neurotransmission. We have also paired these with upconverting nanocrystals (UCNPs), which absorb in the near infrared (NIR) and emit in the visible to excite the ion sensors. We have synthesized a series of UCNPs with increased efficiency in activating the fluorescent sodium sensors; for sensor targeting, we have developed methodology for the controlled covalent attachment of nanocrystals to antibodies. Current efforts are geared toward imaging these nanocrystal-sensor conjugates in neurons, controlling cellular localization to membranes, vesicles, and synapses to monitor neural activity as well as developing analogous tools to detect potassium.

Further, we have demonstrated the efficacy of NIR-emitting UCNPs for deep brain optical imaging and optogenetic stimulation. In a proof of concept imaging experiment, we have used NIR light to excite and image patterned UCNPs through a 2-nm-thick slice of wild-type mouse brain. When the slice was pumped with 980 nm light, we were able to spectrally image the newly-designed UCNP emission through tissue, with a strong enough signal to imply that imaging through cms of tissue should be straight-forward (assuming well-known rates of absorption and attenuation). A next step will be to not only image and stimulate at greater tissue depths, but to employ acoustic wave patterns (currently being developed by Maharbiz et al) for steering the excitation light to specific regions of the tissue.

HIGH-PERFORMANCE CHEMICAL ID.
FOR HYPERSPECTRAL DATA SCIENCE

Principal Investigator(s): (Benjamin P. Bowen)

Project Description

The aim of our OpenMSI research program is to develop open tools for the integration and scientific analysis of very large multi-modal hyperspectral datasets. This LDRD in particular is focused on providing chemical tools for transforming raw mass spectrum images into chemically informative images of identified molecules and molecule classes in analyzed samples. Our approach is to apply probabilistic propagation of molecular identifications across datasets. This research will lead towards establishing OpenMSI as a new science resource, centered at LBNL and used by thousands of researchers around the world. If we succeed, we will establish LBNL as a leader in mass spectral imaging, and will make future extreme data science research and development projects in multimodal hyperspectral imaging achievable. In this project period, we've collaborated with the Lewis Lab (WSU), Northen Lab (LBL) and the MANTISSA project (LBL) to both obtain new, cutting-edge datasets with the most advanced instrumentation and also to develop new computational strategies for analysis.

Accomplishments

To facilitate identification of compounds imaged using MSI, we have developed Pactolus. Pactolus includes high-performance methods to compute all possible fragmentation paths a molecule can follow. Calculation of these fragmentation trees would not be possible without NERSC's supercomputing capabilities. To date we have generated fragmentation trees for >11,000 compounds. Due to the high cost for computing these trees, the resulting fragmentation tree data by itself will be an invaluable resource for the scientific community. Based on these trees, we have developed methods in Pactolus to identify new molecules from raw experimental data. Using this approach will enable OpenMSI users for the first time to search large databases of chemical compounds using large collections of measured fragmentation spectra to rank and identify chemical compounds --- think large-scale Google search for chemical compounds via real, measured data.

To integrate these methods with OpenMSI and to fulfill the promise of a scalable ecosystem for multi-modal mass spectrometry imaging data, we have extended and are in the process of releasing the Berkeley Analysis and Storage Toolkit (BASTet). BASTet standardizes the interfaces that OpenMSI uses for analyses and data and supports: i) integrated data storage for raw and derived data, ii) automatic provenance for reproducible analyses, iii) workflow management and supports iv) the evolution of analysis software from initial development to deployment. Using BASTet enables the direct integration of Pactolus with OpenMSI, enabling the generation and search of Pactolus trees using high-performance computing. We also extended BASTet to support MS/MS data, cleaning the data, detection of peaks, generation of fragmentation trees, searching and comparison of spectra with trees, and statistical analysis of scores across spectra. We have extended BASTet to support such advanced analysis workflows in an easy-to-use, scriptable fashion and extended the capabilities of BASTet to track and record the provenance of analysis workflows. Using BASTet enables us to manage complex analysis workflows, empowers users to reuse, share and interpret the generated derived data products and analysis results.

Project Title:
REINVENTING PRE-CLINICAL 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 approaches 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 paths 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: We have applied for follow-on NIH funding via the R01 mechanism. We have a manuscript in submission to PNAS reporting the development of the algorithm and it's utilities. We have applied our method to large GWAS cohorts in human and mouse. We have discovered epistatic interactions, including non-additive interactions between host genotype and the community architecture of the commensal microbiome. Progress on this aim is very good.

Aim 2: We have a distributable software package for Introspective Learning Machines implementing iterative Random Forests (iRF) and "Unconstrained Surface Mapping" (USM). 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. Our approach uses an ensemble technique to conduct density or response surface estimation in high dimension given finite data. Our algorithm can detect interactions between covariates of high order at the same computational cost as pairwise interactions – making it tractable, for the first time, to discover complex, non-linear structure in extreme-scale datasets. We are now working to combine our algorithm with boosting to generate a class of learning machine that will simultaneously map structure in data and identify and model heterogeneity.

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. We will measure long-term physiological effects and identify interactions between the content of microbiome and organ structure, metabolism, and behavior. 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*. We will make detailed, quantitative measurements of microbiome community structure using genomic techniques. 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 changes in behavior with changes in the microbiome, induced by a variety of pesticides commonly used in California agriculture, while controlling for genetic background. We will also have set up the necessary equipment and environment for future high throughput testing. 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

Our most significant accomplishment has been the isolation and complete genomic sequencing of the bacterial phyla that inhabit the fly gut and determining the microbial and host responses to the herbicides, paraquat and atrazine. We've found that paraquat and to a lesser extent atrazine specifically target *Acteobacter* a genus of acetic acid bacteria characterized by the ability to convert ethanol to acetic acid in the presence of oxygen. These studies were presented at a Symposium of the Genetic and Environmental Toxicology Association of Northern California (GETA) on Nov 17, 2015. We are now testing the affects of additional herbicides on the fly microbiome. We are also in the process of determining the affects of herbicides on isolated microbial species and characterizing changes in metabolites and transcriptional profiling throughout the growth cycle. In addition, we have succeeded in establishing a gnotobiotic facility for the mammalian experiments and published our first studies of genetics and behavior.

4D DYNAMICS OF EPIGENOME REGULATION IN RESPONSE TO ENVIRONMENTAL CHALLENGES

Principal Investigator: Serafin Colmenares

Project Description

The goal of this project is to generate a comprehensive, integrated understanding of how common environmental challenges impact 4D dynamics of epigenome regulation, as well as the persistence of these changes across cellular and organismal generations. We will focus on the fruitfly *Drosophila melanogaster*, a powerful model system that allows us to elucidate components and mechanisms in cultured cells, tissues and organisms. Ultimately, we will use these tools and approaches to investigate how environmental epigenomics impacts human health. We will identify changes in chromatin dynamics and epigenetic modifications induced by three environmental factors known to negatively impact biological systems and human health: radiation, hyperthermia, and bisphenol A (BPA). Radiation triggers extensive chromatin reorganization important for DNA repair, including global heterochromatin expansion and relocalization of damaged sites to the euchromatic space. Hyperthermia simultaneously reduces global transcription, mobilizes heterochromatin proteins, and induces trans-generational transcriptional deregulation in Drosophila. Finally, the estrogen mimic BPA, a common component of plastics, is implicated in birth defects, cancer, and the induction of the H3K27 methyltransferase Enhancer of Zeste (EZH2) which is critical for Polycomb group (PcG)-mediated gene silencing, developmental patterning, and trans-chromosomal interactions. Through this project, we plan to generate a more comprehensive and detailed understanding of the spectrum of epigenetic changes in response to these environmental challenges, and their impact on cells and organisms. Successful completion of this study will provide 'proof of principle' of our ability to comprehensively analyze the interplay between the environment, the epigenome, and fundamental cell and organismal functions.

Accomplishments

We have successfully developed a high-quality ChIPSeq library protocol and ChIPSeq data analysis pipeline to pursue the goals of this project. We have determined that acute ionizing radiation does not perturb global distributions of 4 general histone modifications from Kc cells, suggesting that "readers" of such histone marks are likely responsible for spatiotemporal regulation of chromatin domains in response to DNA damage. We have identified KDM4A as a novel heterochromatin component and regulator of heterochromatic DNA repair, which has been recently submitted for publication. We have also discovered that BPA induces hypermethylation of H3K27me3 in Kc cells but only at endogenous and not ectopic sites. We also discovered higher BPA-induced lethality in female but not male flies, suggesting sex-specific Polycomb-regulated developmental events are targeted by BPA. We have also shown immediate and delayed chromatin changes in fly cells after heat shock, including loss of histone H2A ubiquitination (H2A-Ub) and HP1a spreading into euchromatin. ChIPSeq analyses of H2A-Ub indicate heat shock-induced loss of this modification from PcG target sites but also the formation of new H2A-Ub in other regions. We also detected the gradual return of HP1a cytological localization to heterochromatin and restoration of normal H2A-Ub peaks upon return to physiological temperature. These results highlight the sensitivity of epigenetic machinery to environmental stress but also its robustness in restoration of normal function. Based on these results and others, we expect to publish several interesting stories highlighting the impact of environmental factors on chromatin in the near future, and pursue a NIH grant to further elucidate the mechanisms of environmental epigenetics.

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

Thus far we have made tremendous progress on the goals of our proposal. We have developed detailed designs for increasing the throughput of small angle X-ray scattering (SAXS). We estimate that our new designs will increase our current throughput by a factor of eight or better. Also we will reduce sample size down by a factor of 6. These features will allow for more comprehensive measurements to elucidate the structure of biomolecules in many contexts.

Our design relies heavily on procuring a new liquid handler. Through our LDRD funding we have identified an off-the-shelf system that should serve well. While our LDRD is not sufficiently funded to purchase this system, we have sent proposals to DOE and NIH for this purpose. Since we have identified the liquid handling system and funding looks promising, we have begun to reengineer our beamline to accommodate the new system and integrate its control with other beamline equipment. The increased throughput means 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. Until we have procured the sample handler will test our engineered control systems with the handler we have now.

We have also made tremendous progress in our bioengineering efforts. Two papers are in various stages of publication. The first will be available on December 18th in the journal *Nature*. The publication is titled “Exploring the repeat protein universe through computational protein design”. This collaboration with the Baker laboratory (University of Washington) utilized SAXS to validate 60 computationally designed peptides. The second publication has been submitted to the journal *Science Advances* and is titled “Designing and defining dynamic protein cage nanoassemblies in solution”. In this collaboration we test two designed 600kDa macromolecular complexes and comprehensively asses their structure in a variety of solution conditions. The publication of these two high profile papers places us in good position to request follow-on funding and makes a strong case for our proposals at ALS-U.

A Graphene-Based Platform for Correlative Electron and Super-Resolution Microscopy

Principal Investigator(s): Ke Xu

Project Description

The purpose of this project is to develop a graphene-encapsulation method to enable correlated electron microscopy and super-resolution microscopy of wet cells. Graphene is a two-dimensional material that is just a single layer of bonded carbon atoms. Here we employed graphene as the thinnest possible membrane to encase wet and live cells to allow for electron microscopy of wet samples without the common dehydration requirement of sample preparation. Our design takes full advantages of the unique properties of graphene: while being transparent to both light and electrons, graphene is chemically inert, mechanically strong yet flexible, and impermeable to small molecules. In addition, graphene is an excellent electrical and thermal conductor and so is helpful in minimizing charging and heating effects under electron beams.

High-vacuum operating conditions have fundamentally limited how biological samples can be studied with electron microscopy. Laborious dehydration and embedding procedures are required, which, besides being time-consuming and costly, often lead to structural artifacts. The methods involved also create notable difficulties for correlating results with high-resolution fluorescence microscopy. Our approach achieved facile electron microscopy of wet/live cells with minimal sample preparation, and further enabled facile correlation with super-resolution fluorescence microscopy on the same platform, thus revolutionizing, at a fundamental level, how biosamples can be studied at the nanoscale in their native, fully hydrated state.

Accomplishments

We have shown that graphene can encapsulate and thus protect wet and live mammalian cells from external environments, including liquid and vacuum environments. We then demonstrated that this graphene encapsulation can allow for direct electron microscopy of wet and live cell samples in conventional electron microscopes operated under high vacuum. We found that the graphene encapsulation enabled electron microscopy with excellent resolution and contrast at low accelerating voltages, which can be attributed to the extreme thinness and excellent conductivity of graphene. In contrast, cell samples not protected by graphene were significantly distorted in structure when exposed to vacuum.

We have also realized correlated super-resolution microscopy and electron microscopy imaging on our graphene-based platform. Comparison of the images obtained from the two modes showed excellent correlation/agreement with each other, showing that the graphene protection has been highly effective in protecting cells and preserving the detailed subcellular structures at the nanometer scale in the vacuum environment of electron microscope. We have demonstrated such capabilities for multiple subcellular structures, including cytoskeletal filaments, cell membranes, and mitochondria, in both stained and untreated cells. The capabilities to readily achieve correlated super-resolution microscopy and electron microscopy of wet cells enabled us to utilize the complimentary advantages of the two image modules.

Our results are recently published in *Nature Communications* (below), which, due to their importance and novelty, were highlighted by *Nature* (*Nature* **552**, 394).

SEARCH AND SYNTHESIS FOR THE NEXT GENERATION OF QUANTUM MATTER
PRINCIPAL INVESTIGATOR: JAMES ANALYTIS

Project Description

The purpose of this project is to create new materials manifesting exotic quantum phenomena. This includes Dirac and topological systems, quantum critical materials, unconventional superconductors and quantum magnets. The strategy is to identify specific material properties that are connected to chemical building blocks, and use this identification to drive new materials. This project is therefore based on *both* state-of-the-art measurements of materials as well as synthesis. A good example is iridium-based compounds. In this case the property we identify is the combination of strong spin-orbit coupling and symmetry leads to strongly spin-anisotropic magnetic exchange. Since beginning this project in 2013, we have extended this strategy to develop a deeper understanding of high temperature superconductivity, new routes to quantum spin liquids and quasi-one dimensional superconductors.

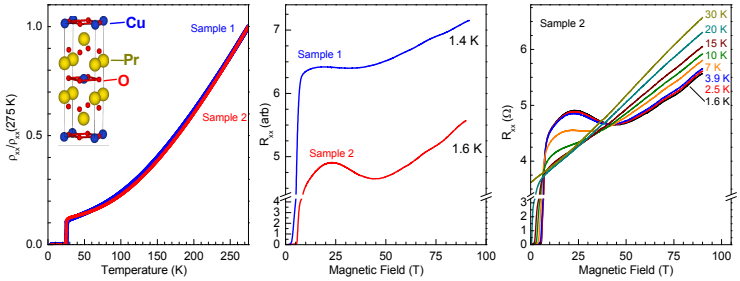


Figure 1; Resistivity and magnetotransport data of Pr_2CuO_4. First panel: resistivity ρ_{xx} versus temperature for two PCO samples. Inset: tetragonal unit cell of Pr_2CuO_4. Second panel: magnetoresistance measured to 90 T for both samples near 1.5 K; note the break in axis scale. Third panel: suppression with temperature of both quantum oscillations, and a region of increased resistance at fields between 5 and 40 T.

Accomplishments

1. **Discovery of a new 3D-honeycomb quantum magnet.** We discovered a new material is very close to a new, theoretically predicted, state of matter known as a quantum spin liquid. Our system is magnetically ordered, but with strongly anisotropic magnetic properties.
2. **Discovery of new field induced magnetic order in Li_2IrO_3.** We have discovered a new field-induced magnetic order that points to a universal microscopic description of 2D and 3D Mott-Kitaev honeycomb materials.
3. **Discovery of new scaling laws in high temperature superconductors.** We recently discovered a new scaling law in the transport of an iron-based superconductor, between the magneto-resistance and the temperature-dependent resistance (Figure 1). This scaling betrays a novel physical mechanism that suggests that B and T are simple different kinds of energy.
4. **Discovery of quantum oscillations in a quasi-1D superconductor.** We synthesize a new material that is *thought* to be a quasi-one-dimensional superconductor, $Ta_4Pd_3Te_{16}$. By measuring our samples in high magnetic fields, we discovered quantum oscillatory effects that unambiguously show that these materials are *two-dimensional.*
5. **Discovery of a new commensurate to incommensurate phase transition in a quasi-one dimensional superconductor.** In addition to our quantum oscillatory work on $Ta_4Pd_3Te_{16}$, we have also found a new phase transition which suggests that this materials is already in charge density wave ordered state before it becomes superconducting.
6. **Discovery of magnetic breakdown effects in high-T_c supercondcutors.** We recently discovered that in high magnetic fields quasiparticles tunnel through Fermi surface hot spots.
7. **First Quantum Oscillations in thin film cuprates.** By utilizing high magnetic fields and ultra-high quality thin films we have observed the *first* quantum oscillations in Pr_2CuO_4, the archetypical cuprate superconductor. We also discovered a new kind of quantum critical point.

Optical and Electrical Characterization of 2-Dimensional Nanosheets without Naturally Layered Structure

Principal Investigator(s): Jie Yao

Project Description

The purpose of this project is to fabricate and characterize ultrathin sheets of layered ZnO, including a unique BN-like phase. ZnO will be transformed into a layered, BN-like structure when it is thinned down to below approximately 1 nm. Currently, ultrathin BN-like ZnO has only been fabricated on metal substrates, or in extremely small (~3 nm) suspended membranes using highly specialized growth procedures. The current method we propose would drastically simplify the growth process and allow the ZnO to be large scale and free standing. This method also allows for easy alloying and doping of ZnO, primarily with aluminum, in order to tune the properties of these ultrathin plates. This phase of ZnO has been theorized to have many unique properties in its monolayer and bilayer forms, and will make another great addition to the exciting and growing field of 2D materials.

We grow the materials using an alternative method from a previously reported technique. Samples are deposited on top of Si/SiO_2 wafers for electrical, photoluminescence, and thickness measurements, and on top of holey SiN membranes for TEM analysis. For electrical measurements, electrodes will be patterned using electron beam lithography (EBL) followed by Cr/Au electrode electron beam deposition and measured using a typical probe station. Photoluminescence will be performed using a home built setup using a 266 nm femtosecond laser. Thickness measurements will be performed using a Veeco Dimensions 3100 AFM. TEM analysis will be performed through NCEM at LBNL in order to verify the correct crystalline structure and, for doping, in order to determine the homogeneity of the doping species. These characterizations should verify the unique properties of the ultrathin layered ZnO theoretically predicted by many papers, including a direct-indirect-direct bandgap transition.

Accomplishments

Our most important accomplishment is the successful synthesis and chemical identification of ZnO for approximately 1-2 nm thick samples, verified using EDX and AFM, that range from 5 to 50 micron in size. Samples have also been created that are below 1 nm, although the chemical identify has not been verified due to the difficulty in measuring such ultrathin species accurately. The method is relatively consistent, which allows us to carry forward with optimization and characterization.

We have also confirmed that both ZnO and aluminum doped ZnO (AZO) exhibit insulating behavior. Even after vacuum annealing processes that normally create conducting ZnO, the samples show a negligible conductance. This is consistent across thicknesses ranging from 1 nm to 10 nm. Further gating experiments will help determine if the insulating behavior is error in fabrication or a true property of the ZnO.

We have also succeeded in fabricating ZnO nanoplates on top of holey SiN TEM grids and have performed initial imaging that show that the ZnO is amorphous, or weakly crystalline. The amorphous behavior may be due to the growth method, as it is prone to forming nanocrystals with poor crystallinity. We are currently investigating high temperature annealing as a way to improve the crystalline quality. In addition, initial EDX measurements on AZO samples show the successful homogeneous incorporation of aluminum in ZnO. This proves that the technique for fabricating ZnO can be used for alloys and doping with consistent compositions.

Artificial Carboxysomes for CO2 Capture and Conversion

Principal Investigator: Raffaella Buonsanti

Project Description

This project explores a new paradigm in CO2 conversion which includes the sequestration of CO2 and its conversion into value-added chemicals in a single object. As the predicted use of fossil fuels continues to grow, different efforts have been pursued to reduce CO2 emissions. In this scenario, carbon capture and carbon-to-fuel conversion are playing major roles. Currently, in electrochemical conversion of CO2, Cu is the only catalyst with the propensity to form hydrocarbons, the most energy dense products of CO2 reduction. Improvement in the reaction selectivity and lowering of the electrochemical potential needed to drive CO2 conversion are still needed to enable sustainable CO2 utilization even for the Cu system. Nature combines carbon capture and conversion in single objects known as Carboxysomes, which are bacterial microcompartments constituted by a protein shell that concentrate CO2 to overcome the catalytic inefficiencies of RuBisCo, an enzyme involved in carbon fixation. This LDRD explores a similar paradigm in artificial systems comprising Cu-based CO2 conversion catalysts and CO2 sorbents intimately bound in a single integrated system.

We will develop robust synthetic approaches to synthesize "artificial carboxysomes" which include Cu nanocrystals (NCs) and metal-organic frameworks (MOFs). We will understand the parameters controlling the nucleation and growth of these hybrid systems, so to achieve an unprecedented level of control. Tunability is crucial to establish meaningful structure/properties relations. After establishing the synthesis method, we will characterize the CO2 adsorption properties and study their ability to convert CO2 into value-added chemicals. Specifically, it would be desirable to increase the Cu selectivity towards higher hydrocarbons and alcohols. The ultimate goal of this proposal is to elucidate the effect of CO2 concentration on catalyst efficiency and, to understand how possible changes of the CO2 molecule configuration affect product selectivity and activation energy of CO2 on Cu electrocatalyst.

Accomplishments

Our most significant accomplishment has been to develop a synthetic approach to construct Cu@Cu-MOF core@shell hybrids. Through our study, we have identified the key reaction parameters to obtain hybrids with uniform morphology and homogeneous spatial distribution of the NCs within the framework materials.

We have also succeeded in positively confirming the ability of the hybrids to adsorb CO2. We are now learning how to integrate them into electrodes and we will test their electrocatalytic properties for CO2 conversion.

In the mean time, we have synthesized Cu NCs of different size and shape and study their behavior as electrocatalysts for CO2 conversion in a custom-build flow cell. These experiments will serve as blank to compare the activity of the same NCs when embedded in the framework.

Hard X-Ray Photoemission for Materials Science

Principal Investigator: Charles S. Fadley

Project Description

The goal of this project 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. Together with this 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 than has been possible previously. 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 is reviewed in publication [7], and a major conference will be held at LBNL in 2017.

Accomplishments

We have further improved the unique facility that has been established for HXPS at Beamline 9.3.1 of the ALS, which is currently an Approved Program with 10% of the beamtime over 2014-2017, with full details concerning this system at: http://www.physics.ucdavis.edu/fadleygroup/Hard.Xray.Photoemission.at.the.ALS.pdf .

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 Himpsel (UW Madison), we used HXPS, together with x-ray absorption spectroscopy, to make very accurate measurements of the band offset at the interface between copper indium gallium selenide (CIGS) and doped diamond, as a promising new pair of materials for photovoltaic cells [1].
- With Bluhm (LBNL CSD), we 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 [2,3].
- With Bibes et al. (Thales, Paris), we studied $BiFeO_3$ and Ca-doped $CeMnO_3$, which again exhibit an interface 2DEG, but with the property of facile electrostatic switching from conducting to insulating state, and the thickness of the 2DEG has been directly measured [4].
- With Louie et al. (LBNL MSD, UCB), we combined SXPS and soft x-ray ARPES with a cumulant expansion Green's function theory to observe and confirm dispersive plasmon satellites in ARPES [5], and to accurately determine valence-band maxima [10].
- With Stemmer et al. (UCSB), we studied multilayer oxide systems composed of:
  --$GdTiO_3$ and $SrTiO_3$, of interest because they exhibit a two-dimensional electron gas (2DEG) and ferromagnetic order at the interface between these two insulating materials [6,8],
  --$LaNiO_3$ and $SrTiO_3$, which show insulating behavior in thin $LaNiO_3$ layers [9].
- 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 [11,12]. We have also obtained additional HXPS and SXPS and ARPES data for these systems that are being analyzed and written up.
- With Chambers et al. (PNNL MSD), we combined SXPS, HXPS and SW-ARPES with local-density theory to study the interface-induced ferroelectricity of $LaCrO_3/SrTiO_3$ [13].

RESPONSIVE NANOPARTICLE ASSEMBLIES

Principal Investigator(s): Brett Helms, Thomas Russell

Project Description

Our goal is to create nanoparticle (NP) assemblies at interfaces that can be controllably reconfigured by external stimuli, generating materials that adapt their properties to changes in the environment. We are considering a diverse range of systems including NPs that become more structurally ordered in response to applied forces, thereby, increasing strength. NPs with tailored responsive ligands will yield materials that undergo reversible aggregation/percolation transitions, with corresponding dramatic changes in optical and electronic properties. NPs, comprised of alloys that undergo rapid phase changes, and possible shape changes, in response to an external stimulus are of interest. We are functionalizing the NPs with responsive ligands that enable controlled disassembly and re-assembly. This involves a competition for interactions with the polymer end groups that can be driven, under non-equilibrium conditions, to a metastable (or kinetically trapped) state, directing the NPs into structures with different properties.

Accomplishments

The electrostatic interaction of amine-terminated polydimethylsiloxane ($PDMSNH_2$) dissolved in a hydrophobic fluid (oil) and carboxlic acid functionalized nanoparticles (NPs) dispersed in water results in the formation and interfacial assembly of NP-surfactants. These assemblies can be controlled by the pH of the aqueous medium. At higher pH, the electrostatic interactions between NPs and the end-capped functionalized polymer ligands are strong, promoting the interfacial formation of NP-surfactants, enabling the fluids to be shaped. With decreasing pH, the weakening of the interaction forces allows the NP-surfactants to be ejected from the interface when the NP-surfactants are compressed as the interfacial area decreases, resulting in restoration of the droplet to its equilibrium spherical shape. The adjustment of pH, can be affected by the photo-triggering of a photo-acid generator, presenting a route toward structured liquids.

We expanded the range of solvents pairs and nanocrystal-polymer pairs by using naked nanocrystals (NCs) and amine end-capped polydimethylsiloxane (PDMS-NH_2) for the interfacial assemblies. We also used naked iron oxide (Fe_3O_4) nanocrystals, allowing us to use magnetic fields to re-structuring the liquids. The Fe_3O_4 NCs were synthesized, then were stripped and redispersed in dimethylformamide (DMF). The PDMS-NH_2 (Mw = 5.2k) was dispersed in a mixture solvent of 20 w% of dodecane and 80 w% of PDMS (50cSt, Mw= 3780). The naked Fe_3O_4 NCs and PDMS-NH_2 assemblies formed an active layer at the liquid/liquid interface and could be jammed as the interfacial area decreased. Jammed spherical droplets could be stretched into non-equilibrium shapes with a magnetic field and kinetically trapped.

We also designed and synthesized several small molecules to that were soluble in the DMF phase and could compete with PDMS-NH_2 for binding to the naked nanocrystal surface. This competitive binding affords an elegant route to jam and unjam the interfacial assembly of the nanoparticles and to control the restructuring of the liquids. The zwitterion 2-(1-butyl-1H-imidazol-3-ium-3-yl)acetate acting as a ligand markedly stabilizes naked Fe_3O_4 NCs dispersion in DMF and weakens the binding between naked nanocrystals and amine function groups. It allows the non-equilibrium structure to relax back to an equilibrium spherical shape. This introduces an entirely new concept of dynamic ligands for controlling assembly.

Synthesis Of Bio-Inspired Adaptive Membranes For Direct Capture Of Co_2 From Biogas

Principal Investigator(s): Nathaniel A. Lynd, Jeffry B. Greenblatt, Corinne D. Scown, and Roger Sathre

Project Description

Biogas derived from the anaerobic fermentation of biomass consists of ca. 50%wt CH_4. However, due to the high content of CO_2 and accompanying high cost of compression, the biogas is typically flared on site. If the CO_2 content of biogas could be effectively reduced via a low energy separation strategy, then biogas streams could be harvested to yield an estimated 410 Petajoules per year with lower greenhouse gas emissions than from other sources. Significantly, this amounts to 0.5% of our annual energy expenditure. Within this context, the US energy landscape would reap significant benefit from an efficient, low energy method of continuous, modular CO_2 removal. The fundamental synthesis of the materials and concepts required to develop this membrane technology are the focus of this LDRD-funded research.

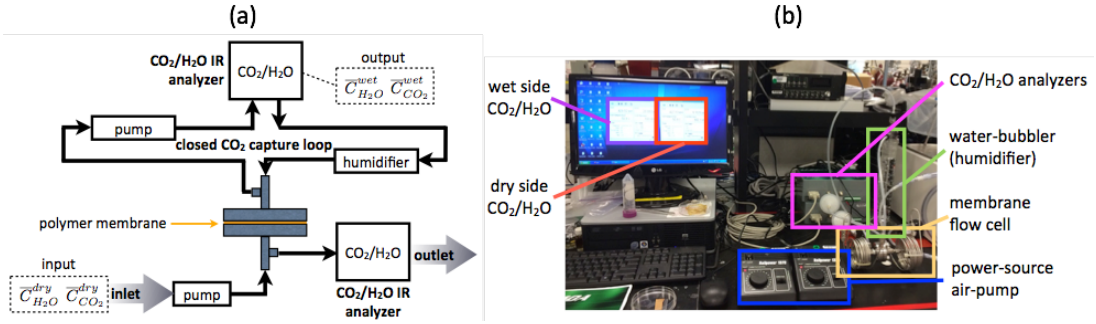


Figure 1. (a) A schematic of an experimental assembly for measuring the relationship between a membrane and a surrounding controlled atmosphere. An image of the actual experimental assembly is shown in (b).

The ultimate objective of our proposed research is to develop the fundamental science that may enable the development of a continuous process of carbon capture using a separate chemical potential driving force.

Accomplishments

Our most significant accomplishment has been to develop a testing methodology that could reliably measure the concentration of carbon dioxide and water on either side of a membrane. A schematic of the instrument is shown in Figure 1(a), and an image of the actual instrument is shown in Figure 1(b). The experimental assembly shown in Figure 1 was then used to measure the interaction between a commercial anion exchange resin and the air volumes on either side. Current efforts are focused on further understanding these phenomena, and on utilizing these concepts in the broader context of efficient membrane-based separations.

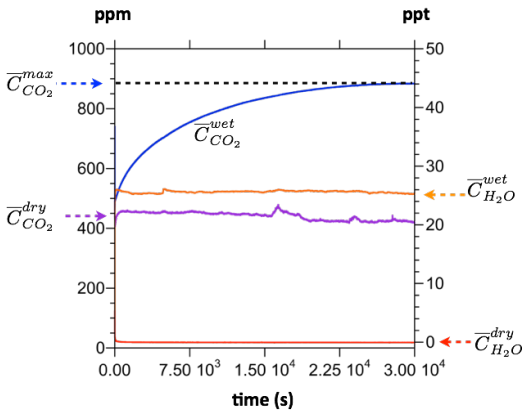


Figure 2. Measurements made on the CO_2/H_2O composition of air volumes separated by a commercial anion exchange membrane. [ppt = parts per thousand]

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. This is evidenced by the fact that all commercial resists in use for EUV today are simply variants of materials developed for 248-nm and 193-nm lithography. Such photoresists are blends of polymers and photoacid generators (PAGs) where the PAG is designed specifically to absorb the DUV photons. Unlike for DUV, however, EUV photons do not directly interact with the PAG and without knowing 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 three 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

In the first year of this LDRD, an experimental program has been implemented to build an understanding of EUV photoexcitation response in a library of materials. Molecular beam mass spectrometry has been coupled to an tunable electron gun (6-2000 eV) , and EUV radiation from beamline 6.3.2 (25 – 1303 eV) and fragmentation spectra, appearance energies and photoionization efficiency curves for the photon energy range of 7.4 – 200 eV have been measured for a series of halogenated phenolic based gas phase resist prototype molecules as well as for currently used PAGs. In addition, quantum-chemistry calculations of excited state forces of photoionized species have been used to predict which chemical bonds are most susceptible to cleavage in initial or relaxed excited states. While molecular beam studies do provide phenomenal insight into the primary EUV induced events in the individual molecules, we also want to understand how the landscape changes when molecules are condensed, as this is the medium in which industrially relevant processes will occur. Velocity map imaging photoelectron spectroscopy on condensed "nanophase" materials is the method chosen to implement this.[i] Such a spectrometer has been build in the first year of this LDRD and has been deployed to measure photoelectron spectra from VUV photoemission and in the near future will be coupled to EUV and low energy electron beam sources.

Computational Design of Smart Complex Oxides with Tunable Quantum Phases

Jeffrey B. Neaton

Project Description

Here, we develop and use computational approaches for discovery and design of functional quantum materials for next-generation energy, computing, and information technologies. In recent years, a new class of materials has emerged that exhibit novel topologically-protected conducting states on their surfaces or in bulk. These materials – topological insulators, Dirac and Weyl semimetals, nodal-line fermion systems, and others – feature noncollinear spin states and strong spin-orbit coupling protected by symmetry that, analogous to graphene, can lead high conductivity and large mobility, desirable for many applications. However, quantum materials with topological phases that have been identified and synthesized thusfar are not optimal; moreover, many such existing materials tend be unstable in ambient environments, limiting their utility. In this proposal, 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 – a 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 class.

Accomplishments

An important accomplishment to date is to develop a workflow to identify new tunable and topological phases with a high-throughput repository, the Materials Project, based on the ICSD. 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. We have identified more than ten new candidate Dirac semimetal phases near structural phase transitions that may be induced via temperature or epitaxial strain. Some of these systems (e.g., BiP2O7 and PbO2) are oxides, which are expected to be stable under ambient conditions. With enlarged pool of material searches and more complete theoretical understanding, it is highly anticipated that many other more accessible and functional topological oxides can be found and designed.

In addition to our high-throughput studies, we have performed detailed "case-study" calculations of a few classes of systems: pyrochlore iridates, which are well known for their metal-insulator transition and the possible existence of Weyl semimetal phases; lead chalcogenides, where a new class of topological materials with "nodal-line" fermions was recently observed PbTaSe2; and line defects in two-dimensional MoSe2, which exhibit an electronic phase transition. We predict that the pyrochlore iridates with a special type of magnetic domain wall undergoes metal-insulator transition. We have further examined whether chemical substitution modifies nodal-line features in the band structure in lead chalcogenides, showing these systems' topological electronic features are quite robust upon changing the chalcogen atom. Finally, we have explained recent STM experiments showing a low-temperature gap in line defects in MoSe2 as arising from the formation of a charge-density wave.

Dynamics of Mesoscale Electronic Ordering in Complex Materials

Principal Investigator: Robert W. Schoenlein

Project Description

The purpose of this project is develop new time-resolved resonant X-ray scattering approaches to advance our understanding of self-organized patterns of charge, spin, and orbital order and the rapid interactions that drive their formation in complex materials. These mesoscale patterns spawn novel states of electronic matter. The competition between such phases leads to important new physics and exotic properties such as metal-to-insulator transitions, high-T_C superconductivity, and colossal magnetoresistance.

A key challenge in understanding and manipulating electronically ordered materials is to disentangle the cause/effect interactions that drive the formation and fluctuating evolution of these competing ordered phases. To this end, we will perturbatively excite specific material modes and track the coupled order parameters in the time domain using advanced X-ray techniques including resonant scattering, spectroscopy, and dichroism at the Advanced Light Source and at the Linac Coherent Light Source. Resonant X-ray scattering is selectively sensitive to charge, spin, and orbital order at the atomic scale. X-ray dichroism can separate spin and orbital contributions to magnetic order. Coupling between these order parameters will be revealed by their disparate time responses. The time-profile of their response will provide insight to fluctuations and glassy behavior that often arise in complex oxides. Broadband THz/mid-IR spectroscopy will reveal how charge transport and lattice vibrations are coupled to different electronic order parameters. In conjunction with resonant optical or mid-IR vibrational excitation, these experiments will allow us to shed light on the salient ultrafast interactions that govern the physics of strongly correlated materials. Our studies will focus on model complex transition-metal oxide materials, and rare-earth lanthanide metals.

Accomplishments

Our most significant accomplishment has been comprehensive studies of spin-helix dynamics in the rare-earth lanthanide metal dysprosium. Time-resolved resonant X-ray scattering reveals the dynamic response of the helical spin order to injection of a transient unpolarized spin current. The observed spin dynamics are significantly slower than that exhibited by the ferromagnetic phase in lanthanide metals and are strongly dependent on temperature and excitation fluence. Theoretical modeling of the spin helix dynamics using a Gross–Pitaevskii formalism provided new insight to the dynamic bottleneck that emerges due to spin structures at the nano-scale.

A second significant accomplishment has been comprehensive studies of the photo-induced insulator-to-metal phase transition in a colossal magnetorestive manganite, PCMO. Time-resolved resonant X-ray scattering studies of the spin-ordering in PCMO reveal that the metallic phase does not fully form for several picoseconds following photo-excitation, in contrast with previous claims. Moreover, comparison with detail ultrafast optical spectroscopy measurements, and principal component analysis shows that phase competition, nano-scale domain formation and associated lattice deformation at domain boundaries are responsible for this unusual behavior. These studies demonstrate that phase separation effects play a significant role in the novel properties of colossal magnetorestive manganites.

Project Title: 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 analysis from single isolated applications to multiple applications in complete workflows. In the case of I/O, we now have information about the data read and written per application and the required lifetime of data files to support scientists' workflows. This big picture view of workflow I/O is necessary to reason about storage requirements, including capacity and performance per storage tier and user interfaces to storage. The results show two common characteristics of workflows: low average reuse of data in input files and short-lived data files for communicating information between workflow stages. The implication is that sufficient bandwidth is needed to stage input files from capacity tiers and interfaces are needed for users or workflow management software to control movement of data between tiers, i.e. prefetching data files and constraining short-lived data files to fast tiers.

We have incorporated a new tool named Procmon (developed by Doug Jacobsen of Berkeley Lab) into our analysis methodology. This tool captures procfs performance data for all processes executed on a compute node within a user job. It allows us to understand more of the data analysis workload, including applications written in interpreted languages and workflow scripts consisting of multiple applications. Analysis of Procmon data shows that some workflow stages are in a good position to transition to architectures with many small cores and extremely limited memory per core (hmmer, psfex, swarp (resample)). However, end-to-end workflow thread scalability is generally disappointing and some workflow stages have high memory footprint per thread emphasizing the importance of architectures with reasonable single thread performance.

We are currently using our findings to inform the APEX procurement. In particular, we have included data intensive workflow requirements in a workflows whitepaper, jointly written by NERSC, SNL and LANL, intended to help our conversations with vendors about delivering a usable architecture for both HPC and data analytics. We have also created a new I/O benchmark, inspired by the Blast bio-informatics application, which will be included in the APEX benchmarks.

Toward Laser Spectroscopy of Transfermium Elements

Principal Investigator(s): Jacklyn M. Gates

Project Description

The purpose of this project is to dramatically increase our understanding of the chemical and nuclear behavior of nuclei at the far reaches of stability by revolutionizing the techniques available to study these nuclei. Transfermium nuclei are produced in nuclear reactions between accelerated beams and rotating targets and at rates of atoms-per-second to atoms-per-year. Currently, the most advanced method for studying atomic properties of transfermium ($Z>100$) elements currently involves using aqueous phase and gas phase chemistry, which must be done on single atoms. Due to this, the current status of knowledge of atomic state energies in transfermium elements results solely from theoretical calculations with errors on the order of 0.3 eV.

With this project, we will develop a more direct method for determining the behavior of the atomic orbitals using laser spectroscopic techniques to obtain high-precision measurements of energy levels of atomic transitions and ionization potentials. These techniques can measure the energies of atomic transitions to within 3×10^{-5} eV, four orders of magnitude better than the current calculations. Detailed knowledge of atomic transitions at this level will greatly increase our knowledge of atomic and nuclear properties of elements at the limits of stability, including energies of atomic transitions, ionization potentials, hyperfine structure and isotope/isomer shifts. This information will allow for the determination of nuclear spins, electromagnetic moments, the change of the nuclear mean square charge radii and chemical properties of the heaviest nuclei.

Accomplishments

At the end of FY2014, we were in the process of commissioning a gas catcher and finalizing the design of the neutralization and re-ionization chamber for a laser spectroscopy system at LBNL. However, within the last year, laser spectroscopy was successfully performed on isotopes of nobelium (Z=102) and lawrencium (Z=103) at the *GSI Helmholtzzentrum für Schewerionen-forschung*. Due to the low production rates of elements with $Z>103$ and the ~1% efficiency of traditional laser spectroscopy setups (like the one being developed for LBNL), performing spectroscopy beyond lawrencium requires a drastic redesign. As such, we have spent the last year developing a new system suitable for studying elements with $Z>103$ at LBNL.

The new design builds on where the traditional method left off: During this year, we have finished commissioning the gas catcher and radiofrequency (RFQ) trap at Argonne National Laboratory and brought both over to LBNL. The gas catcher and RFQ trap have been installed at the exit of the pre-existing Berkeley Gas-filled Separator (BGS - an instrument that is used to separate transfermium nuclei from the beam and unwanted reaction products) and are being modified for LBNL safety standards. With this new instrument, we now have the ability to trap thermal ions in a small, well-defined volume. We have designed a system to excite the electrons of these trapped ions with different wavelengths and observe their decay back to the ground state. Since the ions are trapped in a potential well, we will be able to excite and de-excite each ion multiple times, thus greatly increasing the efficiency of the process and allowing us to extend these studies well beyond $Z=103$.

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 purpose of this project is to develop next-generation codes to support fundamental nuclear physics important to FRIB, the Facility for Rare Isotope Beams under construction at MSU that will be the next flagship facility for DOE nuclear physics. FRIB's scientific focus is the discovery and characterization of new isotopes that are unstable and short-lived under conditions found on earth, but can be stable states in the high-temperature environments of astrophysical explosions. The project supports NSD/CRD collaborations on FRIB physics:

(1) Enormous effort has led to the development of sophisticated 3D numerical 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 via neutrinos. These codes, integrated to typically one second after core bounce, reliably compute the initial conditions for the star's subsequent mantle ejection and neutrino-driven neutron-rich wind. Our project focuses on coupling these initial conditions to the CCSN code CASTRO and the radiation transport code SEDONA, producing an integrate code framework for propagating the explosion to later times, where contact can be made with the nucleosynthetic processes relevant to FRIB as well as to the electromagnetic observables that characterize CCSN.

(2) Some of FRIB's rare isotopes, if captured in atom traps, will open up extraordinary opportunities to improve our understanding of fundamental symmetries such as CP and its violation, due to large enhancements in symmetry violation from the accidental degeneracy of nuclear states. To connect FRIB observations to underlying theory, one must be able to derive from a fundamental UV theory the effective low-energy symmetry-violating nucleon-nucleon interaction responsible for the polarization of FRIB nuclei. We are developing the first rigorous methods for doing this, in the framework of lattice QCD, which provides a numerically exact solution of the strong interaction by discretizing time and space on the lattice.

Accomplishments

A derivation of the CP-violating NN interaction in QCD requires the use of extended nuclear sources as well as techniques to extract, from sources of cubic symmetry, specific spherical partial waves. This capability did not exist prior to our work, as previous studies of NN interactions utilized point nuclear sources, and thus could treat only s-wave interactions. Higher partial waves are necessary in interactions that violate CP. 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), submitting the work for publication. The initial calculations were performed for an effective pion mass of 800 MeV, which will now be systematically lowered too its physical value. Applications to parity violation are underway.

The astrophysics efforts began in summer 2015 with the hiring of Austin Harris. Austin is playing a major role in the continued development of CHIMERA, the 3D CCSN code of the ORNL group. We are now in the process of integrating that code with the local CASTRO/SEDONA suite. The local codes are LBNL candidates for Exascale Applications development.

Next-Generation Neutrino and Rare-Event Detection

Principal Investigator(s): Gabriel D. Orebi Gann

Project Description

The recent development of water-based liquid (WbLS) scintillator has opened up the possibility for a new kind of large-scale detector 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 goals of this project were the development and testing of critical aspects of this new detector technology.

The potential of the proposed WbLS target material has still to be fully understood and characterized in the regime relevant for these physics applications. 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 optimize the final target for maximum physics output. The ultimate goal of this project is to demonstrate successful separation of prompt Cherenkov light from delayed scintillation, thus enabling significantly enhanced background rejection through a combination of ultra-low energy thresholds (below Cherenkov threshold) and directional information.

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. A 200-ml target vessel has been constructed from UV-transparent acrylic, and rests atop an optical transmission medium of the same material. The cylindrical vessel has two flat faces machined to allow various attachments. The target can be excited in one of two ways: 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 5 degrees of vertical. Thus we can characterize the target in both the low-and high-energy regimes. Six 10-inch R7081 Hamamatsu PMTs are used to maximize photon collection from the target, in order to measure the intrinsic light yield. A grid-like array of 12 fast (300ps TTS) 1-inch H11934 Hamamatsu PMTs are positioned vertically beneath the target, in order to image the Cherenkov ring and to measure the time profile of the emitted light. Six 2m-by-1m scintillator panels are arranged around the apparatus in order to veto cosmic muons during source data taking. A 5GHz V1742 CAEN digitizer is used to readout the small, fast PMTs. The high sampling rate allows a precision timing measurement, but the 1024-sample buffer limits the event window to 200ns. The large-area PMTs are read out using a 500MHz V1730 CAEN digitizer. This provides a large dynamic range in order to measure anything from the tens of mV of a single photoelectron signal up to the few hundred photoelectrons that might be expected from a pure scintillator target, with a large buffer that allows a long event window, to catch all delayed scintillation photons.

A complete simulation has been developed and the setup has been calibrated using a pure water target, which can be modeled exactly, allowing a full understanding of the apparatus. Initial light yield measurements have been performed, and we are in the process of obtaining a range of WbLS samples in order to complete the timing measurements, and to understand these characteristics as a function of the target composition.

NEXT GENERATION SI-BASED TRACKING AND MASSIVE ONLINE DATA PROCESSING FOR COLLIDER EXPERIMENTS

Principal Investigator(s): Mateusz Ploskon

Project Description

In the second year LDRD we have focused on new approaches to online and offline data processing, for hadron collider physics experiments with high-intensity beams. The study was based on the ALICE experiment at the Large Hadron Collider at CERN, which will generate an unprecedented raw data rate of 1.1 Terabyte/second following a major upgrade during the LHC Long Shutdown 2 (LS2) in 2018. Such data rates require qualitatively new approaches to detector readout and online processing, to ensure that all physics of interest is recorded for offline analysis with realistically achievable offline computing resources.

Our specific focus is the future ALICE Inner Tracking System (ITS) upgrade. However, this work is to establish a novel strategy for collision data processing that can be applied to any future high rate collider detectors. In the planned approach the paradigm of a standard *event-based* reconstruction is replaced by a *time-stamp* driven analysis of the detector signals. We explored hardware computing architectures with the focus on high-performance facilities as well as software infrastructure for both efficient data compression and data selection in silicon-based tracking detectors, guided by the physics requirements.

Accomplishments

Within the first year of the project we have established a number of benchmark observables of heavy-flavor production at high- and low-energy scales that became a strategic part for the future heavy-ion program at the LHC. These observables connecting the precision of the single particle tracking and full jet reconstruction put stringent requirements on the performance of the new Si-detector developed for experiments at high collision rates. The main performance benchmarks of the principal elements of the readout system have been identified.

Within the second year, and final, of the project we have developed several key algorithms for handling detector data structured in the *time-stamp* (as opposed to traditional *event-driven*) approach. We have prototyped a fully functional digitization algorithms for the silicon detector within a new framework ALFA (ALICE-FAIR software framework). In particular, we have ported ITS chip simulation and raw signal digitization to offline algorithms including the time information of a unit digit data structure from the detector. We note that the new framework is not specific to ALICE ITS and can be used for any other type of detectors. The developments make use of the fault-tolerant (ZeroMQ) messaging service opening possibilities for concurrent process execution that in turn may lead to a parallel computing analysis infrastructure (a possibility to be explored). Moreover, in order to fully profit from the High-Performance Computing clusters we have adopted and commissioned ANALISA (a new tool for management and execution of ALICE jobs) within the NERSC computing farms (Edison, Hopper and Cori). This new setup is a side product but a way to a potential use of the NERSC HPC systems within the LHC/ALICE grid infrastructure. The development provides a transparent submission layer and a worker layer translating parallel MPI jobs into multiple serial jobs. Together with an automatic build infrastructure for the ALICE software stack successfully deployed this allowed for setting up a test simulation facility for the future data processing on HPC. In summary, we arrived at a setup capable of a *time-stamp* based detector reconstruction in a parallel processing infrastructure that carries the key ingredients for a future mass data reconstruction.

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) The multimodality and multi-sensor system, HEMI, was used to refine concepts of 3-D scene reconstruction and gamma-ray fusion to enhance radiation mapping capabilities. During the first year of this LDRD, HEMI was deployed on an aerial platform in Namie town, in the evacuated area in Fukushima Prefecture. Preliminary analysis indicates the gain achievable by the new volumetric imaging concept.

ii) A high resolution, high fidelity model of the Ogi dam basin within the Fukushima prefecture was constructed to include variation in land use and land cover type and complex topography. To obtain an initial hydrologic condition of the domain where a dynamic equilibrium is reached, a "spin-up" simulation was performed utilizing NERSC. Notoriously computationally expensive, a number of techniques were tested to aid in the spin-up simulation time, resulting in the development of new methods for this step in watershed numerical simulations. Preliminary comparisons of water table depth at dynamic equilibrium conditions between the JAEA numerical simulator and ParFlow indicate good agreement.

iii) Uptake and viability was characterized for cells exposed to both forms of cesium. To evaluate cell death, clonogenic survival from external sources of Cs-137 has been measured as control experiments for various doses of acute exposures and for chronic external exposures. For live cells, cells exposed to doses as low as 5 cGy and as high as 70 cGy delivered over a 48-hour time course have been acquired with a small external source of Cs-137 placed inside our microscope. Our bioinformatics pipeline has determined the impact of chronic exposures on cell proliferation, cell death and homeostatic levels for DNA damage. Kinetic measurements from acute data is allowing us to validate a mathematical model to predict the response to chronic exposure.

iv) A key aspect of remediation of Fukushima will be the development of chemical and physical treatments of the Fukushima soils for volume reduction, which relies on the knowledge of Cs speciation in the clays. Spectromicroscopy with the scanning transmission X-microscope (STXM) has been used to characterize the Cs speciation in several simulated Fukushima clays. STXM studies of reference Cs materials has been performed as a basis for understanding the speciation of Cs in the Fukushima soils that is associated with clay constituents of the soil since near-edge x-ray absorption fine structure (NEXAFS) spectroscopy of Cs at the Cs $M_{4,5}$-edges has not been studied in detail. The experimental safety infrastructure was successfully put into place to handle real, radioactive Fukushima soils and several classes of Cs-contaminated soils were received at the ALS for experiments.

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.
- 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. We have developed a new program within the Phenix system, called phenix.real_space_refine, which performs optimization of an atomic model against a cryo-EM reconstruction (map), whilst also maintaining good stereochemistry. The algorithms have been designed to be computationally efficient, so as to provide researchers with rapid feedback in the process of model optimization. It has also been necessary to develop approaches that possess a large radius of convergence, as the starting atomic models often contain significant errors.

With these new algorithms it is possible to refine large atomic models, containing tens of thousands of atoms, in hours and minutes rather than days. The algorithm's overall scaling is between linear and quadratic with the number of atoms in the model. Initial tests with maps and models deposited in the EM Databank and Protein Databank show that it is possible to improve models both in terms of fit to the experimental data and the stereochemistry of the resulting models. A typical example at higher resolution (3.8A) is the TRPV1 ion channel from Yifan Cheng's group at UCSF. Refinement with the new algorithms is able to improve the correlation between the model and map from 0.65 to 0.714, whilst also reducing atomic clashes by a factor of 3 and correcting all side chain rotamer outliers. We also see that large errors in models can be corrected automatically in the course of refinement. Although the algorithms are new, and still being actively developed, they have already been used by several groups, with some results recently published.

PROBING DYNAMICS OF ELECTRON TRANSFER FOR MICROBIAL-BASED ENERGY INTERCONVERSION

Principal Investigator(s): Caroline Ajo-Franklin (Lead), Matthew B. Francis, Naomi S. Ginsberg

Project Description

Enabling more efficient flow of electrons across the boundary between living and human-made systems is critical for bioenergy technologies, including harvesting energy from wastewater and efficient synthesis of fuels from sunlight and CO_2. Over the last 20 years, proteins that mediate electron transfer across this abiotic-biotic interface have been identified, purified, and structurally characterized in isolation. However, the structural basis of how these proteins perform catalysis, i.e. electron transfer, with minerals has remained unknown. This is because the protein-material interface is structurally complex, buried and not crystallizable, and thus has remained inaccessible to traditional structural techniques such as X-ray crystallography, NMR, and AFM. Our overall goal is to address these critical structure-function knowledge gaps so that we can redesign proteins for more efficient electron transfer to materials.

The Mtr pathway of *Shewanella oneidensis* MR-1 is currently the best understood extracellular electron transfer pathway. It consists of a periplasmic decaheme cytochrome *c* (cyt *c*), an outer membrane non-cyt *c* porin-like protein (MtrB, MtrE) and an outer membrane decaheme cyt *c* (MtrC, MtrF, OmcA). The outer membrane decaheme cyts *c* are the most unique and important components of this pathway since these are the proteins that transfer electrons to abiotic surfaces such as minerals or electrodes. These key multi-heme cyts *c* have been recently structurally characterized in isolation, however, it is unknown if these proteins can recognize specific metal oxides and if so, what the structural basis behind this binding is.

Accomplishments

This year our team made several leaps forward in our understanding of structure-function at the protein-material interface. Leveraging our ability to express and purify MtrF, we first probed the ability of MtrF to bind to nanoparticulate α-Fe_2O_3 and α-Al_2O_3. Using both fluorescence quenching and sedimentation assays, we demonstrated that MtrF binds to α-Fe_2O_3 (K_{ads}=12fmol/mm^2), but does not bind to α-Al_2O_3. This difference is striking because both α-Fe_2O_3 and α-Al_2O_3 have the same α-corundum crystal structure, but only α-Fe_2O_3 can be reduced by MtrF. Additionally, we found that the binding affinity of MtrF to α-Fe_2O_3 increases with increasing H^+ concentration, suggesting that binding is mediated by electrostatic interactions.

Next, we used both protein and X-ray footprinting to identify residues that are protected by MtrF binding to α-Fe_2O_3. These techniques probe different binding timescales (μs and hr) and interactions with different sets of amino acids. Nonetheless, both protein and X-ray footprinting showed two key regions, one region bracketed by hemes 6 and 7 and a second region near heme 10, were protected upon α-Fe_2O_3 binding. Each region contained a set of several amino acids, separated by tens of amino acids in primary sequence, that were protected. This strongly suggests that MtrF binds α-Fe_2O_3 through tertiary structure. If this idea proves correct, this will be the first example of a protein using its 3D structure to recognize a material.

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 nanowires functionalized with hydrogen-producing catalysts and living microbes as an autotrophic chassis for the production of value-added fuels and other chemicals from CO_2 and photogenic H_2. Specific aims include (i) development of photocatalytic H_2-producing inorganic nanowire platforms that can operate in aqueous media at physiological pH and ionic strength, as well as (ii) metabolic engineering of H_2-metabolizing organisms to divert carbon fluxes to value added carbon products.

We have focused on different approaches to generating solar-derived reducing equivalents that may be used to drive microbial metabolism of diverse types. In addition, we are developing genetic tools for the engineering of environmental microbes that can fix carbon dioxide and/or nitrogen for various downstream applications

Accomplishments

During this year, we have been developing bio-nano hybrids for the conversion of carbon dioxide to methane using solar input. We have worked with a native methanogen, *Methanococcus barkeri*, which is capable of fixing carbon dioxide to form methane under non-photosynthetic conditions. Under electrosynthetic conditions with a platinum cathode, we have shown that a culture of *M. barkeri* shows chemoselective conversion of CO_2 to CH_4 with high Faradaic efficiencies (up to 86%) and low overpotential (η = 360 mV). The system was long-lived, surviving for < 7 d and also able to produce methane at high productivity (110 mL, 4.3 mmol). We also synthesized a new electrocatalyst from the earth-abundant metal, Ni, that could produce methane at similar efficiency and productivity as with the platinum electrode.

This overall electrocatalytic process was converted into a photocatalytic using a photoactive silicon cathode, which reduced the overpotential to 175 mV upon irradiation with 740-nm light. We also showed that unassisted light-driven methane generation could be achieved using tandem solar absorption by a photoactive n-TiO_2 anode and p-InP cathode assembly. Taken together, the results demonstrate the feasibility of combining compatible inorganic and biological systems to achieve solar-to-chemical conversion from light, H_2O, and CO_2, affording a starting point for the fixation of CO_2 to value-added molecules.

We are currently continuing to work with new systems for solar-driven catalysis in non-model environmental organisms. At this time, we are focusing on developing tools for their genetic modification.

Functional Genomic Encyclopedia of Bacteria and Archaea: Evidence-Based Annotation of the Microbial Tree of Life

Principal Investigator(s): Adam Deutschbauer, Adam Arkin, James Bristow, Matthew Blow

Project Description

The purpose of this project is to bridge the gap between microbial genome sequencing and genome characterization. For example, current gene function annotation pipelines fail to identify a role for 40% genes the typical bacterial genome. In this project, we aim to establish a flexible, rapid, and inexpensive platform for assay mutant phenotypes and predict gene function using high-throughput transposon mutagenesis in bacteria and archaea. After establishing this pipeline, we aim to apply it to ~25 diverse microorganisms and use the resulting data to annotate gene function across the microbial tree of life using functional and comparative genomics. In addition, we will establish computational tools for the analysis and visualization of this large dataset.

Accomplishments

Our first significant accomplishment was the development of a flexible and inexpensive method (random barcode transposon-site sequencing or RB-TnSeq) for assaying the phenotypes of thousands of genes in parallel using transposon mutagenesis and DNA barcode sequencing (BarSeq). The key to the approach is the introduction of random DNA barcodes into the transposon. A mutant library for a given microbe is characterized a single time using the time-consuming and expensive TnSeq protocol. All subsequent assays to measure mutant fitness for thousands of genes in parallel only require the quantification of the DNA barcodes, a simple and inexpensive assay termed BarSeq.

Our most significant accomplishment has been the generation of the largest bacterial functional genomics dataset to date and the demonstration that large-scale functional genomics can be applied rapidly and inexpensively to virtually any genetically tractable microbe. In total, we have applied RB-TnSeq to 26 diverse bacteria and generated over 4,000 whole-genome mutant fitness profiles, representing ~13 million gene fitness measurements. We have identified significant phenotypes for over 20,000 bacterial genes including 7,375 previously uncharacterized genes. Among these genes, 4,690 had phenotypes under a specific experimental condition, or shared phenotypic patterns with a gene of known function, thus enabling specific predictions of gene function. Finally, since 11% of hypothetical genes across all sequenced genomes have at least one ortholog with a phenotype in our dataset, we demonstrate the ability of high-throughput genetics to identify roles for many of the uncharacterized proteins in bacterial genomes. Lastly, we have made our computational experimental tools available to the larger microbiology community and created a website for the comparative analysis and visualization of our data.

Enhancing the Design-Build-Test-Learn Cycle for Metabolic Engineering

Principal Investigator: Nathan J. Hillson

Project Description

There is a strategic imperative for investment in biomanufacturing infrastructure at Berkeley Lab. In the 2013 State of the Union address, Barack Obama said: "I'm announcing the launch of three more of these manufacturing hubs, where businesses will partner with the Departments of Defense and Energy .... And I ask this Congress to help create a network of fifteen of these hubs and guarantee that the next revolution in manufacturing is Made in America." While the complete specifications for these fifteen national manufacturing hubs have yet to be announced, given the Administration's 2012 National Bioeconomy Blueprint, it is very likely that there will be at least one biological manufacturing hub. This FY14-15 lab-wide strategic LDRD aims to place Berkeley Lab in a dominant position from which to lead a competitive effort that brings a biomanufacturing hub to Northern California.

While Berkeley Lab is uniquely positioned to leverage DOE investments in the JGI, NERSC, KBase, JBEI, and the ABPDU for biomanufacturing competitive advantage, the capabilities and expertise at these facilities have yet to be integrated and successfully demonstrated as a 'one-stop-shop' from target molecule identification to industry-ready microbial production strains. Operationally, this requires biomanufacturing pipeline component standardization and interoperability; the ability to generate, QC, and track large numbers of DNA constructs; seamless integration of microbial strain construction with high-throughput functional assessment; and machine intelligence to learn from previous successes and failures to drive forward the next design iteration. This strategic LDRD aims integrate existing and develop new Berkeley Lab capabilities and expertise to create revolutionary biomanufacturing infrastructure. This infrastructure will enable the rapid design, implementation, and assessment of target molecule production by iteratively uncovering and resolving critical biosynthesis bottlenecks. This LDRD aims to tackle a stress-test and a challenging biosynthesis demonstration project to drive a compelling success story narrative, while in parallel addressing key infrastructure gaps. Demonstrating the ability to go from target molecule to functional construct within a year for important and valuable targets will cement Berkeley Lab's leadership in biomanufacturing.

Accomplishments

In early FY15, we completed and validated the construction of the refactored (genes recoded; fully synthetic promoter and ribosomal binding-site genetic components) actinorhodin pathway, transformed the construct into a modified *Streptomyces coelicolor* host lacking its native actinorhodin pathway, and detected the production of actinorhodin, our selected challenge project. This was a very impressive feat, as it constitutes a record-breaking refactored secondary metabolite pathway at 22 genes and 25 kbp in length. Sample preparation and analytical mass spectrometry methods were developed for actinorhodin and other secondary metabolites including violacein, our selected biosynthesis stress-test project target. Significant progress was also made in completing the DNA construction and metabolomic analysis of a subset of a 50,000-variant refactored violacein pathway combinatorial library, identification and initial progress towards molecular "targets of opportunity", the development of machine learning algorithms for processing combinatorial library metabolomics data, and in the further development of DNA construction process tracking and assistance software.

DEVELOPMENT OF A CRISPR/CAS9 KNOCKOUT SYSTEM FOR *STREPTOMYCES VENEZUELAE*

Aindrila Mukhopadhyay

Streptomyces venezuelae is an industrial microbe studied for its production of the complex antibiotics chloramphenicol and jadomycin. *Streptomyces* species in general are noted producers of prized and difficult to replicate natural products, but the bacteria themselves are fastidious and difficult to cultivate or manipulate. *S. venezuelae* itself is somewhat more amenable to laboratory conditions because it grows diffusely and sporulates completely in liquid media, unlike practically every other member of its genus. It also lacks native immune systems, making genetic transformation a much simpler proposition. The Fuels Synthesis group at JBEI has already proven that the organism would be a suitable microbial host for the production of biofuel precursor isoprenoids. The purpose of this LDRD was to further develop *S. venezuelae* for the production of a broad array of polyketide synthase associated chemicals by developing a contemporary genome editing toolkit and knocking out competing biosynthetic pathways.

The plan was to use classical genetics to knock in a marker gene and then to test and optimize the *in vivo* use of Cas9 endonuclease on the genome. Once a reproducible Cas9 protocol was developed, we planned to knock out the chloramphenicol biosynthetic pathway, and to repeat the previous isoprenoids work in the newly edited strain.

Accomplishments

Two papers demonstrating Cas9 usage in *Streptomyces* were published between the submission of this LDRD and its issuance. Relieved of the need to pioneer or optimize Cas9 expression in our bacteria, we instead acquired their constructs as soon as material transfer agreements made it possible. We proceeded with the second part of the plan, which was the removal of biosynthetic pathways. That work is still underway. In the meantime we optimized growth medias, nucleotide extraction protocols, and began gathering plasmids and specialized knowledge about this non-model organism.

In addition to the bench work, we designed and deployed software for the design of CRISPR reagents. This software, TOASTER, is served from JBEI at biostudio.jbei.org and has been disclosed to the IPO (disclosure number 2016-056). It is in heavy use in the Fuels Synthesis group and interested industry groups are seeking to license it.

Tactical High Throughput Computing
Principal Investigator: Stephen Bailey

Project Description

As data sets grow larger, there is an increasing need across multiple LBNL divisions for tools to simplify "High Throughput Computing" (HTC) — the efficient processing of many thousands or even millions of small tasks. Examples include running the same analysis program on many thousands of images or spectra or gene sequences, or running the same simulation with thousands of different input parameters. The traditional batch model of 1 task = 1 script = 1 batch job is impractical for both the batch queue system and the human management of such scripts.

Although multiple groups have solved this problem in a project-specific manner, the solutions fall short of being general enough to be reusable by other projects. At the same time, general-purpose workflow tools are often heavyweight, requiring significant buy-in to the particular tool used. This LDRD developed a lightweight middle ground for "tactical high throughput computing" — general purpose enough to be useable by multiple projects, while being simple enough to quickly deploy, use, and reconfigure.

The model developed under this LDRD separates the list of computing tasks to perform from the batch jobs that process these tasks, with each worker job processing multiple tasks. The assignment of tasks to workers is not pre-determined, allowing flexibility for the worker jobs to scale up and down, and to add more tasks to the queue even after the processing has begun. Tasks can have priorities and dependencies, thus accommodating many different use cases. The state and control of tasks can be done in aggregate, thus simplifying the management of thousands of tasks (e.g. rerun all tasks, list only the failed tasks). The toolkit is written in python, but the tasks themselves can be written in any language.

Accomplishments

In the first year of the LDRD, we reviewed available options, compared two of them in detail, and make scaling and robustness improvements to both. We then focused on further developing the "qdo" toolkit. The second year focused on providing a web interface and testing the usability and scaling of qdo with real-world applications. The underlying postgres database backend was refactored to support many more users, and the ability to remotely use qdo was added.

The results of this LDRD have been used by the Legacy Survey (http://legacysurvey.org) for their data processing of thousands of astronomical images. The Dark Energy Spectroscopic Instrument (DESI; https://desi.lbl.gov) has also used qdo for their data processing pipeline development. Multiple other individuals have used qdo for single-purpose analysis tasks, demonstrating its success at being a lightweight toolkit that is easy to deploy and use.

The code is released as an open source project at https://bitbucket.org/berkeleylab/qdo, which has enabled contributions from a broader community of developers than those who were directly involved with this LDRD.

Higher Performance CCDs for Next Generation Dark Energy Experiments

Principal Investigator(s): Christopher Bebek

Project Description

We have completed the 3rd year of this project to develop advanced charge-coupled devices (CCDs) for use in the next generation of Dark Energy experiments. CCDs developed at LBNL are presently in use at two Dark Energy experiments; the eBOSS experiment that is a continuation of the Baryon Oscillation Spectroscopic Survey, and the Dark Energy Survey that is in its 3rd year of operation. Also, a new camera, Mosaic-3 that utilizes four, 500 μm thick, fully depleted LBNL CCDs is beginning operation at the National Optical Astronomy Observatory Mayall Telescope. Future projects such as the Dark Energy Spectroscopic Survey (DESI) and the Large Synoptic Survey Telescope have adopted the fully depleted CCD technology that was developed at LBNL, but desire further improved performance.

Performance improvement areas that we emphasized in this work are increasing the quantum efficiency (QE), reducing the detector readout noise, increasing the readout speed, and exploring methods to achieve single-photon detection. The QE work requires technology development at the LBNL MicroSystems Laboratory. The other efforts involve LBNL design work and exploration of advanced fabrication steps with our industrial partner Teledyne DALSA.

Accomplishments

In this 3rd year of the project we continued our efforts in QE improvement and developed an improved, broadband anti-reflecting coating consisting of thin films of indium tin oxide, ZrO_2, and SiO_2. We also explored the use of the high refractive index material TiO_2 as a replacement for the ZrO_2 film. The resulting QE was greater than 85% in the wavelength range of interest to DESI, i.e. 550 nm – 1 μm. We also demonstrated single-photon detection with the improved charge-multiplying CCD that was part of the CCD design and fabrication effort in the first year of the LDRD, and that was tested during the 2nd year.

A new wafer layout was generated based on the results of the first two years of the LDRD. The main emphasis was to develop scientifically useful CCDs. A 4k x 4k, $(15\ \mu m)^2$ pixel CCD with low-noise amplifiers was included. DESI has adopted this device for its twenty visible and near-infrared spectrograph channels. This CCD is base-lined for the European Southern Observatory (ESO) Multi Object Optical and Near-Infrared Spectrograph and will be the first thick, fully depleted CCD deployed by ESO. Larger format versions of the charge-multiplying CCD with more multiplication stages were included in the wafer layout. We are in the process of providing charge-multiplying CCDs to a group at NASA Goddard that is interested in the development of instruments for future space-based missions to study exoplanet atmospheres for signs of life. In addition, CCDs with the 2nd generation, sub-electron read noise amplifier technology using a thin gate dielectric in the output transistors were included in order to acquire more data on the reproducibility of this technology.

We have also had on-going efforts throughout the 3 year period of this project to reduce the impact of imaging artifacts that are present in thick, fully depleted CCDs. These artifacts include periodic variations in the pixel response due to the nature of the manufacturing process used for the photomasks needed in the CCD processing, and concentric ring patterns observed under conditions of uniform illumination that arise due to resistivity variations during crystal growth in the high-resistivity, silicon substrates used to produce the CCDs. We have been able to reduce the size of these effects from about the 0.5% level to less than 0.1%.

Advanced Composites for Next Generation Scientific Instruments FY2015

C.Haber (PI,Physics), E. Anderssen, J. Silber, (Engineering) A. Ruminski, J.Urban (Mat.Sci.)

Purpose/Goal: This LDRD proposal is aimed at evaluating and acquiring technical concepts and capabilities which could be crucial aspects of future instrumentation for high energy, relativistic heavy ion, and astro-particle physics, and of accelerator and light source UHV components and superconducting magnets. These aspects bear particularly on requirements for thermal performance, mechanical precision, strength and stability, scale, and reliability. **Approach/Methods:** This study involves advanced materials which combine excellent mechanical and thermal properties, and are ultimately suitable for large scale applications and fabrication. We study special processing, apply measurement and modeling methods, and develop new measurement capabilities needed for characterization and inspection. We utilized Laboratory resources and capabilities including Molecular Foundry and Composites Laboratory.

Cyanate Ester (CE) Resin Qualifications for Application to Superconducting Magnets and Large Structures: Calorimetric studies initiated in FY2014 were completed.

Vacuum Compatible Polymers for Accelerators: CE resins already used in composite structures were qualified for use in vacuum applications at CXRO at 'High Vacuum' (10^{-9} Torr), compatible with ALS experimental (end station) vacuum. This effort was completed.

Air-Cooled Low-Mass Structures: A custom air flow test stand was constructed to measure pressure and thermal differentials when passing air through candidate non-metallic foam material in FY2014. Our CVD material was evaluated further and shown to perform significantly better than the older RVC (reticulated vitreous carbon) material. A test 0.5 meter “stave” structure with a CVD core was fabricated and tested for temperature drop, for a variety of flow rates and for power densities between 0.5 and 0.1 watts per square cm. The results can be scaled to practical 1 m long stave configurations. For future applications with reasonable power densities and material budgets this becomes a very attractive alternative to liquid and bi-phase cooling.

Resin modification: An extensive survey of candidate non-metallic particle additives for thermal enhancement of structural resins was initiated in FY2014. A notable success was a high purity micron scale graphitic powder, which enhanced the base resin's thermal conductivity (0.3 W/m*K) by an order of magnitude at 25%-30% volume fraction. This material was the focus of study in FY2015. Spreading behavior versus volume fraction was evaluated. Test “stavelets” were built and their thermal performance was studied with IR imaging. The electrical properties of the powder/resin system was studied and the material was shown to have an important effect on electrical conductivity. An electrical grounding and shielding test structure was fabricated and sent for testing to our collaborators at UC Santa Cruz. Thermal test samples were also exchanged with collaborators and BNL and Queen Mary/UK, and these demonstrated consistent results. Additional resins were identified and one was studied using the new filler.

Instrumentation for Precision Inspection: A large area multi-purpose test stand which integrates precision metrologic capabilities was fabricated. Efforts focused on software control, data acquisition, and test. A user control interface was designed and programmed. Mechanical stability was addressed with modifications to the support arch. Alternative support structures were also conceived and designed. A confocal multi-point line sensor was acquired and integrated. Studies of scanning and image matching were carried out. Issues of calibration and point-to-point matching were resolved. The confocal probe was compared to the laser triangulation sensor for vibrometric applications.

Searches for the Supersymmetric Particles at the LHC in Run-2 and Beyond
Principal Investigator(s): Beate Heinemann

Project Description

The purpose of this project is to search for supersymmetric (SUSY) particles at the Large Hadron Collider (LHC) using data from the ATLAS experiment. The idea for the existence of supersymmetric particles (sparticles) stems from the 70s and it is widely thought to be a likely extension of the Standard Model as it solves several problems with the SM, e.g. it provides a natural candidate for Dark Matter and it addresses the hierarchy problem. Searching for such particles in the 2nd run of the LHC provides an exciting opportunity for finding them.

Accomplishments

We have used the 2015 dataset to search for sparticles. The dataset corresponds to a luminosity of 3.2 fb-1: this is sufficient to search for high mass SUSY particles produced via the strong interaction, in particular gluinos, with a sensitivity beyond that of run-1. However, it is not sufficient to search for direct production of the SUSY partners of top quarks or electroweak gauge bosons as originally foreseen in this proposal. Thus the strategy was slightly adapted to do two related but different analyses with this dataset:

1. A search for strong production of sparticles decaying into a final state containing a Z boson, jets and large missing transverse energy (Etmiss). A diagram of an example of such a process is shown in Fig. 1. We selected this search as during the first LHC run there was an excess of events seen in this analysis with a statistical significance of 3 standard deviations. This search was performed requiring a Z boson candidate in the dielectron or dimuon decay mode, Etmiss greater than 225 GeV and the total transverse energy in the event to be above 600 GeV. The observed dilepton mass distribution is shown in Fig. 1. The data agree well with the background estimate in most of the mass range but in the Z mass region near 90 GeV there are more data events than expected from the background estimate. The significance of this excess is 2.2 standard deviations. This result has been released in preliminary form and is currently being updated for final publication. The publication is expected in 1-2 months.

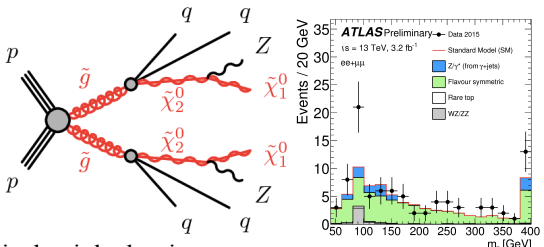


Fig. 1: Left diagram for the production of gluinos decaying to Z bosons, jets and neutralinos. Right: Dilepton mass spectrum for events selected by the analysis. The data are shown as points and the backgrounds are shown as colored histograms.

1. A search for a quasi-stable gluino that hadronises and has a lifetime larger than 0.4 ns. The signature of such a gluino is that it hadronises before it decays and thus can be a charged particles moving relatively slowly (β<1) through the detector. This causes the particle to have a larger ionization energy loss than SM particles traveling with β=1. Using the ATLAS pixel detector (which was largely designed and built in Berkeley) we measure the ionization energy loss of particles and can measure the mass as m=p/(βγ). In addition to requiring a high momentum charged particle a requirement is placed on large Etmiss to ensure the event passes the ATLAS trigger. Fig. 2 shows the measured mass distribution compared to the background and several gluino mass hypothesis. The data agree with the background and are used to derive lower limits on the gluino mass as function of the lifetime. These limits are also shown in Fig. 2: the extend beyond 1.5 TeV for lifetimes above 10 ns. This result has not yet been fully approved but is currently being reviewed within the collaboration, and I expect it to be published in 1-2 months.

I plan to continue both analyses using the 2016 data of the LHC, where about 30 fb^{-1} are expected, a 10-fold increase in statistics. This will clarify the nature of the excess in the first analysis and significantly improve the sensitivity of the 2nd analysis.

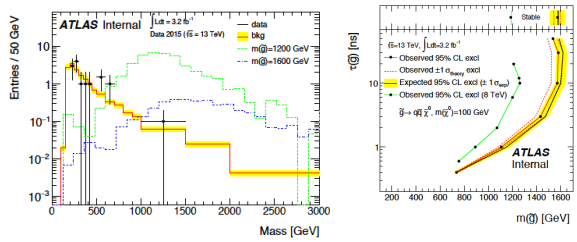


Fig.2: Left: Reconstructed mass distribution in the search for quasi-stable gluinos for data, background and example gluino signals. Right: gluino lifetime versus mass plane showing the 95% CL limits from the run-1 analysis (green) and the run-2 analysis (this LDRD).

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

Principal Investigator: Adrian Lee

Project Description:
The purpose of this project is to develop detector technology for next-generation Cosmic Microwave Background (CMB) polarimetry experiments. “B-mode” CMB polarization pattern, which have a handedness, carries information about primordial gravitational wave generated during inflation, sum of mass of neutrino masses and evolution of dark energy. Current generation of CMB polarimetry experiments detected B-modes from gravitational lensing and put the tightest constraint on amplitude of primordial gravitational waves. Current CMB experiments are deploying of order 1,000 detectors and experiments with order 10,000 detectors will deploy within few years. The community is gaining momentum for next stage of CMB experiment (CMB-S4) to definitively characterize B-mode polarization with an order 500,000 detector count. The desire to increase detector count by up to two orders of magnitude requires a fresh approach. We identified components in current detector systems that are currently not scalable, and we developed methods to improve their scalability.

Accomplishments:
This year, we explored micro-fabrication foundary to fabricate CMB detectors. We identified foundary that has potential to fabricate CMB detectors. We worked with foundary to come up with design that is compatible with their capability. We are planning to continue pursuing detector fabrication effort in FY16. We successfully fabricated monolithic superconducting resonator for frequency multiplexing readout in FY14. We improved fabrication method to bring yield of integrated superconducting resonator package to be higher than 98%. We improved antireflection coating uniformity of thermal spray coated lenslet array by moving lenslet array in planetary motion. We demonstrated quality control and packaging scalability method we developed last year with POLARBEAR-2 detector modules.

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 Dark Matter searches at collider, supersymmetric gauge-mediated models, natural Higgs sector models of "Neutral naturalness", novel flavor models and the connection between the Standard Model Higgs and inflation.

The investigation of the power of "mono-X" searches for Dark Matter at the Large Hadron Collider has been extensively performed and the related publications will be presented in the near future. We have found that such searches in many models tend to be less powerful then other more conventional new physics searches such searches for supersymmetry and exotic resonances and extra Higgs bosons and we have identified the areas where mono-X searches genuinly provide an improvement.

Further development of the software package Atom has progressed alongside its usage. Better description of detector effects has been implemented and parallelization of the code is underway. New LHC Run I analyses, especially those looking for multi-lepton signatures have been added.

On the model building end, S.Knapen studied the applications of orbifold constructions in theories with color-neutral top partners. This let to a new class of Twin-Higgs inspired models, in which the UV sensitivity is cancelled without the presence of an explicit Z_2 symmetry. Further research along this line is in progress as a continuation of this LDRD. He furthermore constructed a new mechanism to generate the standard model mass hierarchies, in which the structure of the CKM matrix is not related to hierarchies in the mass spectrum.

On the topic of supersymmetry, Knapen performed a complete study of the low energy spectra of general gauge mediation. He also showed that in gauge mediation A-terms can arise at tree-level and that adding collective symmetry breaking to minimal gauge mediation can elegantly reproduce a mini-split spectrum.

On the front of the connections between particle physics and cosmology H.Yoo also investigated and continue research on the behavior of the Standard Model Higgs during Inflation, and the possible compatibility of our Universe with the Higgs vacuum instabilities at high energy in case no extra beyond the Standard Model physics is present.

ENOS: ESnet Network Operating System

Principal Investigator(s): Inder Monga

Project Description

We propose to build a network operating system, ENOS, as a prototype next-generation ESnet architecture for handling data-intensive science workflows. The concept of a 'network operating system', a software layer that enables applications to get information about the network and to program it to meet its needs, has been around in academic papers for a while but appears to be feasible now due to the wide adoption of the Software-Defined Networking (SDN) paradigm. The SDN paradigm constitutes a network architecture that separates the control plane from the distributed data plane and provides logical centralization of the network control and state. These logical central control plane capabilities can be evolved to become the operating system through which the network policies are implemented across the entire network and applications can program network behavior.

At a high-level, an operating system interacts with hardware using device drivers while providing an environment with sufficient abstractions where multiple applications can run. The current vendor marketplace is focusing on SDN controller platforms that are equivalent to the 'device drivers' in a generalized OS model. In addition, since this is early days in the evolution of this concept, there is no industry or academic accepted model of a 'network operating system'. We propose taking the lead in the Research and Education domain by researching and developing an architectural framework for the OS with a focus towards serving science workflows and build an experimental version of the software applied towards specific science use-cases.

Given the trends and the uptake of SDN in the industry, our efforts will be complemented by hardware efforts already in progress within the industry. In addition, Open Networking Foundation (ONF) is standardizing the OpenFlow protocol that defines the interaction between the network operating system and hardware data plane. There are multiple examples of 'device drivers' or OpenFlow controllers that have been developed and open-sourced – this is not an area we will focus our efforts, other than making a choice of the appropriate open-source package.

Accomplishments

Over the LDRD year, we have focused on developing the architecture and proof of concept implementation of ENOS. As articulated in the LDRD, we have developed over the past few months:

- Detailed ENOS architecture
- Abstract API to interact with multiple network controllers especially OSCARS and Open Daylight, with an ability to build and load dynamically new software modules
- Security architecture and design to deal with multiple applications run-time environment over the operating system
- Virtual representation of network topology including verification of topology and routing metrics
- Python-based execution environment for customer-build applications

The above functionality with the proposed demonstration of a multi-site, multi-point connectivity using this prototype code, was demonstrated in the first week of May. These concepts were presented as two accepted conference talk to the R&E (University and Lab) community at the Technology Exchange 2015.

The prototype version of the Network Operating system has already influenced the direction of the recently funded ASCR SENSE project, of which I am the lead PI. It is also being used to manage the ESnet 100G SDN Network Testbed that is being opened to researchers in early 2016.

In addition, investigation into the 'Building a programmable container API to enable multiple applications to interact with the network' task led to an interesting new field of exploration. Instead of building programmatic APIs to the network like we had done for OSCARS, we explored the concepts of building 'intent-based' application APIs. This is the focus of the FY16 LDRD extension to ENOS.

Publications List

Accelerator (LPA) and Assessment of its Utility for Potential Biomedical Applications
AT-Schenkel LB13001 Probing Point Defect Dynamics in Solids with Short Ion Beam Pulses

Journal Publications

P. A. Seidl, W. G. Greenway, S. M. Lidia, A. Persaud, M. Stettler, J. H. Takakuwa, W. L. Waldron, T. Schenkel, J. J. Barnard, A. Friedman, D. P. Grote, R. C. Davidson, E. P. Gilson, I. D. Kaganovich, "Short intense ion pulses for materials and warm dense matter research", Nucl. Instr. Meth. A 800, 98 (2015), arXiv:1506.05839

AT-Vay LB14002 High-Accuracy Scalable Solvers for Modeling of Future Ultrafast Photon Sources

Journal Publications

R. Lehe, M. Kirchen, I. A. Andriyash, B. B. Godfrey, J.-L. Vay, "A spectral, quasi-cylindrical and dispersion-free Particle-In-Cell algorithm", http://arxiv.org/abs/1507.04790 , submitted to Computer Physics Communications (2015).

B. B. Godfrey, J.-L. Vay, "Improved numerical Cherenkov instability suppression in the generalized PSTD PIC algorithm", Computer Physics Communications, 196, 221-225, (2015), http://dx.doi.org/10.1016/j.cpc.2015.06.008 .

P. Lee, J.-L. Vay, "Efficiency of the Perfectly Matched Layer with high-order finite difference and pseudo-spectral Maxwell solvers", Computer Physics Communications, 194, 1-9, (2015), http://dx.doi.org/10.1016/j.cpc.2015.04.004 .

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

Journal Publications

J. Ruppe, T. Zhou, C. Zhu, J. Nees, R. Wilcox, A. Galvanauskas, "Cascading of Coherent Pulse Stacking Using Multiple Gires-Tournois Interferometers", Advanced Solid State Lasers 2015, Oct. 7, 2015. https://www.osapublishing.org/abstract.cfm?uri=ASSL-2015-AW3A.4

AL-Shapiro LB13038 Ultra-high Resolution Microscopy of Nano-materials by Scanning X-ray Diffraction Microscopy

Journal Publications

Li, Y., et al, Nanoscale variation of Li-insertion rate controls compositional spatio-dynamics within battery primary particles, submitted to Science

Shi, X., et al, Imaging nanoscale magnetic and structural correlations in thin SmCo5 films using soft x-ray ptychography, submitted to Applied Physics Letters

Wu, Y., et al, In-situ Multimodal Imaging and Spectroscopy of Mg Electrodeposition at Electrode-Electrolyte Interfaces, submitted to Nanoscale

Shapiro, D.A., et al, A new apparatus for soft x-ray tomography at the Advanced Light Source, in preparation for Rev. Sci. Inst.

Farmand, M., et al, Near-edge X-ray Refraction Fine Structure Microscopy of Nano-materials, submitted to Nature Photonics.

Yu, Y.S., et al, Ultra-high resolution chemical state tomography, in preparation for Nature Materials

Venkatakrishnan, V., et al, Robust X-ray Phase Ptycho-Tomography, submitted to IEEE Signal Processing Letters

Y. Li, et al, Effects of Particle Size and Incoherent Nanoscale Crystallite Domains on the Sequence of Lithiation in LiFePO4 Porous Electrodes, 2015, accepted by Advanced Materials.

S.-C. Bae, et al, Soft X-ray Ptychographic Imaging and Morphological Quantification of Calcium Silicate Hydrates (C-S-H), 2015, accepted by JACERS.

Yu, Y-S, et al, Dependence on crystal size of the nanoscale chemical phase distribution and fracture in LixFePO4, Nano Letters, 15 (7), pp 4282–4288 (2015)

D.A.Shapiro, et al, Chemical Composition Mapping with Nanometre Resolution with Soft X-ray Microscopy, Nature Photonics, 8, 765-769 (2014).

AL-Steier LB14003 Novel Accelerator Techniques for Diffraction Limited Light Sources

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

AL-Yang LB15003 High Efficiency Soft X-ray In-situ Spectroscopy (HESIS) for ALS-II Energy Sciences

Journal Publications

R. Qiao, L.A. Wray, J.-H. Kim, N.P.W. Pieczonka, S.J. Harris, W. Yang, "Direct Experimental Probe of the Ni(II)/Ni(III)/Ni(IV) Redox Evolution in LiNi0.5Mn1.5O4 Electrodes", The Journal of Physical Chemistry C, November 11, 2015. http://pubs.acs.org/doi/10.1021/acs.jpcc.5b07479

R. Qiao, K. Dai, J. Mao, T.-C. Weng, D. Sokaras, D. Nordlund, X. Song, V.S. Battaglia, Z. Hussain, G. Liu, W. Yang, "Revealing and suppressing surface Mn(II) formation of Na0.44MnO2 electrodes for Na-ion batteries", Nano Energy, September 2015. http://www.sciencedirect.com/science/article/pii/S2211285515002785

H. Zhao, R. Qiao, C. Zhu, Z. Zheng, M. Ling, Z. Jia, Y. Bai, Y. Fu, J. Lei, X. Song, V. S. Battaglia, W. Yang, P. B. Messersmith, G. Liu, "Conductive Polymer Binder for High-Tap-Density Nanosilicon Material for Lithium-Ion Battery Negative Electrode Application" Nano Letters, 9, 7927, 2015. http://pubs.acs.org/doi/10.1021/acs.nanolett.5b03003

W. Yang, R. Qiao "Soft x-ray spectroscopy for probing electronic and chemical states of battery materials", Chin. Phys. B 25, 017104 (2016). .(review) http://cpb.iphy.ac.cn/EN/Y2016/V25/I1/17104

X. Liu, Y. J. Wang, B. Barbiellini, H. Hafiz, S. Basak, J. Liu, T. Richardson, G. Shu, F. Chou, T.-C. Weng, D. Nordlund, D. Sokaras, B. Moritz, T. P. Devereaux, R. Qiao, Y.-D. Chuang, A. Bansil, Z. Hussain, W. Yang "Why LiFePO4 is a safe battery electrode: Coulomb repulsion induced electron-state reshuffling upon lithiation" Phys. Chem. Chem. Phys., 17, 16369 (2015). http://pubs.rsc.org/en/content/articlelanding/2015/cp/c5cp04739k

CH-Hartwig LB14005 Design of Mesoscale Catalyst Networks

Journal Publications

H. M. Key, P. Dydio, D. S. Clark, and J. F. Hartwig "Beyond Iron: Multi-Dimensional Preparation and Evolution of Artificial Metalloenzymes containing Noble Metal-Porphyrins for New Enzymatic Reactions"Nature accepted with minor revisions (2016).

CH-Head-Gordon, M LB13036 New Algorithms for Performing and Analyzing Large-Scale Electronic Structure Calculations

Journal Publications

R.J. Azar and M. Head-Gordon, "Similarity-Transformed Perturbation Theory on Top of Truncated Local Coupled Cluster Solutions: Theory and Applications to Intermolecular Interactions", J. Chem. Phys. 143, 024113 (2015).

R.J. Azar, P.R. Horn and M. Head-Gordon, "Adaptive basis functions from fragment-localized zeroth-order solutions: Frugal yet accurate density functional theory calculations of intermolecular interactions", (manuscript in preparation).

CH-Head-Gordon, T LB14006 Designing Fluctuations and Dynamics of Enzyme Catalytic Networks

Journal Publications

L. Ruiz, N. Mardirossian, M. Head-Gordon, T. Head-Gordon (2016). Characterization of meta-GGA functionals for bulk water. In preparation.

D. H. Brookes and T. Head-Gordon (2015). The family of oxygen-oxygen radial distribution functions for water. J. Phys. Chem. Lett. 6 (15), 2938-2943.

A. Bhowmick, S. Sharma, and T. Head-Gordon (2016). Computational directed evolution of of Kemp Eliminase KE15. In preparation

A. Bhowmick, S. Sharma, and T. Head-Gordon (2016). The role of side chain entropy and mutual information for improving the de novo design of Kemp Eliminases KE07 and KE70. submitted

A. Bhowmick and T. Head-Gordon (2015). A Monte Carlo method for generating side chain structural ensembles. Structure 23(1):44-55.

L. E. Felberg, A. Doshi, G. L. Hura, J. Sly, V. A. Plunova, R. Miller, J. E. Rice, W. C. Swope, T. Head-Gordon (2016). Controlling the structural transition of polymers with pH using chemical composition and star polymer architecture. Submitted.

L. E. Felberg, D. H. Brookes, J. E. Rice, T. Head-Gordon, and W. Swope (2015). Role of hydrophilicity and length of diblock arms for determining star polymer physical properties. J. Phys. Chem. B (William Jorgensen Festschrift) 119 (3), 944–957

Presentations

Advanced Potential Energy Surfaces for Condensed Phase Simulation Symposium on Synergistic Relationships between Computational Chemistry and Experiment, Pacifichem, December 15-20, 2015.

Advanced Potential Energy Surfaces for Water Simulations. Symposium on Liquids and Glassy Soft Materials: Theoretical and Neutron Scattering Studies, Materials Research Society, November 29 - December 4, 2015, Boston, Massachusetts.

New Solutions to the Poisson Boltzmann Equation. Mathematical Biosciences Institute Workshop 2: Multiple Faces of Biomolecular Electrostatics. Columbus, Ohio, October 12-16, 2015.

Determining the Structural Ensemble of Intrinsically Disordered Disease Peptides combining Theory and Experiment: Applications to Alzheimer's Disease Biology. Telluride Workshop, July 13-17, 2015.

Development and Deployment of Chemical Software for Advanced Potential Energy Surfaces. Telluride Workshop. THG, J. Ponder, J. Essex, co-organizers, June 14-20, 2015.

Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis. Albany 2015: The 19th Conversation, University of Albany, New York, June 9-13, 2015.

Progress in Solvation Science. German Bunsen-Society for Physical Chemistry, Bunsentagung 2015, Ruhr-Universität Bochum, Germany, May 14-16, 2015

Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis. Physical Chemistry Seimar, University of Oregon, May 4, 2015.

Determining the Structural Ensemble of Intrinsically Disordered Disease Peptides combining Theory and Experiment: Applications to Alzheimer's Disease Biology. Lorentz Center Workshop on Amyloid Aggregation: Single Molecule Approaches to a Many Molecule Problem, Leiden University, Netherlands April 13 - 17, 2015

Determining the Structural Ensemble of Intrinsically Disordered Disease Peptides combining Theory and Experiment: Applications to Alzheimer's Disease Biology. ACS PHYS. Denver, Colorado, March 22, 2015.

Advanced Potential Energy Surfaces for Water Simulations. ACS COMP. Denver, Colorado, March 25, 2015.

Advanced Potential Energy Surfaces for Condensed Phase Simulation. Frontiers in Materials Science Lecturer. Pacific Northwest National Laboratories. Jan. 26, 2015.

The Future of Molecular Simulation. NSF Conceptualization Workshop. Houston, Texas Jan. 22-24, 2015.

New Polarizable Models for Water. Workshop on Fundamental Problems in the Physics and Chemistry of Water. Houston, Texas Jan. 16, 2015.

Statistical Fluctuations, Dynamics and De Novo Enzyme Catalysis. CCP-BioSim, Leeds, UK Jan. 7-9, 2015.

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

Journal Publications

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, "Stochastic methods for aerosol chemistry: a compact molecular description of functionalization and fragmentation in the heterogeneous oxidation of squalane aerosol by OH radicals", Physical Chemistry Chemical Physics, 2015 DOI: 10.1039/c4cp05093b.

F. A. Houle, W. D. Hinsberg, and K. R. Wilson, "Reaction of OH radical with a model alkane aerosol: connecting surface accommodation to the reactive uptake coefficient", Physical Chemistry Chemical Physics, 2015, DOI: 10.1039/C5EE01434D.

A. A. Wiegel, S. H. Kessler, M. Liu, J. H. Kroll, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, "Large gradients in the chemical and physical properties of a semisolid organic aerosol upon heterogeneous oxidation by OH radicals", in preparation.

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, "The evolution of the chemical and physical properties of organic aerosol oxidized in the atmosphere as a function of viscosity and diffusion coefficient.", in preparation.

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, "Accelerated free radical chemistry on the surface of semisolid organic aerosols during the heterogeneous oxidation by OH radicals in the presence of NO and SO2.", in preparation.

M. Liu, A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, and F. A. Houle, "Aerosol growth and chemical mechanisms in the heterogeneous oxidation of aqueous citric acid aerosol by OH radicals.", in preparation.

Presentations

F. A. Houle , W. D. Hinsberg, K. R. Wilson, On the connection of organic aerosol ageing to viscosity, American Chemical Society National Meeting, Denver, March 22-26, 2015

A. A. Wiegel , K.R. Wilson, W. D. Hinsberg, F. A. Houle, A stochastic approach to diffusion modeling of the fragmentation processes during heterogeneous oxidation of organic aerosol, American Chemical Society National Meeting, Denver, March 22-26, 2015

K.R. Wilson, "Aerosol Mass Spectrometry and Heterogeneous Chemistry," 25th Australian and New Zealand Society for Mass Spectrometry (ANZSMS), Brisbane, Australia, July 18th – July 24th, 2015

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle, "Investigating the effect of phase state on the fragmentation and evaporation processes during heterogeneous

oxidation of organic aerosol using a stochastic reaction-diffusion kinetics model" Gordon Research Conference, August 2 – 6, 2015.

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle, "Investigating the effect of phase state on the fragmentation and evaporation processes during heterogeneous oxidation of organic aerosol using a stochastic reaction-diffusion kinetics model" The International Conference for Carbonaceous Particles in the Atmosphere, August 11 – 13, 2015.

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle, "A stochastic reaction diffusion kinetics model of the fragmentation processes during heterogeneous oxidation of organic aerosol", 34th Annual American Association for Aerosol Research Meeting, October 12 – 17, 2015.

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle, "Investigating the effect of phase state during the heterogeneous oxidation of model organic aerosols using a stochastic reaction-diffusion kinetics simulation", International Aerosol Modeling Algorithms Meeting, December 9 – 11, 2015.

CR-Adams LB15004 High Performance Geometric Mulitgrid (HPGMG) For a New TOP500 Computer Architecture Benchmark

Journal Publications

Mark F. Adams, Jed Brown, John Shalf, Brian Van Straalen, Erich Strohmaier, Samuel Williams, "HPGMG 1.0: A Benchmark for Ranking High Performance Computing Systems", LBNL Technical Report, 2014, LBNL 6630E,

Mark Adams, Samuel Williams, Jed Brown, HPGMG, Birds of a Feather (BoF), Supercomputing, November 2014,

Presentations

Samuel Williams, HPGMG-FV, FastForward2 Proxy App Presentation, December 2014

CR-Bell LB15006 Surrogate Model Algorithms for Optimization Problems

Journal Publications

J. Mueller, R. Paudel, C.A. Shoemaker, J.D. Woodbury, Y. Wang, N. Mahowald, "CH4 Parameter Estimation in CLM4.5bgc Using Surrogate Global Optimization", Geosci. Model. Dev., 8, 3285-3310, 2015, http://www.geosci-model-dev.net/8/3285/2015/gmd-8-3285-2015.html

J. Mueller, "MISO: Mixed-Integer Surrogate Optimization Framework", Optimization and Engineering, published online June 20, 2015, http://link.springer.com/article/10.1007%2Fs11081-015-9281-2

J. Mueller, O. Rouhani, C.A. Shoemaker, H.O. Gao, "Surrogate Model Optimization for Discrete Transportation Network Design Problems", INFORMS Transportation Science, submitted

J. Mueller, J.D. Woodbury, "GOSAC: Global Optimization with Surrogate Approximation of Constraints", INFORMS Operations Research, submitted

O. Rouhani, J. Mueller, C.A. Shoemaker, H.O. Gao, "A Surrogate Optimization Algorithm for Solving Discrete Transportation Network Design Problems", Computers & Operations Research, submitted

CR-Buluc LB14008 Graph-Based Analysis and Visualization of Multimodal Multi-Resolution Large-Scale Neuroimaging Data

Journal Publications

S.Y. Oh, O. Dalal, K. Khare, B. Rajaratnam, "Optimization Methods for Sparse Pseudo-Likelihood Graphical Model Selection", Neural Information Processing Systems (NIPS), 2014

S. Murugesan, K. Bouchard, J, Brown, B. Hamann, W. Seeley, A. Trujillo, G.H. Weber. "Brain Modulyzer: Interactive Visual Analysis of Functional Brain Connectivity" under review for IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB).

Presentations

P. Koanantakool, A. Azad, A. Buluc, D. Morozov, S.Y. Oh, L. Oliker, K. Yelick. "Communication-Avoiding Parallel Sparse-Dense Matrix-Matrix Multiplication", accepted to 30th IEEE International Parallel & Distributed Processing Symposium (IPDPS), 2015

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 preparation

CR-de Jong LB14009 Advanced Computational Chemistry and Semantic Data Tools for Mesoscale Science

Journal Publications

D.M.L. Brown, H.M. Cho, W.A. de Jong, "Bridging experiment and theory: a template for unifying NMR data and electronic structure calculations", J. Cheminformatics, submitted (2015)

Presentations

D. Ozog, A. Kamil, Y. Zheng, P. Hargrove, J. Hammond, A. Malony, W.A. de Jong, K. Yelick, "A Hartree-Fock Application using UPC++ and the New DArray Library ", accepted to 30th IEEE International Parallel & Distributed Processing Symposium (2016)

W. Lavrijsen, C. Iancu, W.A. de Jong, X. Chen, K. Schwan, "Exploiting Variability for Energy Optimization of Parallel Programs", submitted to PPoPP '16: 21th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (2016)

M. Chabbi, W. Lavrijsen, W.A. de Jong, K. Sen, J. Mellor-Crummey, C. Iancu, "Barrier Elision for Production Parallel Programs", in PPoPP '15: 20th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (2015)

H. Shan, S. Williams, W.A. de Jong, L. Oliker, "Thread-Level Parallelization and Optimization of NWChem for the Intel MIC Architecture", in PMAM 2015: The 2015 International Workshop on Programming Models and Applications for Multicores and Manycores, pp 58-67 (2015).

CR-Kemper LB13010 Computational Approaches to Understanding Ultrafast Science

Journal Publications

A.F. Kemper, M. A. Sentef, B. Moritz, J. K. Freericks, and T. P. Devereaux, "Amplitude Mode Oscillations in Pump-Probe Photoemission Spectra of Electron-Phonon Mediated Superconductors", Physical Review B, December 2015 http://journals.aps.org/prb/abstract/10.1103/PhysRevB.92.224517

M.C. Langner, S. Roy, A.F. Kemper, Y.-D. Chuang, S.K. Mishra, R. Versteeg, Y. Zhu, M.P. Hertlein, T.E. Glover, K. Dumesnil, R.W. Schoenlein, "Scattering Bottleneck for Spin Dynamics in Metallic Helical Antiferromagnetic Dysprosium," Physical Review B, November 2015 http://journals.aps.org/prb/abstract/10.1103/PhysRevB.92.184423

Shuolong Yang, J.A. Sobota, D. Leuenberger, A.F. Kemper, J.J. Lee, F.T. Schmitt, W. Li, R.G. Moore, P.S. Kirchmann, and Z.-X. Shen, "Thickness-Dependent Coherent Phonon Frequency in Ultrathin FeSe/SrTiO3 Films," Nano Letters, June 2015 http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.5b01274

D. Leuenberger, J. A. Sobota, S.-L. Yang, A.F. Kemper, P. Giraldo-Gallo, R. G. Moore, I. R. Fisher, P. S. Kirchmann, T. P. Devereaux and Z.-X. Shen, "Classification of Collective Modes in a Charge Density Wave by Momentum-Dependent Modulation of the Electronic Band Structure," Phys. Rev. B, May 2015 http://journals.aps.org/prb/abstract/10.1103/PhysRevB.91.201106

M.A. Sentef, M. Claassen, A.F. Kemper, B. Moritz, T. Oka, J.K. Freericks and T.P. Devereaux, "Theory of pump-probe photoemission in graphene: Ultrafast Tuning of Floquet Bands and Local Pseudospin Textures," Nature Communications, May 2015 http://www.nature.com/ncomms/2015/150511/ncomms8047/abs/ncomms8047.html

S. Gerber, D. Leuenberger, J. J. Turner, T. Wolf, Y. Zhang, P. S. Kirchmann, J.-S. Lee, Y.-D. Chuang, Z.-X. Shen, D. Zhu, R. G. Moore, A. Mehta, Z. Hussain, T. P. Devereaux, W.-S. Lee, N. Plonka, A.F. Kemper, C.-C. Kao, M. Yi, M. Chollet, H.-H. Kuo, B. Moritz, G. L. Dakowski, J. M. Glownia, I. R. Fisher, K. W. Kim, "Direct characterisation of photo-induced femtosecond lattice dynamics in BaFe2As2," Nature Communications, April 2015 http://www.nature.com/ncomms/2015/150608/ncomms8377/abs/ncomms8377.html

M.A. Sentef, A.F. Kemper, A. Georges, C. Kollath, "Theory of light-enhanced phonon-mediated superconductivity," Under review at Physical Review B

J.P. Hinton, E. Thewalt, Z. Alpichshev, F. Mahmood, J.D. Koralek, M.K. Chan, M.J. Veit, C.J. Dorow, N. Barisic, A.F. Kemper, D.A. Bonn, W.N. Hardy, Ruixing Liang, N. Gedik, M. Greven, A. Lanzara, J. Orenstein, "The rate of quasiparticle recombination probes the onset of coherence in cuprate superconductors," Under review at the Proceedings of the National Academy of Sciences

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

Journal Publications

L. Lin, "Localized spectrum slicing", submitted to Math. Comp., 2015, http://arxiv.org/abs/1411.6152

L. Lin, J. Lu, "Sharp decay estimates of discretized Green's functions for Schrodinger type operators", submitted to Sci. China Math., 2015 http://arxiv.org/abs/1511.07957

X. Li, L. Lin, J. Lu, "Boundary conditions of open Kohn-Sham systems with discrete Dirichlet-to-Neumann map", in preparation, 2015

CR-Oliker LB13007 High-Performance Parallel Analysis for Key Genomics Computations

Presentations

V. Strnadova, J. Gonzalez, J. Chapman, J. Gilbert, D. Rokhsar, L. Oliker, "Efficient and Accurate Clustering for Large-Scale Genetic Mapping", IEEE International Conference on Bioinformatics and Biomedicine (BIBM), Nov 2014

V. Strnadová, A. Buluç, J. Chapman, J. Gilbert, J. Gonzalez, L. Oliker, "Efficient Large-Scale Genetic Mapping", ACM Conference on Bioinformatics, Computational Biology, and Health Informatics (ACM BCB), September 2015

CR-Saye LB14010 High-Order Implicit Interface Methods for Complex Fluid Flow and Multiple Interface Dynamics

Journal Publications

R. Saye, "High-Order Quadrature Methods for Implicitly Defined Surfaces and Volumes in Hyperrectangles", SIAM Journal on Scientific Computing, 2015, http://dx.doi.org/10.1137/140966290

R. Saye, "Interfacial Gauge Methods for Incompressible Fluid Dynamics", in preparation.

CR-Tull LB13009 SPOT Suite - Towards an End-to-End Solution for Light Source Data

Journal Publications

"High performance data management and analysis for tomography", Blair, Justin and Canon, Richard S and Deslippe, Jack and Essiari, Abdelilah and Hexemer, Alexander and MacDowell, Alastair A and Parkinson, Dilworth Y and Patton, Simon J and Ramakrishnan, Lavanya and Tamura, Nobumichi and others, book"SPIE Optical Engineering+ Applications", pp. 92121G--92121G, 2014, International Society for Optics and Photonics

"Fast Analysis of Time-Resolved Scattering Data", Hexemer, Alexander and Kumar, Dinesh and Venkatakrishnan, Singanallur and Sarje, Abhinav and Patton, Simon and Li, Sherry and Deslippe, Jack and Tull, Craig and Dart, Eli and Liu, Feng and others, Bulletin of the American Physical Society, Volume 60, 2015, APS

"ALS User Meeting Highlights Accomplishments and Challenges", Troutman, Keri and Arenholz, Elke and Parkinson, Dula and Hexemer, Alexander and Shapiro, David and MacDowell, Alastair and Tull, Craig and Yang, Wanli and Ralston, Corie and Gupta, Sayan and others, Synchrotron Radiation News, Volume 28, Number 1, pp. 2--8, 2015, Taylor & Francis

"Spade: Decentralized orchestration of data movement and warehousing for physics experiments", Patton, Simon and Samak, Taghrid and Tull, Craig E and Mackenzie, Cindy, book"Integrated Network Management (IM), 2015 IFIP/IEEE International Symposium on", pp. 1014--1019, 2015, IEEE

Presentations

"Workflow management for real-time analysis of lightsource experiments", Deslippe, Jack and Essiari, Abdelilah and Patton, Simon J and Samak, Taghrid and Tull, Craig E and Hexemer, Alexander and Kumar, Dinesh and Parkinson, Dilworth and Stewart, Polite, book"Proceedings of the 9th Workshop on Workflows in Support of Large-Scale Science", pp. 31--40, 2014, IEEE Press

"Data optimised computing for heterogeneous big data computing applications", Yang, Erica and Ross, Derek and Nagella, Srikanth and Turner, Martin and Kockelmann, Winfried and Burca, Genoveva and Pouzols, Federico Montesino, book"Big Data (Big Data), 2015 IEEE International Conference on", pp. 2817--2819, 2015, IEEE

ES-Ceja Navarro LB15016 The Soil Metazoan Microbiome: A Key Functional Compartment of Importance to Plant Health and Root C Stabilization

Journal Publications

Ceja-Navarro, J.A., Arellano, A., Kvietok, M., Brodie, E.L. Populations of soil arthropods and their microbiome are key players in soil nutrient cycling. In preparation. To be submitted to the ISME Journal.

ES-Freifeld LB15018 Fracture Characterization During and After Multistage Hydraulic Fracturing in Unconventional Gas Reserves Using Temperature Data

Journal Publications

B Yingqi Zhang and Barry Freifeld, "Using Distributed Temperature Sensing to Detect Gas Flow Along the Well Casing," Draft

ES-Kueppers LB13041 Using Experiments and Numerical Models to Examine Ecosystem and Land Management Interactions with Atmosphere and Climate

Journal Publications

Lu, Y., J. Jin, and L. M. Kueppers. 2015. "Crop growth and irrigation interact to influence surface fluxes in a regional climate-cropland model (WRF3.3-CLM4crop)." Climate Dynamics 45:3347–3363 doi: 10.1007/s00382-015-2543-z.

Lu, Y. and L. M. Kueppers. 2015. "Increased heat waves with loss of irrigation in the United States." Environmental Research Letters. 10: 064010, doi:10.1088/1748-9326/10/6/064010.

Meromy, L., N. P. Molotch, M. Williams, K. Musselman, and L. M. Kueppers. 2015. "Snowpack-climate manipulation using infrared heaters in subalpine forests of the Southern Rocky Mountains, USA." Agricultural and Forest Meteorology 203: 142-157 doi:10.1016/j.agrformet.2014.12.015.

Conlisk, E., C. Castanha, A. Moyes, M. Germino, T. T. Veblen, J. Smith, P. de Valpine, M. S. Torn, J. B. Mitton, L. M Kueppers. "Declines in warm-edge subalpine tree populations outpace cool-edge population expansion with warming." In revision for PNAS.

Lu, Y., K. Harding, and L. M. Kueppers. "Irrigation effects on land-atmosphere coupling strength in the United States." In review at Journal of Climate.

Fernández, M. H. Hamilton, and L. M. Kueppers. 2015. "Back to the future: using historical climate variation to project near-term shifts in habitat suitable for coast redwood." Global Change Biology 21:4141-4152 doi: 10.1111/gcb.13027.

ES-Lammers LB15033 Clay Interlayer Stratification: Implications for Ion Exchange and the Mobility of Neutral Molecules in Shales

Journal Publications

K. Kolluri, L.N. Lammers, "Interlayer ion exchange and interstratification in anhydrous clay minerals," J. Colloid Interface Sci., In preparation.

Presentations

K. Kolluri, L.N. Lammers, "Kinetics of interlayer ion migration in non-swelling clays: An atomic-scale study," Oral presentation, AGU Fall Meeting, (2015).

ES-Nico LB14015 Quantifying the Dynamics of Natural Organic Matter Conformation and Reactivity

Journal Publications

Lee, N.; Schuck, P. J.; Nico, P. S.; Gilbert, B., Surface Enhanced Raman Spectroscopy of Organic Molecules on Magnetite (Fe3O4) Nanoparticles. Journal of Physical Chemistry Letters 2015, 6 (6), 970-974;

Lee, N, Shuck, PJ, Nico, P &Gilbert, B Goldschmidt Abstracts, 2015 1807

ES-Wan LB13019 Extracting Natural Surfactant from Earth Sediments for Economical Oil/Gas Recovery

Journal Publications

Bikkina, P., J. Wan, Y. Kim, T. J. Kneafsey, T. K. Tokunaga, Influence of wettability and permeability heterogeneity on miscible CO2 flooding efficiency, Fuel 166, 219-226, 2015.

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

Presentations

B. Gerke, M. McNeil, and T. Tu, "International Database of Efficient Appliances (IDEA): A Novel Tool for Efficiency Program Development and Evaluation", International Energy Program Evaluation Conference 2015, August 2015. http://www.iepec.org/wp-content/uploads/2015/papers/026.pdf

EE-Kiliccote LB14012 Application of Virtual Grind-Integration Laboratory (VirGIL)

Journal Publications

S. Chatzivasileiadis, M. Bonvini, J. Matanza, R. Yin, T. Nouidui, E. C. Kara, R. Parmar, D. Lorenzetti, M. Wetter, and S. Kiliccote. VirGIL: A co-simulation platform for cyber-physical modeling of distributed resources for distribution system operations. Proceedings of the IEEE. Accepted http://arxiv.org/abs/1505.00078

Presentations

S. Rotger-Griful, S. Chatzivasileiadis, J. Matanza, R Hylsberg Jacobse, M. Wetter, Hardware-in-the-Loop Co-simulation of Distribution Grid for Demand Response, 19th Power Systems Computation Conference, Submitted

EE-McCloskey LB14029 Using Differential Electrochemical Mass Spectrometry to Characterize Catalytic Processes in Li-Air Batteries

Journal Publications

McCloskey, B. D.; Burke, C. M.; Nichols, J. E.; Renfrew, S. E. "Mechanistic insights for the development of Li-O2 battery materials: addressing Li2O2 conductivity limitations and electrolyte and cathode instabilities." Chemical Communications (2015), 51, 12701-12715.

Burke, C. M.; Pande, V.; Khetan, A.; Viswanathan, V.; McCloskey, B. D. "Enhancing electrochemical intermediate solvation through electrolyte anion selection to increase nonaqueous Li-O2 battery capacity." Proceedings of the National Academy of Sciences (2015), 112(30), 9293-9298.

Giordani, V.; Tozier, D.; Tan, H.; Burke, C. M.; Gallant, B. M.; Uddin, J.; Greer, J. R.; McCloskey, B. D.; Chase, G. V.; Addison, D. "A molten salt lithium-oxygen battery." Minor revisions requested, Journal of the American Chemical Society (2016).

Richey, F. W.; McCloskey, B. D.; Luntz, A. C. "Mg anode corrosion in aqueous electrolytes and implications for Mg-air batteries." Submitted, Journal of the Electrochemical Society (2016).

Knudsen, K. B.; Nichols, J. E.; Vegge, T.; Luntz, A. C.; McCloskey, B. D.; Hjelm, J. "An electrochemical impedance study of the capacity limitations in Na-O2 cells." In preparation for submission to Journal of Physical Chemistry C (2016).

Knudsen, K. B.; McCloskey, B. D.; Vegge, T.; Hjelm, J. "Revealing the surface and solution-based mechanisms in the Li-O2 battery by electrochemical impedance spectroscopy." In preparation for submission to the Journal of Physical Chemistry C (2016).

EE-Saxena LB13045 Transforming the Electricity & Automotive Markets with the LBNL Vehicle-to-Grid Simulator (V2G-Sim)

Journal Publications

S. Saxena, J. MacDonald, S. Moura, "Charging ahead on the transition to electric vehicles with standard 120V wall outlets", Applied Energy, 2015, http://dx.doi.org/10.1016/j.apenergy.2015.05.005

J. Greenblatt, S. Saxena, "Autonomous taxis could greatly reduce greenhouse-gas emissions of US light-duty vehicles", Nature Climate Change, 2015, http://dx.doi.org/10.1038/nclimate2685

S. Saxena, C. Le Floch, J. MacDonald, S. Moura, "Quantifying EV battery end-of-life through analysis of travel needs with vehicle powertrain models", Journal of Power Sources, 2015, http://dx.doi.org/10.1016/j.jpowsour.2015.01.072

T. Markel, A. Meintz, … S. Saxena, "Multi-Lab EV Smart Grid Integration Requirements Study", NREL technical report, 2015, http://www.nrel.gov/docs/fy15osti/63963.pdf

S. Saxena, J. MacDonald, D. Black, S. Kiliccote, "Quantifying the Flexibility for Electric Vehicles to Offer Demand Response to Reduce Grid Impacts without Compromising Individual Driver Mobility Needs", SAE Technical Paper, 2015, http://dx.doi.org/10.4271/2015-01-0304

EE-Todd LB15013 Behavior Analytics

Journal Publications

L. Jin, S. Borgeson, A. Spurlock, A. Todd, "Whipping Load Data Into Shapes: Behavior Insights from Load Shape Clustering in the Context of Program Targeting", Draft.

Fredman, S. Borgeson, L. Jin, A. Spurlock, A. Todd, "This American Life (style Group): Defining and Interpreting Energy Lifestyles Using Smart Meter Data", Draft.

S. Patel, S. Borgeson, A. Spurlock, A. Todd, "Which Households Respond? Exploring Heterogeneity in Response to Experimental Pricing Programs Using Pre-treatment Smart Meter Data", Draft.

Presentations

T. Kim, D. Lee, J. Choi, A. Spurlock, A. Sim, A. Todd, K. Wu, "Extracting Baseline Electricity Usage with Gradient Tree Boosting", Proceedings of 2015 International Conference on Big Data Intelligence and Computing, December 2015, https://sdm.lbl.gov/perf/DataCom2015-91-final.pdf

GN-Wei LB13022 Developing Epigenomic Technologies to Interrogate Genome Functions Relevant for Environment and Bioenergy

Journal Publications

Chew Yee Ngan, Chee-Hong Wong, Cindy Choi, Yuko Yoshinaga, Katherine Louie, Jing Jia, Cindy Chen, Benjamin Bowen, Haoyu Cheng, Lauriebeth Leonelli, Rita Kuo, Richard Baran, José G. García-Cerdán, Abhishek Pratap, Mei Wang, Joanne Lim, Hope Tice, Chris Daum, Jian Xu, Trent Northen, Axel Visel, James Bristow, Krishna K. Niyogi, Chia-Lin Wei. "Lineage-Specific Chromatin Signatures Reveal a Regulator of Lipid Metabolism in Microalgae." Nature Plants, 1: 15107 (2015)

Fan-Suo Geng, Marion Coolen, Øyvind Drivenes, Anja Baresic, Thomas Hawkins, Wigard Kloosterman, Yubo Zhang, Chia-Lin Wei, Stephen W. Wilson, Boris Lenhard, Silke Rinkwitz, Laure Bally Cuif, and Thomas S Becker. "Transcriptional control of miR-9 in embryonic and adult neural precursor cells by large enhancer arrays." Accepted in Scientific Reports.

Gina Turco, Kaisa Kajala, Govindarajan Ramamoorthy, Chew-Yee Ngan, Andrew Olson, Shweta Deshphande, Barbara Waring, Scott Stelpflug, Patricia Klein, Shawn Kaeppler, Doreen Ware, Chia-Lin Wei, Peter Etchells, and Siobhan Brady DNA Methylation and "Gene Expression Regulation Associated with Vascularization in Sorghum bicolor." Submitted to Plant Physiology

Chew Yee Ngan, Denis Tolkunov, Rita Kuo, Richard Dannebaum, Chee-Hong Wong, Jennifer Chiniquy, Eleanor Wong, Hope Tice, Cindy Choi, Benjamin J. Cole, Chris Daum, Govindarajan Kunde Ramamoorthy, Axel Visel, Chia-Lin Wei. "Genome-wide single-molecule sequencing reveals regulatory roles of 6 methyladenine in eukaryotes." Under review.

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

Journal Publications

D. Doud, T. Woyke. "Novel approaches in function-driven single-cell genomics", in preparation.

D. Doud, N. Ivanova, S. Singer, T. Woyke. "Substrate-directed single-cell genomics of active cellulose degraders", in preparation.

GN-Zhu LB14018 Development of a Cas9 Based Resource for Genome Engineering

Presentations

Dickel DE, Osterwalder M, Zhu Y, Yuzawa Y, Mannion B, Afzal V, Plajzer-Frick I, Pickle C, Akiyama JA, Rubin EM, Visel A, Pennacchio LA. Systematic deletion screens of distant-acting in vivo enhancers in mice. Talk at the 2015 Cold Spring Harbor Laboratory Genome Engineering: The CRISPR/Cas Revolution Meeting, September 24-27, 2015, Cold Spring Harbor, NY.

Dickel DE, Zhu Y, Osterwalder M, Mannion B, Afzal V, Plajzer-Frick I, Fang A, Pickle C, Akiyama JA, Rubin EM, Visel A, Pennacchio LA. Large-scale in vivo enhancer deletion with CRISPR/Cas9. Talk at the 2015 Cold Spring Harbor Laboratory Biology of Genomes Meeting, May 5-9, 2015, Cold Spring Harbor, NY.

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

Journal Publications

Curt R. Fischer, Oliver Rübel, Benjamin P. Bowen, An accessible, scalable ecosystem for enabling and sharing diverse mass spectrometry imaging analyses, Archives of Biochemistry and Biophysics, Available online 11 September 2015, ISSN 0003-9861, http://dx.doi.org/10.1016/j.abb.2015.08.021. (http://www.sciencedirect.com/science/article/pii/S0003986115300473)

LS-Brown LB14027 Reinventing Pre-Clinical and Environmental Testing Paradigms

Journal Publications

Stoiber MH, May G, Duff M, Obar R, Artavanis-Tsakonas S, Brown JB*, Graveley BR, Celniker SE. "Extensive cross-regulation in Drosophila post-transcriptional regulatory networks". Genome Research. 2015. doi:10.1101/gr.182675.114 *co-senior author, corresponding author, Stoiber is Brown Lab.

Mao, JH, Langley SA, Huang Y, Hang M, Bouchard KE, Celniker SE, Brown JB, Jansson JK, Karpen GH, and Snijders AM. "Identification of genetic factors that modify motor performance and body weight using Collaborative Cross mice." Scientific reports. 2015. 5: 16247.

Brown JB, Celniker SE. "Lessons from modENCODE". Annual Reviews of Genomics and Human Genetics. 2015, In Press, available online: DOI: 10.1146/annurev-genom-090413-025448

Wessel J, et al. "Low-frequency and rare exome chip variants associate with fasting glucose and type 2 diabetes susceptibility". Nat Commun. 2015, (6):5897. doi: 10.1038/ncomms6897.

LS-Celniker LB15022 Microbiome Adaptation in Response to Environmental Challenges

Journal Publications

J. Mao, S. Langley, Y. Huang, M. Hang, K. Bouchard, S. Celniker, J. Brown, J. Jansson, G. Karpen and A. Snijders, "Identification of genetic factors that modify motor performance and body weight using Collaborative Cross mice", Scientific Reports. 2015 5:16247, http://www.nature.com/articles/srep16247

LS-Xu LB14011 A Graphene-Based Platform for Correlative Electron and Super-Resolution Microscopy

Journal Publications

M. Wojcik, M. Hauser, W. Li, S. Moon, and K. Xu, "Graphene-enabled electron microscopy and correlated super-resolution microscopy of wet cells", Nature Commun.6, 7384 (2015).

MS-Analytis LB13040 Search and Synthesis of the Next Generation of Topological Insulators

Journal Publications

I. M. Hayes, Nicholas P. Breznay, Toni Helm, Philip Moll, Mark Wartenbe, Ross D. McDonald, Arkady Shekhter, James G. Analytis, "Magnetoresistance near a quantum critical point", arXiv:1412.6484

Kimberly A Modic, Tess E Smidt, Itamar Kimchi, Nicholas P Breznay, Alun Biffin, Sungkyun Choi, Roger D Johnson, Radu Coldea, Pilanda Watkins-Curry, Gregory T McCandless, Felipe Gandara, Z. Islam, Ashvin Vishwanath, Julia Y Chan, Arkady Shekhter, Ross D McDonald, James G Analytis, "Realization of a three-dimensional spin–anisotropic harmonic honeycomb iridate", Nature Communications 5, 4203 (2014).

Sylvia Lewin, James G. Analytis, "Angle-dependent magnetoresistance oscillations of cuprate superconductors in a model with Fermi surface reconstruction and magnetic breakdown", Phys. Rev. B 92, 195130 (2015)

Toni Helm, Robert Kealhofer, James Analytis, "Quasi-one dimensional order in superconducting Ta4Pd3Te16", in preparation

Sylvia Lewin, James G. Analytis "Magnetic breakdown in YBa2Cu3O7-x" in preparation

Alejandro Ruiz, Nicholas Breznay, James G. Analytis "Vestigial magnetic order in β-Li2IrO¬3" in preparation

Nicholas Breznay, James G. Analytis "Quantum oscillations suggest hidden quantum phase transition in the cuprate superconductor Pr2CuO4±δ" arXiv:1510.04268

MS-Buonsanti LB15023 Artificial Carboxysomes for CO2 Capture and Conversion in a Single Object

Journal Publications

Ignacio Luz, Anna Loiudice, Daniel T. Sun, Wendy L. Queen, Raffaella Buonsanti, "Understanding the Formation Mechanism of Nanocrystal@MOF-74 Hybrids.", submitted.

Anna Loiudice,Peter Lobaccaro, Esmail A. Kamali,Timothy Tao, Brendon Hung, Joel Ager, Raffaella Buonsanti, "Tailoring Cu Nanocrystals Towards C2 Products in Electrochemical CO2 Reduction", submitted.

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

Journal Publications

M. Kapilashrami, G. Conti, I. Zegkinoglou, S. Nemšák , C. Conlon, T. Törndahl, V. Fjällström, J. Lischner, S. G. Louie, A. Riazanova, L. Belova, R. J. Hamers, L. Zhang, J. Guo, C. S. Fadley, F. J. Himpsel, "B-doped diamond films as donor electrodes in photovoltaics: an x-ray absorption and hard x-ray photoemission study", J. Appl. Phys. 116, 143702 (2014)-October 14, 2014.

S. Nemšák, A. Shavorskiy, O. Karslioglu, I. Zegkinoglou, P. K. Greene, E. C. Burks, K. Liu, A. Rattanachata, C. S. Conlon, A. Keqi, F. Salmassi, E. M. Gullikson, S.-H. Yang, H. Bluhm, C. S. Fadley, "Chemical-state resolved concentration profiles with sub-nm accuracy at solid/gas and solid/liquid interfaces from standing-wave ambient-pressure photoemission", Nature Communications 5, 5441 (2014), November, 2014.

O. Karslıoğlu, S. Nemšák, I. Zegkinoglou, A. Shavorskiy, M. Hartl, F. Salmassi, E.M. Gullikson, M.L. Ng, Ch. Rameshan, B. Rude, D. Bianculli, A.A. Cordones-Hahn, S. Axnanda, E.J. Crumlin, P.N. Ross, C.M. Schneider, Z. Hussain, Z. Liu, C.S. Fadley, H. Bluhm, "Aqueous Solution/Metal Interfaces Investigated in operando by photoelectron spectroscopy", Faraday Soc. Disc., 2015, 180, 35 (2015), doi: 10.1039/C5FD00003C .

M. Marinova, J. E. Rault, A. Gloter, S. Nemšák, G. K. Pálsson, J.-P. Rueff, C. S. Fadley, C. Carrétéro, H. Yamadag, K. March, V. Garcia, S. Fusil, A. Barthélémy, O. Stéphan, C. Colliex, M. Bibes, "Depth profiling charge accumulation from a ferroelectric into a doped Mott insulator", Nano Letters 15, 2533−2541 (2015), April, 2015.

Johannes Lischner, G. K. Pálsson, Derek Vigil-Fowler, S. Nemsak, J. Avila, M. C. Asensio, C. S. Fadley, and Steven G. Louie, "Satellite Band Structure in Silicon Caused by Electron-Plasmon Coupling", Phys. Rev. B 91, 205113 (2015), May, 2015.

S. Nemšák, G. Conti, G.K. Pálsson, C. Conlon, S. Cho, J. Avila, M.-C. Asensio, P. Moetakef, C. Jackson, A. Janotti, C. G. Van de Walle, C. M. Schneider, S. Stemmer, and C. S. Fadley", "Observation by resonant angle-resolved x-ray photoemission of a critical thickness for 2-dimensional electron gas formation in SrTiO3 embedded in GdTiO3", Applied Phys. Lett. 107, 231602 (2015); http://dx.doi.org/10.1063/1.4936936. An Editor's Pick selection.

C.S. Fadley, "Hard X-ray Photoemission: An Overview and Future Perspective", invited introductory chapter to appear in the book Hard X-ray Photoemission, J. C. Woicik, Editor, Springer (2015), review of 37 pages and 20 figures. in press.

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 a two-dimensional electron gas at the buried interface between GdTiO3 and SrTiO3", submitted to Physical Review X, http://arxiv.org/abs/1508.01832 .

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", submitted to Physical Review B, http://arxiv.org/abs/arXiv:1510.06600 .

J. Lischner, S. Nemšák, G. Conti, A. Hloskovsky, G. K. Pálsson, W. Drube, S.G. Louie, C.S. Fadley, in preparation, "Accurate determination of the valence band

edge in hard x-ray photoemission spectra by means of GW theory", in preparation, to be submitted to Applied Physics Letters.

S.Nemšák, H. Fang, G. Conti, 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, to be submitted to Physical Review B.

S.Nemšák, H. Fang, G. Conti, C. Conlon, G. K. Pálsson, C. Battaglia, A. Javey, C.S. Fadley, "Angle-resolved photoemission and photoelectron microscopy from semiconductor membranes of WSe2 and MoS2", in preparation, to be submitted to Physical Review Letters.

R.B. Comes, S.-C. Lin, C.-T. Kuo, S.M. Heald, S.R. Spurgeon, D.M. Kepaptsoglou, Q.M. Ramasse, M. Engelhard, J. Rault, S. Nemsak, P.V. Sushko, C.S. Fadley, and S.A. Chambers, "Interface composition and electronic structure of LaCrO3/SrTiO3 from standing wave- and resonant core- and valence- photoemission", in preparation, to be submitted to Nature Materials

MS-Helms LB14028 Responsive Nanoparticle Assemblies

Journal Publications

T. Feng, D.A. Hoagland, and T.P. Russell, "Assembly of Acid-Functionalized Single-Walled Carbon Nanotubes at Oil/Water Interfaces," LANGMUIR 30(4), 1072-1079, DOI: 10.1012/la404543s, (January 2014).

T. Pham, A.P. Goldstein, J.P. Lewicki, S.O. Kucheyev, C. Wang, T.P. Russell, M.A. Worsley, L. Woo, W. Mickelson, and A. Zetti, "Nanoscale Structure and Superhydrophobicity of sp(2)-bonded Boron Nitride Aerogels," NANOSCALE 7(23), 10449-10458 (2015).

K. McEnnis, A.D. Dinsmore, and T.P. Russell, "Solid Particles Adsorbed on Capillary-Bridge-Shaped Fluid Polystyrene Surfaces," LANGMUIR 31(19), 5299-5305, DOI: 10.1021/acs.langmuir.5b00372, (May 19, 2015).

K. Bryson, T. Lobling, A.H.E. Muller, T.P. Russell, and R.C. Hayward, "Using Janus Nanoparticles to Trap Polymer Blend Morphologies during Solvent-Evaporation-Induced Demixing," MACROMOLECULES 48(12), 4220-4227, DOI: 10.1021/ace.macrmol.5b00640, (June 23, 2015).

C. Huang, Z. Sun, M. Cui, F. Liu1, B. A. Helms, T. P. Russell, "pH Resppnsive Structured Liquids" ADV. MAT, under review.

C. Huang, F. Liu1, B. A. Helms, T. P. Russell, "Assembly of Carboxylated Nanoparticles at the Water/Oil Interface", LANGMUIR, submitted.

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

Presentations

D. Frank Ogletree, Paul Ashby, Kristina Closser, Yi Liu, David Prendergast, Deirdre Olynick, Musa Ahmed, Oleg Kostko, Bo Xu, Suchit Bhattarai, Patrick Naulleau, "EUV Radiation Chemistry Fundamentals: Novel Experiments and Simulations," 2015 International Symposium on Extreme Ultraviolet Lithography, Maastricht Netherlands, October 5-7, 2015, proceedings available from LBNL Center fo X-ray Optics, Berkeley, CA.

P. Naulleau, C. Anderson, W. Chao, S. Bhattaria, A. Neureuther, “Multivariate Poisson Propagation Model and Resist Stochastics,” 2015 International Symposium on Extreme Ultraviolet Lithography, Maastricht Netherlands, October 5-7, 2015, proceedings available from LBNL Center fo X-ray Optics, Berkeley, CA.

O. Kostko, B. Xu, K. D. Closser, S. Bhattarai, D. L . Olynick, D. G. Prendergast, P. D. Ashby, D. F. Ogletree, Y. Liu, P. Naulleau, M. Ahmed, “Fundamental understanding of EUV radiation induced chemistry on a molecular level,” 2015 International Symposium on Extreme Ultraviolet Lithography, Maastricht Netherlands, October 5-7, 2015, proceedings available from LBNL Center fo X-ray Optics, Berkeley, CA.

Kristina D. Closser, David Prendergast, Musa Ahmed, Paul Ashby, Oleg Kostko, Yi Liu, Frank Ogletree, Deirdre Olynick, Bo Xu, Patrick Naulleau, “Interaction of EUV radiation with novel photoresist materials,” 2015 International Symposium on Extreme Ultraviolet Lithography, Maastricht Netherlands, October 5-7, 2015, proceedings available from LBNL Center fo X-ray Optics, Berkeley, CA.

Suchit Bhattarai, Shaul Aloni, Gong Chen, Andreas Schmid, Andrew R. Neureuther, Patrick P. Naulleau, “Investigation of Low Energy Electron Mean Free Path and Energy Delivery in EUV Resists,” 2015 International Symposium on Extreme Ultraviolet Lithography, Maastricht Netherlands, October 5-7, 2015, proceedings available from LBNL Center fo X-ray Optics, Berkeley, CA.

Dominik Ziegler, Andreas Amrein, Ken Matthews, Adrian Nievergelt, Arnaud Benard, Travis Meyer, Frank Ogletree, Deirdre Olynick, Patrick Naulleau, Andrea Bertozzi, Paul Ashby, “Improving Scan Speed and Resolution of AFM for Elucidating Resist Dissolution Dynamics,” 2015 International Symposium on Extreme Ultraviolet Lithography, Maastricht Netherlands, October 5-7, 2015, proceedings available from LBNL Center fo X-ray Optics, Berkeley, CA.

MS-Neaton LB15026 Computational Design of Smart Complex Oxides with Tunable Quantum Phases

Journal Publications

L. M. Schoop, L. S. Xie, R. Chen, Q. D. Gibson, S. H. Lapidus, I. Kimchi, M. Hirschberger, N. Haldolaarachchige, M. N. Ali, C. A. Belvin, T. Liang, J. B. Neaton, N. P. Ong, A. Vishwanath, and R. J. Cava, "Dirac metal to topological metal transition at a structural phase change in Au2Pb and prediction of Z2 topology for the superconductor," Phys. Rev. B 91, 214517 (2015)

S. Barja, S. Wickenburg, Z.-F. Liu, Y. Zhang, H. Ryu, M. M. Ugeda, Z. Hussian, Z.-X. Shen, S.-K. Mo, E. Wong, M. B. Salmeron, F. Wang, M. F. Crommie, D. F. Ogletree, J. B. Neaton, and A. Weber-Bargioni, “Observation of charge density wave order in 1D mirror twin boundaries of single-layer MoSe2”, submitted to Nature Physics (2015)

MS-Schoenlein LB14025 Dynamic Studies of Mesoscale Electronic Ordering in Complex Materials

Journal Publications

M.C. Langner, S. Zhou, G. Coslovich, Y.D. Chuang, Y. Zhu, J. S. Robinson, W.F. Schlotter, J.J. Turner, M.P. Minitti, R.G. Moore, W.S. Lee, D.H. Lu, D. Doering, P. Denes, Y. Tomioka, Y. Tokura, R.A. Kaindl, and R.W. Schoenlein, "Ultrafast x-ray

and optical signatures of phase competition and separation underlying the photoinduced metallic phase in Pr1-xCaxMnO3," Phys. Rev. B 92, 155148 (2015).

M.C. Langner, S. Roy, A.F. Kemper, Y.-D. Chuang, S.K. Mishra, R.B. Versteeg, Y. Zhu, M.P. Hertlein, T.E. Glover, K. Dumesnil, and R.W. Schoenlein, "Scattering bottleneck for spin dynamics in metallic helical antiferromagnetic dysprosium," Phys. Rev. B, in press (2015).

NE-Wright LB14026 Codesigning Big Iron for Big Data

Presentations

2014 C. S. Daley, L. Ramakrishnan, S. Dosanjh, N. J. Wright, "Analyses of Scientific Workflows for Effective Use of Future Architectures", The 6th International Workshop on Big Data Analytics: Challenges, and Opportunities (BDAC-15) in cooperation with the 27th IEEE/ACM International Conference for High Performance Computing, Networking, Storage, and Analysis (SC15), November 16 2015, Austin, TX, USA.

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

Presentations

Anthony Mezzacappa, E. J. Lentz, S. W. Bruenn, W. R. Hix, O. E. B. Messer, E. Endeve, J. M. Blondin, J. A. Harris, P. Marronetti, K. N. Yakunin, and E. J. Lingerfelt, "A Neutrino-Driven Core Collapse Explosion of a 15 Solar Mass Star," talk presented at ASTRONUM 2014, arXiv:1507.05680 (to appear in the Proceedings) http://arxiv.org/abs/1507.05680

K. N. Yakunin, P. Marronetti, A. Mezzacappa, O. E. Bronson, E. J. Lentz, S. W. Bruenn, W. R. Hix, and J. Austin Harris, "Multimessengers from 3D Core-Collapse Supernovae," talk presented at the 50th Recontres de Moriond on Gravitation, arXiv:1507.05901 (to appear in the Proceedings) http://arxiv.org/pdf/1507.05901

E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P. M. Vranas, and A. Walker-Loud, ``Two-Nucleon Higher Partial-Wave Scattering from Lattice QCD," arXiv:1508.00886 http://arxiv.org/abs/1508.00886

T. Kurth, A. Polchinsky, A. Sarje, S. Syritsyn, and A. Walker-Loud, "High Performance I/O: HDF5 for Lattice QCD," talk presented at the 32nd Symposium on Lattice Field Theory, arXiv:1501.06992 (to appear in the Proceedings) http://arxiv.org/abs/1501.06992

NS-Ploskon LB14020 Next Generation Si-Based Tracking and Massive Online Data Processing for Collider Experiments

Journal Publications

M. Fasel et al., "Using NERSC High-Performance Computing (HPC) systems for high energy nuclear physics applications with ALICE", to be submitted, February 2016

NS-Vetter LB15028 Multi-Disciplinary Research to Enhance Understanding of Transport, Risks, and Mitigation of Radioisotopes for Improved Radiological Resilience

Journal Publications

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," to be submitted to Phys. Rev. B.

S. Costes, D. Sridharan, S. Gauny. D. An, A.-C. Heuskin, 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.

Andrew Haefner, Ross Barnowski, Paul Luke, Mark Amman, Lucian Mihailescu, Kai Vetter. "Handheld Real-time Volumetric 3-D Gamma-ray Imaging" in preparation.

Andrew Haefner et. al. "3-D Gamma-ray Compton Imaging from an Unmaned Aerial System in Fukushima, Japan." In preparation.

Presentations

E.R. Siirila-Woodburn, C.I., Steefel, K.H., Williams, J.T., Birkholzer, "An integrated hydrologic modeling approach to cesium-137 transport in forested Fukushima watersheds" 2015 American Geophysical Fall Meeting. In preparation 2015.

PB-Ajo-Franklin LB13027 Probing Dynamics of Electron Transfer for Microbial-based Energy Interconversion

Journal Publications

H. Jensen, M. TerAvest, M. Kokish, C. Ajo-Franklin, "CymA and exogenous flavins improve extracellular electron transfer and couple it to cell growth in Mtr-expressing Escherichia coli," ACS Synthetic Biology, in revision.

T. Fukushima, S. Gupta, R. Mizrahi, B. Rad, C. Ralston, C. M. Ajo-Franklin, "The Electron Transfer Protein MtrF Uses Tertiary Structure to Recognize Minerals" Proceedings of the National Academy of Sciences USA in preparation.

Presentations

C. Ajo-Franklin, "Controlling Organisms Electrically with Synthetic Biology," 2015 Synthetic Biology: Engineering, Evolution & Design (SEED). June 13, 2015.

M. TerAvest, C. Ajo-Franklin, "Transforming exoelectrogens for biotechnology using synthetic biology," Biotechnology & Bioengineering, September 8, 2015.

C. Ajo-Franklin, "Understanding native exoelectrogens & engineering new ones," 2015 International Society of Microbial Electrochemistry & Technology (ISMET). October 1, 2015.

PB-Chang LB15037 Interfacing Chemical and Biological Catalysis for Solar-to-Fuel Conversion

Journal Publications

E. Nichols, J. Gallagher, C. Liu, Y. Su, J. Resasco, Y. Yi, Y. Sun, P. Yang, M. Chang, C. Chang "Hybrid bioinorganic approach to solar-to-chemical conversion", Proc. Natl. Acad. Sci. U.S.A. 2015, 112, 11461-11466. (http://www.pnas.org/content/112/37/11461.full.pdf)

PB-Deutschbauer LB13028 Functional Genomic Encyclopedia of Bacteria and Archaea: Evidence-Based Annotation of the Microbial Tree of Life

Journal Publications

B.E. Rubin, K.M. Wetmore, M.N. Price, S. Diamond, R.K. Shultzaberger, L.C. Lowe, G. Curtin, A.P. Arkin, A. Deutschbauer, S.S. Golden "The essential gene set of a photosynthetic organism" Proc Natl Acad Sci USA 2015. http://www.pnas.org/content/112/48/E6634.long

K.M. Wetmore, M.N. Price, R.J. Waters, J.S. Lamson, J. He, C.A. Hoover, M.J. Blow, J. Bristow, G. Butland, A.P. Arkin, A. Deutschbauer "Rapid quantification of mutant fitness in diverse bacteria by sequencing randomly bar-coded transposons" mBio 2015. http://mbio.asm.org/content/6/3/e00306-15

PH-Bailey LB14022 Tactical High Throughput Computing: Improving Interdisciplinary Tools for High Throughput Computing at NERSC and Beyond.

Journal Publications

S. Alam, F. D. Albareti, C. Allende Prieto et al., "The Eleventh and Twelfth Data Releases of the Sloan Digital Sky Survey: Final Data from SDSS-III," Astrophysical Journal Supplement 219 (2015) 12 http://arxiv.org/abs/1501.00963 http://www.sdss.org/dr12/

PH-Bebek LB13033 Higher Performance CCDs for Next Generation Dark Energy Experiments

Journal Publications

C.J. Bebek et al, "CCD development for the Dark Energy Spectroscopic Instrument," J. Instrum., 10, C05026, 2015. http://iopscience.iop.org/article/10.1088/1748-0221/10/05/C05026

S.E. Holland, C.J. Bebek, W.F. Kolbe, and J.S. Lee, "Physics of fully depleted CCDs," J. Instrum., 9, C03057, 2014. http://iopscience.iop.org/article/10.1088/1748-0221/9/03/C03057

S.E. Holland, C.J. Bebek, F. Dion, R. Frost, R. Groulx, J.S. Lee and G. Wang, "Technology and device-design enhancements for improved read noise performance in fully depleted CCDs," Proc. of SPIE, 9154, 91541E-1, 2014. http://spie.org/Publications/Proceedings/Paper/10.1117/12.2057219

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

Presentations

ATLAS Collaboration, "A search for Supersymmetry in events containing a leptonically decaying Z boson, jets and missing transverse momentum in $\sqrt{s}$=13 TeV pp collisions with the ATLAS detector", ATLAS-CONF-2015-082, https://cds.cern.ch/record/2114854

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

Journal Publications

K. Rotermund et al., Planar Lithographed Superconducting LC Resonators for Frequency- Domain Multiplexed Readout Systems. J. Low Temp. Phys., 2016. doi:10.1007/s10909-016-1554-4

O. Jeong et al. Broadband Plasma-Sprayed Anti-reflection Coating for Millimeter Wave Astrophysics Experiments. J. Low Temp. Phys., 2016. doi:10.1007/s10909-015-1442-3

A. Suzuki et al. The Polarbear-2 and the Simons Array. J. Low Temp. Phys., 2016. doi: 10.1007/s10909-015-1425-4

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

Journal Publications

S.Knapen, D.Redigolo, D.Shih, "General Gauge Mediation at the Weak Scale", accepted in JHEP, http://arxiv.org/abs/arXiv:1507.04364

S.Knapen, D.Robinson, "Disentangling Mass and Mixing Hierarchies", Phys.Rev.Lett. 115 (2015) 16, 161803, http://arxiv.org/abs/arXiv:1507.00009

J.Kearney, H.Yoo, K.Zurek, "Is a Higgs Vacuum Instability Fatal for High-Scale Inflation?", Phys.Rev. D91 (2015) 12, 123537, http://arxiv.org/abs/arXiv:1503.05193

A.Basirnia, D.Egana-Ugrinovic, S.Knapen, D.Shih, "125 GeV Higgs from Tree-Level A-terms", JHEP 1506 (2015) 144, http://arxiv.org/pdf/1501.00997.pdf

N.Craig, S.Knapen, P.Longhi, "The Orbifold Higgs", JHEP 1503 (2015) 106, http://arxiv.org/abs/1411.7393.pdf

SN-Monga LB15032 ESnet Network Operating

Presentations

Inder Monga, Network Operating Systems and Intent APIs for SDN Applications, Technology Exchange Conference, October 6, 2015,

Eric Pouyoul, ENOS: A Network Operating System for ESnet Testbed, Technology Exchange Conference, October 6, 2015