LBNL-103E

Laboratory Directed Research and Development Program FY 2014

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Report on
Ernest Orlando Lawrence
Berkeley National Laboratory

Laboratory Directed Research and Development Program

FY 2014

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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, and energy technologies in a manner that ensures employee and public safety and 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 to 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 support DOE's Strategic Themes that are codified in DOE's 2011 Strategic Plan (DOE/CF-0010), with a primary focus on Scientific Discovery and Innovation. For that strategic theme, the Fiscal Year (FY) 2014 LDRD projects support each one of the four goals through multiple strategies described in the plan. In addition, LDRD efforts support the four goals of Energy Security, the two goals of Environmental Responsibility, 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. The 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 LDRD program also play 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, breast cancer and accelerator research supported by the Department of Defense, detector and engineering technologies that should be useful to the Department of Homeland Security, and particle detection that will be valuable to the Environmental Protection Agency.

The *Berkeley Lab Laboratory Directed Research and Development Program FY2014* 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.

The Berkeley Lab LDRD program is a critical tool for directing the Laboratory's forefront scientific research capabilities toward vital, excellent, 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 capability, and permits exploration of exciting new opportunities. All projects are work in forefront areas of science and technology. Areas eligible for support include the following:

- 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 maintain compliance 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 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 FY2014, 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 ~3.5% of Berkeley Lab's FY2014 projected operating and capital equipment budgets. This funding level was provided to develop new scientific ideas and opportunities and allow the Berkeley Lab Director an opportunity to initiate new directions. In all about $23.5M was expended for operating expenses.

In FY2014, scientists submitted 206 proposals, requesting about $54.2M in funding prior to assessing laboratory overhead. Eighty three projects were funded, with awards ranging from $16K to $700K.

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
Researcher(s): Hann-Shin Mao (Postdoc)

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, (1) design of a gas jet capable of providing 1-10 MeV electrons, (2) development of a hollow core fiber suitable for transporting the necessary laser energy, and (3) establishing a program to evaluate the efficacy of LPA produced electrons as a radiation source. The gas jet target uses a gas profile featuring a sharp density transition to reduce the 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

Simulations have successfully shown 1-10 MeV electron beam generation with about 10 mJ of laser energy. This is achieved by relying on breaking of a laser excited plasma wave at a sharp density transition. To realize this density profile with step, a special gas jet has been developed with two distinct gas regions. The second gas region has half the electron density of the first region, and the density transition occurs in a few 10's of μm that, according to the simulations, is expected to allow electron injection with small amounts of laser energy. The total length of the gas cell is 350 μm, sufficiently small to act as an internal target during treatment.

Guided by the simulation results, a design was developed to physically achieve such a density profile. This jet design uses two converging diverging nozzles that are pressure matched at the nozzles' exit. The resulting flow is known as a slip line where two regions of disparate density can exist in steady state. In order to demonstrate the initial design, the gas jet was constructed at a scale that is fourteen times larger than the original design. This enables easier manufacturing and a rather straightforward measurement of the density drop. Furthermore, the enlarged device would act as an initial laser target for comparison to simulation. A provisional patent was submitted for this novel two-stream gas jet technique.

Currently, we are in the process of integrating the target into an existing target chamber that is powered by an existing10 TW laser system. This includes modifying several components of the system to accommodate the new target. In initial experiments, high power laser beams have been focused on the gas target with the longitudinal profile of plasma recombination light showing evidence of a density drop. Quantifying the longitudinal gas density and studies to establish the minimum amount of laser energy that is needed to generate e-beams are scheduled for FY15. Additionally, a second round of simulations that includes ionization effects for the scaled up target is being performed to benchmark experimental results.

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 (ns), intense ion beam capability available at LBNL and in the second 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 second year of this LDRD we have routinely used pulses of lithium and potassium ions (~300 keV) with tunable pulse lengths of (15-600 ns), and with up to $2x10^{11}$ ions/pulse/cm^2 to implant samples. When ions from such a pulse impinge on targets such as single crystal silicon samples lattice atoms can be dislodged and a cascade ensues, where many vacancies and interstials are formed, followed by rapid cooling and recombination of defects. We probed the built-up and relaxation rates of defects during ion pulses by making use of the channeling effect. Ions can channel deeply into pristine crystals, but defects scatter ions out of channeling trajectories. We quantify the fraction of channeling ions *in situ* by time resolved measurements of ion transmission through membranes. *In situ* ion transmission measurements allow us to track damage built-up with a time resolution of ~1 ns. Figure 1 shows the intensity of ions that channel as a function of the tilt angle. In year 2, we increased the time resolution (by tuning to shorter pulses and by designing a faster diagnostics), we performed systematic measurements for a

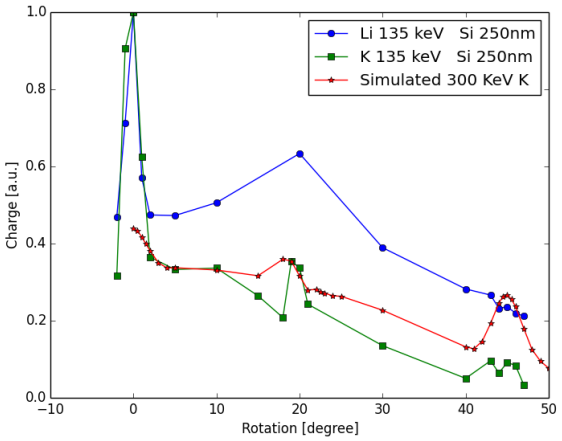


Fig. 1: Transmission of ions through single crystal silicon membranes as a function of the tilt angle. The peaks at 0, 20 and 45 degree show that a fraction of the ions in the intense pulse channel through the crystal lattice. Monitoring of the channeled ion fraction as a function of time during intense ion pulses is a very sensitive way to track the formation and recombination dynamics of defects.

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

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

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

One of our most significant accomplishments is the development of a novel method for high-fidelity modeling of the propagation of electromagnetic waves on a supercomputer. The unprecedented level of flexibility in the tuning of accuracy and locality of our method enables very high (spectral-like) accuracy while preserving scalability to a very large number of computer cores. Our new solver also offers larger time steps than conventional solvers by removing the standard limitations due to the well-known Courant-Friedrich-Levy condition.

Another significant accomplishment is the analysis of the so-called “numerical Cherenkov” instability for our solver in various modes that has lead to the successful development of novel methods that mitigate the instability. The mitigation method has been automated in our Particle-In-Cell code Warp and is now successfully used by collaborators at other institutions.

Strong scaling of the new method was demonstrated on NERSC’s supercomputers Hopper and Edison, yielding near-linear scaling up-to 50,000 cores. During the scalability studies, we also worked to analyze the performance variability of Edison at larger core counts and developed methods to ascertain scalability in the time-sharing environment with the newer Cray Aries interconnect with Dragonfly topology. The scalability of our solver was also contrasted to the scaling of standard global FFTs. The results were presented at the international SC’14 conference and will be documented in a journal publication.

We are beginning to develop and study the scalability of the solver on test-bed next generation computers through portable implementations of the solvers, via heterogeneous and emerging programing models. The solver is critical to the further development of the Warp code, which has been selected in a highly competitive competition as a first tier NERSC NESAP (NERSC Exascale Science Application Program) application. We are also in the process of extending our methods to three dimensions and applying them to large-scale simulations of laser plasma accelerators.

Magnetic-Field-Induced and Transient Quantum Phases in Correlated Materials

Principal Investigators: Elke Arenholz and R. Ramesh

Project Description

We continued the development of resonant soft x-ray scattering (RSXS) into a novel technique for the study of quantum phases exhibiting unique properties in conductance, magnetism and structure.

Accomplishments

We have optimized our resonant soft x ray scattering setup at ALS BL4.0.2 for experiments involving interfaces in nano- and mesoscale heterostructures. For example, detector and sample motion are synchronized with tuning the photon energy of the beamline which allows scanning through the $L_{3,2}$ edges of transition metals monitoring the intensity of Bragg scattering features. In addition to the original diodes installed for detection of the scattered intensity, the system is now equipped with a CCD that allows capturing an angle range of 10º horizontally and 10º vertically which is invaluable for measuring the scattered intensity near the specular reflection in small angle scattering experiments.

We have studied three prototypical systems to develop the tools for RSXS studies of interfaces and domain walls in oxide heterostructures on the nano and mesoscale:

1. Self-organized functional multiscale arrays in form of columns in a matrix were synthesized by codepositing a transition metal oxide with spinel structure and another transition metal oxide with perovskite structure This approach uniquely allows the coupling of order parameters at the interfaces between column and matrix. RSXS at absorption edges allowed us probing selectively the electronic and magnetic structure at interfaces taking advantage of the periodicity of the self-assembled nanostructure.

2. Domain walls corresponding to a rotation of the ferroelectric polarization by e.g. 71° or 109° exist in $BiFeO_3$, a multiferroic that exhibits canted antiferromagnetism as well as ferroelectricity at ambient temperature. By carefully choosing the layer thickness, periodic domain arrays with evenly spaced domains separated by walls of only one type have been created by our team. These refined periodic arrays then served as a model diffraction lattice for soft x-rays. A pronounced dichroism is observed and its detailed analysis as a function of photon energy will provide new insights into the electronic and magnetic structure of the domain walls.

3. RSXS can be made uniquely sensitive to the interfacial electronic structure of layered oxide systems. For a super lattice with sublayer thicknesses of m and n unit cells, the scattering factor will vanish for any reflections with $L=u+v$ if u, v are integers and $u/v=m/n$. In these geometries for which a superlattice reflection is forbidden by symmetry, the residual intensity is a sensitive measure of the difference in scattering factors at the interface as compared to the bulk of the layers. Monitoring the photon energy dependence of the scattered intensity provides new insights into the electronic and spin structure at the interfaces.

Ultra-High Resolution Microscopy of Nano-Materials by Scanning X-Ray Diffraction Microscopy

Principal Investigator: David Shapiro

Project Description

The goal of this proposal is to develop the scientific user community for the next generation soft x-ray spectro-microscopy and tomography based on x-ray ptychography. X-ray ptychography is a robust diffraction imaging method that can take full advantage of the high brightness of the ALS and which is not limited in resolution by the x-ray optics. The technique we have developed enhances the already high resolution scanning transmission x-ray microscope (STXM) with the addition of diffraction data and is able to probe chemical species, molecular orientation, magnetization, and structural morphology at <10 nm resolution. We will apply this method to difficult problems in the material sciences with a focus on materials for energy and carbon cycle research. In particular, we will study chemical phase transformations in nano-crystals of active battery electrodes, hydration reactions in calcium silicate hydrate, pore evolution in sintered zirconia, and magnetic domain structure in thin magnetic films. Finally, we will further develop in situ methods for high resolution microscopy of electrochemical and hydration reactions in these materials. These studies require the ability to visualize 10 nm scale features embedded in a micron-scale matrix with sensitivity to the chemical species however there currently is no imaging technique with such capabilities. We will develop soft x-ray scanning diffraction microscopy with the study of these systems and provide a microscopy program that will directly and efficiently benefit from the very high brightness of the new COSMIC beamline at the ALS and future beamlines at the ALS-U. This program will readily be extended to other problems in the materials sciences such as the study of porous zeolites for carbon capture and catalysis and the characterization of materials by design like self-assembled nanoparticle aggregates for replacement of non-renewable resources in batteries and solid state devices. Finally, this project will leverage the computational resources at NERSC for the reconstruction of Giga-element datasets and potentially provide experimental feedback to material computation efforts.

Accomplishments

Using the unique spatial resolution and chemical sensitivity of our imaging method we have directly visualized a two phase chemical transformation and the complicated chemical domain pattern present in the smallest available nano-crystals of $LiFePO_4$. Our measurements were also correlated with high resolution transmission electron microscope images of many such particles to show that these small particles do not suffer from material fracture (as do larger particles) but still display a complicated domain pattern which does not correlate with the material crystallographic axes as was expected. These results seem to indicate that the superior electrochemical performance of the small particles is due primarily to mechanical issues rather than the fundamental character of the phase transformation itself and provides critical insight into how to engineer higher performing batteries.

We have also used our high resolution imaging technique to measure the magnetic domain wall width distribution in a thin film of CoPd, the pore size distribution in sintered Yttria stabilized zirconia, and the x-ray magnetic circular dichroism spectrum in magnetotactic bacteria all with spatial resolutions which are not achievable at any other x-ray facility worldwide.

Novel Accelerator Techniques for Diffraction Limited Light Sources

Principal Investigator: Christoph Steier

Project Description

Storage ring based light sources have been extremely successful over the years, enabling forefront science in many areas. Recent developments in accelerator technology and lattice design open the door for very large further 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. While there are no showstoppers, work was necessary to reduce risk and cost, enable a timely execution, and optimize the properties of the source to the needs of the science case and prospective user community. The goal of this project was to investigate, demonstrate and improve critical technologies necessary for diffraction limited storage ring light sources at the subsystem level. At a later stage, tests will be carried out with some of those new systems using beams in existing light sources.

Accomplishments

There were three main goals for year one: Achieve a firm understanding of the possible performance of a soft x-ray diffraction limited storage ring; establish the feasibility of the needed accelerator technologies; provide the technical know-how necessary for an upgrade proposal guided by an excellent science case. These high level goals were achieved by the end of year one by putting development effort into the following detailed sub-areas:

1. Fast rise-time pulsed magnets for the swap-out injection
2. Very small aperture vacuum chambers with NEG coating
3. Bunch lengthening, phase transients, third harmonic cavities
4. Advanced radiation producing devices (Superbends, Undulators)
5. Physics design optimization, Code development and benchmarking

As result of the work during year one, a candidate configuration for a soft–ray diffraction limited light source was developed. The performance of the proposal was optimized in conjunction with the development of the science case, with the capability to deliver diffraction-limited light throughout the soft x-ray range. The feasibility of the underlying technologies was studied and all were shown to be feasible. As a result of the studies, several design optimizations were made to provide for better performance.

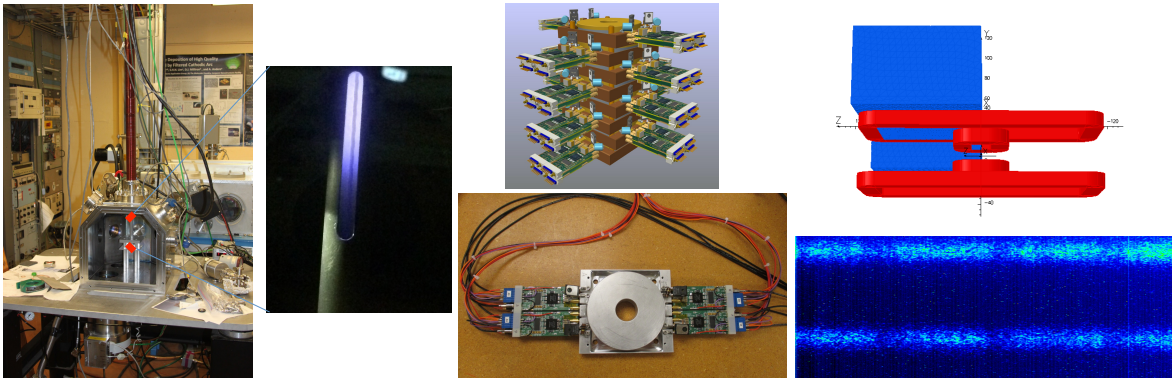


Figure 1: Examples of results from year one: Coating setup for very small aperture NEG chambers; fast injection pulser; concept of a superbend magnet; transient beam loading measurements with tailored fill-patterns.

Next Generation Gratings for X-ray Spectroscopy and Pulse Manipulation

Principal Investigator: Dmitriy Voronov

Project Description

There is a great need in advanced diffraction gratings at the ALS and other synchrotron facilities. To provide high spectral resolution and high diffraction efficiency the gratings are required to have a variable line spacing (VSL), perfect blazed grooves, and smooth groove surface. For Reflective Zone Plates (RZP) elliptical lines are required to provide two dimensional focusing. Fabrication of such gratings with holographic recording and mechanical ruling is challenging. Due to limitations of conventional techniques one can only design gratings within a very limited set of variables. New approaches for fabrication of high quality grating in a cost effective manner should be found to make advanced diffraction gratings available.

This work aims development of a new grating fabrication process based on Direct Write Lithography (DWL) technique which is used in semiconductor industry for making high resolution MEMS structures, nanostructures, and consumer microelectronics. A grating pattern can be written by scanning a focused laser or electron beam over a substrate surface coated with a photoresist. The DWL technology will be used as a pattering technique for making diffraction gratings of arbitrary groove density variation and groove shape complexity. The best available DWL systems will be used for making grating prototypes which will be characterized in terms of groove position accuracy, imaging performances, and diffraction efficiency.

DWL process will be optimized and eventually combined with wet anisotropic etch technique for making highly efficient blazed gratings. Deposition of multilayer coatings on saw-tooth substrate will allow a new kind of x-ray gratings, Multilayer-coated Blazed gratings which will be a basis for a new generation of high resolution and high throughput x-ray instrumentation.

Accomplishments

1. A procedure and software for generation of Reflective Zone Plate (RZP) patterns which are two-dimension gratings has been developed. Design of the patterns was optimized to provide required precision of elliptical grooves and reasonable size of a RZP data file.
2. A full process for in-house making of lamellar gratings using optical direct write lithography has been developed. Photo-resist spin-coating, exposure of resist-coated substrates with DWL66 machine, and plasma etch have been improved to reduce line edge roughness of grating patterns. A lamellar VLS grating for ALS Beamline 12.0.1 was fabricated, tested, and installed in the beamline monochromator.
3. A process of wet anisotropic etch of asymmetrically cut Si substrates has been optimized for making x-ray blazed gratings with extremely small blaze angles. A prototype of a blazed grating with a blaze angle of 0.65° for BL12.0.1 demonstrated 3-fold improvement in diffraction efficiency as compared to the original commercial grating.
4. Electron beam lithography as a direct write technique for grating fabrication has been tested.
5. Optimization of multilayer coated blazed gratings (MBG) for Querlin RIXS spectrometer has been done via diffraction efficiency simulation.
6. New record efficiency of a EUV multilayer blazed grating has been achieved.
7. This work is summarized in five publications and was reported at Optics and Photonics SPIE conference in 2014. One manuscript has been prepared for publication and submitted in Optics Express.

Probing Dynamics with Multi-color, Multi-pulse Laser and Synchrotron Photons

Musahid Ahmed & Daniel Slaughter

Project Description:
The flow of energy and electric charge in molecules are central to both natural and synthetic molecular systems that convert sunlight into fuels and evolve over a multitude of timescales. Understanding and controlling these processes remains a fundamental science challenge. We address this challenge by probing chemically complex systems in the gas phase by combining the precise time information of ultrafast spectroscopy techniques with the chemical sensitivity characteristic of synchrotron radiation. An ultrafast pulse pair with VUV or soft x-ray photons from the synchrotron are used to make measurements with atomic-site specificity. With access to photons spanning the range of terahertz to hard X-rays that is provided by a synchrotron, coupled with the rich spectroscopy available in the UV-VIS-IR region provided by table top ultrafast lasers, a multi-dimensional tool to probe dynamics is enabled.

Accomplishments:
We have developed a portable transient absorption experimental apparatus to perform time-resolved analysis of two color (ultraviolet + tunable infrared) laser excitation schemes applicable to a variety of gaseous systems. This setup is currently deployed at the soft x-ray Beamline 6.0.2 at the Advanced Light Source, where we are interrogating the excited state spectroscopy and dynamics of nitrophenols: Here one ultrafast pulse (in the present experiments 263nm) excites o-nitrophenol while a second ultrafast infrared pulse (1100 nm – 2500 nm, tuned to a resonance) promotes the system to nearby vibronic state after a suitable time delay. The transmitted IR light is detected by a photodiode and a high-sensitivity photon spectrometer to determine the absorption as a function of IR wavelength and time delay. These experiments will be performed in parallel with laser-synchrotron experiments as a complementary diagnostic tool, allowing for the precise control of the electronic states in model chromophores that is crucial towards developing ultrafast laser-synchrotron multicolor spectroscopy.

We have measured ion momentum images of o-nitrophenol following photoexcitation and photoionization from its electronic ground state by soft x-rays tuned near the core-level resonances of oxygen and nitrogen, at Beamline 6.0.2 at the Advanced Light Source. Ultraviolet pulses, produced from the 3rd harmonic of a Ti:sapphire laser system that is synchronized to the ALS storage ring and the 4kHz repetition rate of the soft x-ray Beamline, were also employed in these experiments in an effort to measure the products of laser photodissociation by core-level ion momentum spectroscopy. Our subsequent improvements to the reliability of the laser systems have increased the laser pulse energies from a few hundreds of nanojoules to above 10 microjoules for each of the UV and IR laser beams that will be used for the 3 color experiments. With all the hardware and staff in place experiments are underway to probe the dynamics of evolving excited states in gas phase systems.

Confined Catalysts Based on Metal-Organic Frameworks

John F. Hartwig, Jeffrey Long, F. Dean Toste, Douglas S. Clark.

Project Description: The general goal of this research program is to develop catalysts that can be used as part of a multi-step, multi-catalyst system, termed a "catalytic network," in which mutually incompatible catalysts are made compatible by confinement and the rates of catalytic reactions can ultimately be regulated by feedback mechanisms. To this end, we have sought to achieve reactivity from catalyst sites contained in metal-organic frameworks, to create novel, artificial catalysts within an enzyme active site, and to develop multistep catalytic processes with phase separated small-molecule catalysts.

Accomplishments: We have prepared metal-organic frameworks containing site-isolated, high-valent iron-oxo species that functionalize C-H bonds. Reaction of the iron-containing framework $Fe_{0.1}Mg_{1.9}$(dobdc) [$dobdc^{4-}$ = 2,5-dioxido-1,4-benzenedicarboxylate] with N_2O in the presence of ethane forms ethanol in 60% yield (with respect to iron). Weaker C-H bonds, such as those found in 1,4-cyclohexadiene also give oxidized products. We are currently expanding this chemistry to other iron-based frameworks with the aim of developing catalysts and reaction conditions that will be easier to incorporate into a catalytic network. As such, we are also exploring the use of different oxidants and substrates.

In parallel, we have developed a dual catalyst system to homologate *alpha*-olefins to tertiary amines by sequential hydroformylation and reductive amination (Figure 1). Hydroformylation occurs in the organic phase of the reaction medium and is 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. 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.

Finally, we have prepared artificial enzymes by two methods, In the first, we prepared noble metal-porphyrin active sites in myoglobin. Based on prior reconstitution of myoglobin with both abiotic protoporphyrins ([M]-PPIX) and [M]-salen complexes, we incorporated new Ir, Rh, Co, and Ru-based cofactors into myoglobin mutants in which the axial ligand and secondary coordination sphere are varied. In the past year, we developed a new, highly efficient method for the generation of artificially metallated myoglobins based on the direct expression and purification of apo-myoglobins. Using these new myoglobin-based catalysts, we have shown for the first time that an artificially-metallated PPIX-binding protein can catalyze organic reactions that cannot be catalyzed by the same protein binding its native Fe-PPIX cofactor. In particular, Ir(Me)-PPIX-myo catalyzes cyclopropanation of internal olefins and carbene insertion into C-H bonds, while Co-salen-myo catalyzes intramolecular hydroamination of unbiased substrates.

In the second approach, we developed artificial metalloenzymes for transformations for which there are no known metal catalysts. We are doing so by a bottom-up approach in which we identify by high throughput screening of unrestricted metal-ligand combinations a model reaction using reagents and conditions compatible with proteins. We then conjugate this catalytic site into a protein hosts, using covalent or non-covalent interactions; the catalytic properties of the conjuagates are then be evaluated, and the activity of the enzyme fined-tuned by modification of the ligand used. Following this proposed methodology, identified a metalloenzyme for regioselective halogenation of (poly)aromatic substrates. A Cobalt cofactor covalently bound to nitrobindin catalyzes the halogenation of a simple, water-soluble arene.

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

The electron-electron correlation energy is negative, and attractive dispersion interactions are entirely a correlation effect, so the contribution of correlation to intermolecular binding is commonly assumed to be negative, or binding in nature. However, we have discovered that there are many cases where the long-range correlation binding energy is *positive*, and therefore anti-binding, with certain geometries of the water dimer as a prominent example. We have also undercover the origin of this effect, which is the systematic overestimation of dipole moments by mean-field theory, leading to reduced electrostatic attraction upon inclusion of correlation. Thus, EDA's that include correlation but do not correct mean field electrostatics are sub-optimal, especially those that describe all of the correlation energy as dispersion. This result has major implications for the correct design of new EDA's, which we look forward to taking up in future post-LDRD work.

Our second 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 (CC) calculations can be accurate approximated by a starting point where the CC calculation is 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). The question is whether this approach can improve the often-questionable accuracy of PT, without the prohibitive computational cost of a full CC calculation 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. Work is presently underway to explore whether this result can be improved by using orbitals relaxed in the cluster environment, and how to obtain such orbitals more efficiently than brute force solution as if the cluster is a super-molecule.

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.

Some inspiration for our approach to catalytic network design is derived from another highly successful biomimetic approach- laboratory directed evolution (LDE)- an experimental strategy based on the principle of natural selection(1). The goal is to alter the protein through multiple rounds of mutagenesis and selection to isolate the few new sequences that exhibit enhanced catalytic performance, selectivity, or protein stability, or to develop new functional properties not found in nature in the creation of new biocatalysts(2, 3). Given the limitations of our understanding of the structure-function relationship(4), LDE provides an attractive alternative to rational design approaches and is highly flexible in application to different biocatalysis reactions. However, there are still outstanding problems when transferring LDE into new optimization strategies for new biocatalysts. First the finite size and composition of the LDE libraries may be limiting for the optimization of enzymes that act on, for example, solid substrates(5), and there has been little effort devoted to developing LDE libraries for optimizing biocatalytic activity in the context of chemical networks. Furthermore, although often highly successful, LDE is an opaque process because it offers no rationale as to why the mutations were successful, and therefore stands outside our ability to systematically reach novel catalysis outcomes.

This proposal is a theoretical study to offer new rational design strategies for building an artificial chemical network of biocatalytic reactions that execute complex but now non-biological catalytic functions using computational directed evolution (CDE). Traditionally enzyme optimization is often focused on the energetics of active site organization but there is correspondingly little effort directed toward optimizing entropic or dynamical effects that are also equally relevant for improvements in catalytic activity. Therefore we propose a new CDE design strategy that considers not only energetics but novel physical and theoretical concepts

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 might exist in the atmosphere not as well mixed liquids – the traditional description, and their general state when they are formed - 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 initially liquid aerosols are transformed into glassy ones, in particular by gas phase oxidizers. 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 parameters for 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 liquid-solid transitions. Our goal is to examine the complex coupling of oxidative ageing chemistry with environment- and history-dependent viscosity, and 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. This approach is uniquely enabled using stochastic simulations. The main components required are (1) a description of uptake of gas reactants, (2) a description of the free radical chain over many product generations, and (3) a description of dynamic perturbations by environmental factors such as temperature, pollutant plumes and humidity and internal factors such as immiscibility of products.

Accomplishments

In the first year of this LDRD we have made significant progress on the first two components: modeling uptake and the free radical chain. We have focused on a system for which there are extensive experimental data in the literature, the reaction of squalane ($C_{30}H_{62}$) aerosols with OH over a broad range of pressures. Using only kinetics from the literature we have shown that the current understanding of uptake is at best incomplete – it is not simply the sticking probability of reactants to particle surfaces followed by reactions. Rather, the uptake coefficient is inseparable from the intrinsic internal transport rate (viscosity) of the aerosol itself relative to the gaseous reactant-aerosol collision rate, and is therefore *an emergent property of the system*. This represents a fundamentally new insight that promises to impact thinking on transformations of aerosols and liquid films. The free radical chain reaction that ensues after the initial reaction between OH and squalane aerosol is complex, involving many generations of addition of oxygen-containing functional groups forming hundreds of distinct products as well as fragmentation that transform the composition of the aerosol and cause it to shrink. In work led by the postdoctoral researcher in this project, Aaron Wiegel, we have developed a compact description of this chemistry that fully reproduces experimental observations. The free radical reaction model, which uses only literature kinetics, describes molecules as collections of functionalities and is therefore inherently general. It is the core of a universal free radical oxidation scheme that can be used to apply to a broad range of molecular systems.

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.

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.

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

Our most significant accomplishment is the development of the Global Arrays/GASNet Interface called GAGA. This work was done in collaboration with members of the DEGAS project. The current implementation has been demonstrated to work efficiently on Infiniband clusters and Cray platforms, with significant faster performance and better CPU utilization for the coupled cluster single doubles capability in NWChem. Going forward we will further improve performance of the one-sided operations.

Key two-electron algorithms were analyzed, and in collaboration with the SUPER institute we were able to obtain a 25% increase in performance and we improved the load-balancing algorithm on conventional CPUs. Similar performance improvement was found for Intel Xeon Phi, however the absolute performance is lacking relative to CPUs. We optimized the Fock build capability in NWChem and two-electron integrals to increase their efficiency on Intel's next-generation Intel Xeon Phi processors. In addition, a distance based screening algorithm to enable O(N) computing was implemented that will reduce redundant computation of expensive multi-center two-electron integrals in large systems.

A first version of CML in NWChem has been made available to collaborators in industry (Kitware and Hyper). The work was presented at IUPAC in 2014 and we are in the process of writing a proposal to the organization for support to develop a consistent dictionary and ontology for chemical sciences. We are partnering with Kitware, using their MongoChem infrastructure to build a demonstration case for heavy element chemistry, linking computational and experimental data in a semantically rich framework.

An Optimization-based Strategy for Computational Design of Nanoporous Carbon-Zero Materials

Principal Investigator: Maciej Haranczyk

Project Description

Our goal is to create a computational framework that will allow the *in silico* design of metal organic framework (MOF) materials through a strategy based on structure optimization with respect to property. Efficient global optimum search algorithms will be utilized to efficiently navigate the space of possible structures. By performing this search on a broad space of MOFs, we thereby remove limitations on the search space encountered by currently utilized enumeration-based strategies. We plan to explore two approaches. In the first, we abstract molecular models of MOF building blocks as geometrical – or alchemical – building blocks, defined by a number of continuous parameters, which are optimized using gradient-based techniques. In the second, we perform the search in a discrete space of real molecular building blocks and employ Genetic Algorithm (GA)-based search techniques.

Although the proposed approaches are general and can be used to design a MOF material with almost any desired property, our work will focus on properties critical for gas separation and storage. We aim to enable design of materials for carbon capture and natural gas storage. Therefore properties of interest include high surface area, large pore diameters and adsorption properties of gas(es) of interest. Our framework for MOF design comprises three components: (i) MOF assembly module; (ii) rapid property estimation module(s); and (iii) structure optimization control module. The key aspect of each component is modularity: these components can be substituted or extended to include other building block representation schemes, property estimation modules, scoring functions and optimization/search algorithms.

Accomplishments

We have developed and deployed algorithms and software for assembling MOF structure models: module (i) - allows for automatic assembly of MOFs from metal and organic building blocks (ligands). The latter are placed in 3D space and connected according to a predefined topology. This new functionality is now a part of an open-source Zeo++ software package available to the computational material science community.

Furthermore, we have worked on a new approach to the optimization-based MOF design approach based on discrete optimization algorithms within the space of known, commercially-available compounds and reactions converting the later into materials' building blocks (in the earlier years of the project we focused on approaches involving gradient-based optimization). In our initial work, we have used a database of ca. 40,000 readily available compounds and a database of ca. 100 reactions. We have used GA-based optimization to search the space of compounds/reactions finding combinations leading to optimal materials. We have focused on the following design objectives: internal gravimetric surface area, volumetric surface area and the combination of these two. As a result we have successfully identified many previously unexplored materials whose high surface areas suggest they are promising candidates for gas storage.

High-Performance Parallel Analysis for Key Genomics Computations

Principal Investigator: Leonid Oliker

Project Description

Technological advances in computers and sequencing technology have enabled bioinformatics to develop at an unprecedented rate, especially in terms available data volume that require analysis. However, biologists face significant challenges in effectively studying these data sets due to the complexity of optimizing these classes of computations on modern computational systems. The goal of this project is to deliver unprecedented computational capability to large-scale analytics for key bioinformatics applications, via the development and integration of flexible and high-performance software packages.

Recent work is targeting the analyses of high-throughput "next generation" genome sequencing technologies that are producing a flood of inexpensive genetic information, which is invaluable to genomics research. Sequences of millions of genetic markers are being produced, providing genomics researchers with the opportunity to construct high-resolution genetic maps for many complicated genomes. However, the current generation of genetic mapping tools were designed for the small data setting, and are now limited by the prohibitively slow clustering algorithms they employ in the genetic marker-clustering stage.

Accomplishments

Our most significant accomplishment focuses on the first step of genetic mapping, which involves clustering markers into linkage groups. This is traditionally performed by various standard clustering algorithms applied to a similarity graph of the markers, which creates a significant bottleneck for large numbers of markers. Our work developed a fast clustering algorithm that circumvents the computation of all similarities by exploiting prior knowledge about the specific structure of the marker data: linkage groups (i.e., chromosomes) have an intrinsically linear substructure that remains reflected in the similarity measure. After sorting, the algorithm creates a specific sketch that respects both the geometry and quality of the data. Using synthetic and real-world data, including the grand-challenge wheat genome, we demonstrate that our approach can quickly process orders of magnitude more genetic markers than existing tools while retaining — and in some cases even improving — the quality of genetic marker clusters.

An important application of our method is in the efficient construction of ultra-dense genetic maps for large and complex genomes that are filled with repetitive sequences that frustrate genome assembly but do not limit the number of genetic markers. The most economically important of these genomes are various grasses, including crops grown for food (e.g., barley and wheat, whose genome sizes are two- to seven-fold larger than the human genome) or as biofuel feedstocks (e.g, switchgrass and miscanthus, polyploids that contain multiple, subtly different copies of a basic genome).

Numerical Methods for Multiple Evolving Interfaces

Principal Investigator: Robert Saye

Project Description

The aim of this project is to develop advanced, high-order accurate, numerical methods for the computational simulation of multi-physics processes involving multiple moving interconnected interfaces. To achieve this, we are developing a new computational framework for complex fluid flow problems based on discontinuous Galerkin embedded boundary methods. The framework capitalises on mathematical and computational advantages provided by implicitly-defined representations of geometry, as used for instance in the level set method for single interfaces, and the recently developed Voronoi Implicit Interface Method (Saye & Sethian, 2011-2013) for multiphase physics. In particular, we are developing new projection methods for incompressible fluid flow which are high-order accurate in space and time as well as new techniques for consistent coupling of fluid-solid motion. The goal is to enable high-fidelity simulation of multi-physics interface dynamics, especially when the dynamics of the interface produce small scale features such as boundary layers that would not be captured by existing lower-order methods. The new framework holds promise for enabling high-accuracy simulation in complex geometries and offers advantages over other numerical methods in regards to high-performance supercomputing. We expect that the 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

In laying the foundation for our work on advanced high-order interface methods, during this first year of the LDRD we have successfully developed several new computational techniques and algorithms, including:

New high-order discontinuous Galerkin (dG) methods for implicitly-defined geometry which captures curved interfaces 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. These algorithms have been successfully used in the above dG framework and will continue to be of core importance in future work.

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 and have been used in combination with Voronoi Implicit Interface Methods to perform image segmentation for rebuilding 3D structure from materials sampled at the ALS.

Interlinkage of Cross-Disciplinary Mathematical Technologies

Principal Investigator(s): J. Donatelli, M. Haranczyk, S. Marchesini, B. Preskill, R. Saye, D. Ushizima, J.A. Sethian

Project Description

Applied and computational mathematics can steer discovery in the DOE facilities, providing advanced algorithms and computational methodologies to efficiently extract data, interpret results, and guide experiments. As examples, new mathematics is increasingly instrumental in providing tools to reconstruct structure and properties from synchrotron light sources, direct the hunt for new materials for batteries and gas separation, and model and optimize steps in the production of biofuels. We have been building mathematical models, algorithms, and technologies to attack problems within LBNL and DOE that are brand-new, and require core advancements, with particular focus on (i) New Reconstruction Methods for the Advanced Light Source; (ii) Fast Throughput Screening in New Materials Design; (iii) Mechanical Modeling of Biological Cell Clusters; and (iv) Advanced Imaging Capabilities in Material Analysis.

Accomplishments

Following on our FY13 work, we have accomplished the following:

In new reconstruction methods, we have focussed on nanocrystallography, grazing incidence small angle scattering (GISAXS), and ptychographic analysis. In x-ray nanocrystallography, we have built a new multi-step computational technique to solve the twinning ambiguity. We built an algorithmic framework to determine crystal size, incident photon flux density, and orientation in the presence of the indexing ambiguity. We showed that phase information can be computed from nanocrystallographic diffraction using an iterative phasing algorithm, without extra experimental requirements, atomicity assumptions, or knowledge of similar structures required by current phasing methods, and then tested the approach on simulated data with parameters and noise levels common in current experiments. In GISAXS, we build a high performance simulation code based on the discrete wave Born analysis, which is orders of magnitude faster than before. In ptychographic analysis, we have developed a new, fast reconstruction method, and begun moving the code to a high performance computing environment. In biological modeling, we built a complete simulation of cell cluster dynamics, evolving under the combined effects of hydrodynamic, elastic, and geometric forces. We have been adding inelasticity and adhesion to the computational infrastructure. We have developed a computational methodology based on a non-linear elasticity model to compute acini forces and collagen stretching. In image analysis, we have built techniques to analyze high-resistance ceramic composites under strain, using data optain from the ALS. In new materials design, we have built new optimization algorithms to assemble components to meet design objectives. As an example, we designed record-breaking high surface area materials. In materials analysis, we have developed a new method for tracking multiphase interfaces in materials, including applications to grain metal boundaries, liquid and solid foams, and in semiconductor failures. We have applied these techniques to image segmentation for rebuilding 3D structure from materials sampled at the ALS using micro-tomography (beamline 8.3.2).

We have obtained follow on funding from DOE through FY 15. We were asked to submit a white paper for additional funding, and have done so. On the basis of that, we have been asked to prepare a formal proposal, which we are now doing

Modeling Subsurface Reactive Transport Processes From Mineral-to-Pore-to-Continuum

Principal Investigator: David Trebotich

Project Description

The overall objective of this project is to develop new approaches for representing pore scale processes in Darcy continuum scale numerical models of subsurface reactive transport. We hypothesize that a quantitative, mechanistic understanding of coupled physical and chemical processes at the pore-and-grain scale is possible, and that such an understanding can form a rational basis for upscaling fluid dynamics and geochemical kinetics to field scale systems. By carefully understanding processes at the pore scale, the ultimate goal of this research is to bring such knowledge to bear on the macroscopic scale of a reservoir, which is the relevant scale for carbon sequestration and other important subsurface flow problems such as environmental remediation and storage of nuclear wastes.

The foundation for the multiscale approaches presented here is highly resolved pore scale simulation data. To this end, we have previously developed a high performance simulation capability, called Chombo-Crunch, that models pore scale reactive transport processes associated with carbon sequestration at unprecedented scales. With this capability we have been able to show the effect of pore scale flow on average geochemical reaction rates using straightforward volume averaging over the domain volume. In general, we would expect that volume averaging does not retain heterogeneity in the flow. However, volume averaging can be used *locally* where it is appropriate without reservation. The question is what is the 'local' scale relative to a representative elemental volume (REV) for the continuum Darcy model? It would be of no surprise to discover that highly resolved pore scale data were to violate Darcy assumptions and display non-Fickian behavior, which our preliminary results indicate.

Accomplishments

We have been able to establish high resolution pore scale simulation as a credible basis for upscaling. Our direct numerical upscaling approach is to resolve the entirety of a continuum scale domain with pore scale resolution and to use flux-weighted averaging together with finite volume techniques based on the discrete divergence theorem on a local volume to obtain upscaled parameters like permeability. As an example, we simulated steady-state flow and reactive transport in a 2D heterogeneous continuum domain of 1 meter in length packed with approximately 100,000 spheres. We distributed each subdivided box of 256^2 grid cells of the domain on each of 16,384 cores using the NERSC Cray XE6, Hopper. The grid resolution was 7.6 microns. This domain decomposition produces the sweet spot for load balancing where each subdivided box in the domain corresponds to a local volume that can be correlated to a representative elemental volume (REV) of the continuum Darcy model. We will continue to explore the relationship between the local volume and a REV and ultimately demonstrate the necessity of representing pore scale processes in continuum scale models using direct numerical upscaling.

In addition, we are using high resolution pore scale data and direct numerical upscaling to guide and verify more selective approaches to upscaling. In these more formal multiscale methods we are relying on adaptive modeling and/or statistical characterization of the pore space to sample pore scale data. Examples include adaptive model refinement and information theory.

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. In FY 2014 we added two new ALS beamlines – 7.3.3 SAXS/WAXS (scattering) and 12.3.2 micro-diffraction. As of November 2014 SPOT had processed ~150,000 datasets (>900 TB) and launched >1.3M jobs on NERSC resources in realtime (10x wrt FY 2013).

We successfully conducted 2 data demos of the prototype for SC14. The first demo involved hooking non-ALS BES light source beamlines to the SPOT pseudo-production prototype to study the ability of a central ASCR Scientific Data Facility (SDF) to handle multiple BES facilities. We successfully connected 2 beamlines at the LCLS (SLAC), processing 125 TB of raw data (psana, cctbx) in real time inside SPOT for an experiment on photosynthesis and nanocrystallography. The beamline scientists' first view of real data was on the SPOT Suite portal. We successfully ran 3DXANES under SPOT and simulated ~2 weeks of data taking at NSLS (BNL) for a 3D chemical mapping experiment of battery material measuring in real time the spatial distribution of three components (Fe, $FePO_4$, $LiFePO_4$). Finally, we ran a new tomographic reconstruction code (TomoPy) and utilized a new tomographic-optimized HDF5 data file format (Exchange) from the APS (ANL) and simulated 1-2 weeks of a wide variety of datasets representing all possible data collection schemes and dataset sizes for that APS beamline.

The second Data Demo tested co-scheduling beamtime at an ALS beamline, NERSC MPP time, and OLCF Titan time. We conducted 2 experiments, one in which we studied Nafion (an ionomer polymer based proton conductive membrane used for fuel cells). The second experiment involved slot-die printing Organic PhotoVoltaics (OPVs) and measuring the crystallization of the OPV as it dries. In both cases, we automatically transport data from ALS BL7.3.3 to NERSC (Spade), perform on-the-fly calibration and processing (GIXSGUI, dpdak) at NERSC, transfer data to OLCF (Globus Online+Spade) and process data on Titan using HipGISAXS simulation for the OPV and HipRMC fitting for Nafion (also at Edison). We successfully ran the full chain for both experiments. But, though we could keep up in real-time for the Nafion RMC calculations, the HipGISAXS calculations were 60x too slow to keep up, even using all of Titan.

We also developed and integrated a new remote visualization capability using VisIt that allows end users to launch VisIt servers on Edison, view, manipulate, and share with collaborators their 3D reconstructed datasets at full resolution with nothing installed on their desktop, laptop, tablet, or smart phone other than a web browser. We also integrated filtered and segmented data from QuantCT into the SPOT data browser, and a specialized set of data displays for analysis of flexible sandstone.

Quantitative Image Analysis for Computational Modeling

Principal Investigator: Daniela Ushizima

Project Description

The purpose of this project was to develop image analysis, pattern recognition, and quantification algorithms in support to understanding experimental data produced at DOE and potential new funding sources such as NIH and NSF. The main data sources explored as part of this LDRD were:

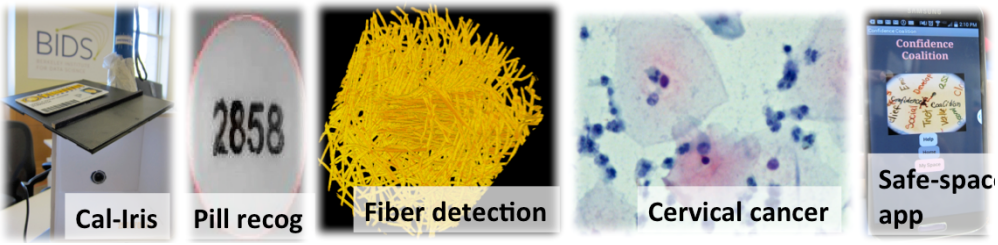
- Microtomography imaging of geological samples and other materials coming from ALS beamline 8.3.2, in collaboration with Dula Parkinson.
- Electron tomography imagery of films for future integrated circuits coming from NCEM, in collaboration with Peter Ercius.
- Optical microscopy of biological samples, for example cervical cells coming from simulations and real experiments in collaboration with Australian Centre for Visual Technologies at the University of Adelaide, Australia and Federal University of Ouro Preto, Brazil.

The goal was to develop algorithms and software to systematically address large amounts of images and/or providing computerized methods to quantify composites/samples in terms of structures and other properties relevant in the identification impurities, defects, and other abnormalities. These data enabled development and deployment of software infrastructure to address image-based experiments, and comparative evaluation of samples.

We developed new software, for example QuantCT software for microCT segmentation, F3D software for general purpose image processing for large volumetric data and Super Pixel representation using Voronoi Diagrams (SPVD) for optical microscopy, which individually and together have been applied to address analysis tasks needed within DOE and other scientific communities.

Accomplishments

Our most significant accomplishment has been to develop a reproducible protocols for analyzing image-based experiments. Our methods include advanced algorithm refactorization and hybrid architectures to solve computational problems that require scaling. For example, our filter kernels are implemented in OpenCL and can be called from our Java code through JOCL, which is a Java library that provides Java bindings to OpenCL architecture. Here, F3D tool provides original and unique gray-level MM operators are one-pass constant time methods that can perform morphological transformations with a line-structuring element oriented in several directions. Another feature of F3D is the ability to generate formatted instructions that permit using the plug-in as part of Fiji macro-scripts. The formatted instructions are based on JSON, and allow user-friendly interaction and promote model-based filtering to recover tubular structures. This work has allowed to springboard innovative ideas that are now part of the Center for Applied Mathematics for Energy Research Applications (CAMERA) and BIDS.



Numerical Algorithms and Mathematical Software Tools for Computational Material Science and Chemistry

Principal Investigator(s): Lin Lin and Chao Yang
Computational Research Division

Project Description

The goals of this project are to develop efficient and reliable numerical algorithms and mathematical software tools for computational material sciences and chemistry. Such tools are becoming increasingly important in the design of new materials for harvesting alternative energy and the development of efficient catalyst to separate greenhouse gas from fossil plants. In the three years of the funding period, we have achieved significant progress in terms the development and implementation of numerical algorithms to accelerate large scale electronic structure calculations.

Recent Accomplishment:

We have successfully integrated the previously developed pole expansion and selected inversion (PEXSI) method for evaluating electron density with the SIESTA software package for massively parallel materials simulation. We can make efficient use of more than 10000 processors on high performance machines. We demonstrate the performance and accuracy of the SIESTA-PEXSI method using several examples of large scale electronic structure calculations, including 1D, 2D and bulk problems with insulating, semi-metallic, and metallic character. Using the SIESTA-PEXSI method, we have successfully computed electronic structure properties of large scale graphene nanoflake to unprecedented size (11700 atoms).

We have a developed a posterior error analysis for a domain decomposition technique for solving the Kohn-Sham density function theory problem that make use of discontinuous Galerkin methodology to construction adaptive basis functions.

We have successfully developed accurate numerical integration methods for ab initio many-electron self energy calculations within the GW approximation for the computation of excited state electronic structure properties. Our scheme evaluates the convolution of a Green's function with a screened Coulomb potential on the real axis in the GW approximation of the self energy, and takes the zero broadening limit in Green's function first, replaces the numerator of the integrand with a piecewise polynomial approximation, and performs principal value integration on subintervals analytically. We analyzed the error bound of our numerical integration scheme and show by numerical examples that it is more reliable and accurate than the standard quadrature rules such as the composite trapezoidal rule.

We have surveyed techniques for computing density of states (DOS) systematically. DOS based techniques allow to estimate the spectral density function at much lower cost for large, Hermitian matrices. We analyzed the error for computing the DOS with different numerical techniques using a modified weak norm indicating the intended resolution of the DOS, and identified that Lanczos based techniques is superior to the Kernel Polynomial Method and similar methods. This could also have impact in the estimation of the excitation spectrum within time dependent density functional theory, and we are currently pursuing this direction.

Computational Approaches to Understanding Ultrafast Science

Principal Investigator(s): Alexander Kemper, Chao Yang

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.

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 have focused on s-wave superconductivity. We correctly reproduce the equilibrium behavior, as well as the basic ideas regarding superconductivity, e.g. supercurrents. Proceeding on to pumping, we have results indicating 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.

Secondly, we completed and published our findings regarding the time-resolved photoemission response in the weak pumping limit. Following this, we further extended the code to allow for the self-consistent calculation of the electron Green's function, which allowed us to observe the effect of strong pumping on the interactions. Recent experimental results indicated that upon illuminating the sample with a strong pump, the hallmarks of electron-phonon coupling known as "kinks" weaken. This was attributed to the decoupling of the electrons from the lattice. Our results showed that this is not the case; rather, the electrons (which are coupled to the lattice) are scattered to higher energies, leading to a similar reduction in the kink, although the coupling remains constant. In fact, we showed that there is a conserved sum rule for the electron-phonon interactions, indicating that this is a conserved quantity. This work provides a framework for future discussion of results in the field, where one needs to go beyond quasi-equilibrium models and consider the full effects of the pump.

Developing a mechanistic high-latitude biological soil carbon and nitrogen cycle module for site, regional and global land models.

Principal Investigator: Nicholas Bouskill

Project description:

This LDRD integrates existing ESD expertise in ecosystem modeling and environmental microbiology to develop a modeling capability for the carbon (C) and nitrogen (N) cycle in high-latitude soils. High-latitude permafrost soils underlie approximately 26 % of terrestrial ecosystems and have the potential to significantly impact the future balance of Earth's C and N cycles. Several models suggest that up to 90 % of the near-surface Arctic permafrost could thaw by 2100 affecting the structure and function of the microbial communities that mediate the majority of biological C and N cycling. These thermal, hydrological, geochemical and biological changes could lead to substantial increases in atmospheric CO_2, CH_4 and N_2O. The efflux magnitudes of these gases from thawing permafrost are largely dependent on complex feedbacks centering on the *in situ* diversity of C- and N-cycling microorganisms, the availability of N, and the physical changes that occur as permafrost thaws. Therefore, the development of a framework for simulating the emergence of microbial community structure based on a few physiological and genomic traits is a critical first step towards predicting how microbial communities will respond to the geochemical, thermal and hydrological changes accompanying permafrost thaw. A further outcome of understanding community emergence is the accurate prediction of rates (e.g., decomposition, N-fixation or N_2O production) that is a consequence of the emergence of particular microbial communities.

Accomplishments:

Research over this part year has focused on one of the main goals of this LDRD, improvements of Earth System models using mechanistically focused trait-based models. Specifically, we have been developing a trait-based model of nitrogen fixation that will improve both the mechanistic approach the Community Land Model takes to predicting global and local rates of nitrogen fixation, and address fundamental questions regarding the limitation of ecosystem processes by nitrogen across local and regional scales. We take a comprehensive approach to modeling high-latitude microbial ecosystems, including the explicit representation of autotrophic and heterotrophic nitrogen fixers, and heterotrophic bacterial and fungal decomposers. Our model includes representations of both the phosphorus and molybdenum cycles and more broad environmental factors (e.g., temperature, soil moisture) that limit microbial activity. Our approach also accounts for physiologically important processes, including microbial nutrient use efficiency. This approach is important for understanding the interactions between the carbon and nitrogen cycle.

The carbon cycle in high-latitude ecosystems (and many other ecosystems) is chronically limited by nitrogen availability. Our approach sets out to answer why nitrogen is chronically limited, and also address how the niche of nitrogen fixing organisms might change over the coming decades, and the feedback this will have with the carbon cycle.This model couples the carbon, nitrogen and phosphorus cycles in an approach that has rarely been applied prior to our current work. This work will continue through additional funding from the NGEE-Arctic and NGEE-Tropics SFAs.

Integrative Mapping of Soil Heterogeneity at the Microbial Scale
Principal Investigator(s): PI: Eoin Brodie; Co-PIs: Peter Nico, Janet Jansson, Hoi-Ying Holman, Margaret Torn, Jonathan Ajo-Franklin, Bill Moses, Jim O'Neil, Manfred Auer, Trent Northen, Tanja Woyke, Susannah Tringe and Dylan Chivian

Project Description

The aim of the project is to develop a predictive understanding of soil biochemistry by determining how µm-scale physics, chemistry and biology interact to control C and N biogeochemical cycles in soil. Most of our current knowledge of soil biogeochemistry is based on bulk analyses, and fine scale spatial (nm-µm) microbial interactions are often overlooked. Soils provide many valuable ecosystem services from carbon sequestration to food production. Studying soil physical, chemical and biological heterogeneity at a scale relevant to microbes will improve our understanding of the factors that regulate microbial activity in soils. We aim to discover a set of universal interactions between microbial functions, soil chemistry and physical properties that are deterministic on biochemical cycles. We are currently focusing on CH_4 oxidation and nitrogen fixation in soils which are important contributors to C and N fluxes in many ecosystems yet are poorly understood due to their spatial heterogeneity. This project integrates different methods and technologies to characterize biochemically active CH_4 oxidation and N_2 fixation "hot-spots" and to develop models to determine factors governing microbial activity in soils.

Accomplishments

Our most significant accomplishment to date is the further development of an experimental workflow for multi-modal characterization of microbial functional distribution in soils. To detect activity hot-spots in the soils we have developed approaches using short-lived ^{11}C and ^{13}N radioisotopes. We have successfully imaged $^{11}CO_2$ fixation through photosynthesis in plants and biological soil crusts, ^{11}C-CH_4 retention by methane oxidizing bacteria and have shown preliminary data supporting our ability to visualize $^{13}N_2$ fixation through endophytic nitrogen fixers. These labeling methods have been coupled with Positron Emission Tomography or Radio Phosphor Storage imaging. We have developed a workflow to sort soil individual aggregates (1mm to 50µm) from soils under sterile conditions and to characterize their surface chemical composition non-destructively via Fourier Transform Infrared (FTIR) spectroscopy equipped with an ATR (Attenuated Total Reflectance) prism. Aggregates are then clustered into chemotypes based on their chemical spectra. Aggregate scale genomic techniques have been developed to determine the microbial composition and metabolic potential microbial composition, these include efficient DNA extraction and purification procedures and novel picogram scale high throughput DNA sequencing library construction methods – the first of their kind for soil systems. We are attempting to define relationships between microbial metabolic potential and aggregate chemical and physical properties. To determine the physical constraints on microbial activity at the aggregate scale we have further developed X-ray micro/nano-computed tomography (sCMT) to achieve nanometer scale measurements of pore volume and pore network topography – these data are now being used to parameterize pore scale models of microbial activity. We have continued to test our improved experimental workflow on several contrasting soils (Alaskan tundra, Californian grassland and Midwestern Prairie) and successfully analyzed their biogeochemical properties. Three manuscripts are in draft form and a fourth has been published.

High-throughput Isolation and Functional Screening (HIFS) of Microbes Relevant to Today's Carbon Cycling and Bioenergy Needs

PI: Romy Chakraborty

Project description:

In the past two years, the isolation platform has been developed and tested successfully. In FY14, this renewal seeks to develop the rapid functional screening platform based on microbial respiration/activity. Our goal is to be able to trap evolved gas from substrate utilization in miniaturized incubation chambers using microtiter plates, which has the advantage of being cheap, portable, compact and high-throughput and amenable to be used on-site during fieldwork. This contraption when coupled with a portable plate reader can enable rapid characterization of soil (microbes present in soil) and their response to different C substrates.

Accomplishment:

We assembled and test prototypes of miniaturized incubation chambers. We used microtiter plates as the platform and explored appropriate sealing manifolds to devise individual, sealed compartments. Microtiter plate wells were supplemented/spotted with test substrates. These included different C-compounds. Various polymers were both tested for their efficacy of trapping the evolved gas from the different substrates provided. Various indicator dyes and fluorescent indicators were tested for their ability to detect the evolved gas. Suitable indicators were identified that provided quantitatively measurable results.

TROPICAL FOREST ECOSYSTEMS UNDER A CHANGING CLIMATE

Principal Investigator: Jeffrey Chambers

Project Description

Increasing levels of atmospheric CO_2 from anthropogenic activities is causing the Earth's climate system to warm resulting in costly societal impacts. However, ~50% of our CO_2 emissions are removed from the atmosphere by vegetation and ocean processes, with old growth tropical forests estimated to account for ~50% of the total terrestrial carbon sink. In addition to these direct effects of rising atmospheric CO_2 on net atmospheric carbon exchange, changing precipitation patterns and elevated surface temperatures are expected to cause a reduction in the terrestrial sink through vegetation mortality, primarily in tropical forests. Elevated disturbance regimes in tropical forests will result in shifting tree species composition, and commensurate shifts in the atmospheric exchange of mass and energy. This LDRD project will improve representation of these important processes in Earth system models (ESMs), leading to improved climate change predictions for the 21st Century, and is focused on the following three questions:

Q1: What are the key uncertainties associated with the old-growth tropical forest carbon sink and how can we improve model treatment of these processes?

Q2: How do land models currently treat drought-induced mortality, and what structures are required to improve forest response to altered precipitation patterns?

Q3: How will shifts in gap-phase dynamics and community composition under elevated disturbance regimes act to amplify climate system feedbacks?

To address these questions we will build on our existing Berkeley Lab expertise, including (*i*) extensive research activities with the Community Land Model (CLM) and DOE's Earth system modeling (ESM) efforts, (*ii*) new hires with expertise in ecosystem demography modeling, and (*iii*) the PI's 20 years of tropical forest ecosystem field research experience.

Accomplishments

This LDRD project started in May 2013. A postdoctoral researcher with extensive experience with ecosystem demography modeling was hired in June 2013 (R. Knox), and significant progress has been made addressing all questions. Jennifer Holm and Robinson Negron-Juarez also participated in LDRD activities. These activities included completing a sensitivity analysis using a version of the Ecosystem Demography model (ED2; co-developed by R. Knox) to rising atmospheric CO_2, and a comparison of that CO_2 response to extensive field data from a Central Amazon site in Brazil. The modeling and analytical work for this activity has been accomplished, and a manuscript is just about ready to submit (Knox et al. in prep). We also made significant progress integrating ED2 functionality into the larger CLM framework, including developing a testbed with data from the Central Amazon site, which enables exploration of drought-mortality interactions in a landscape context. Additional work focused on model structures required to simulate shifts in disturbance regimes. Work carried out under this LDRD was instrumental in Berkeley Lab being tasked by DOE-BER to lead the Next Generation Ecosystem Experiment (NGEE) Tropics (~100M anticipated over a 10 year project duration), and the PI of this LDRD has been tasked to lead NGEE Tropics as Director. The NGEE Tropics proposal is currently under review, with a final decision expected late February 2015.

Isotopic Probe of Ion Migration Processes in Li-ion Batteries

John N. Christensen (ESD), Ian C. Bourg (ESD), Vincent S. Battaglia (EETD)

Project Description

Despite the ubiquity of Li-ion batteries, they are not considered a mature technology and the basic science underlying their function is still a matter of intense research. Developments in Li-ion battery and related technologies are driven by the need to produce higher capacity, efficient discharge, and quicker recharge, while maintaining favorable weight/volume ratios, geometric flexibility, long lifetimes, safety and reliability. The migration of ions across the electrochemical system is a key process that affects the energy efficiency, capacity and voltage output of Li-ion batteries. However, the phenomena that determine ion migration rates for processes such as transport through the bulk electrolyte, through the solid-electrolyte interface (SEI), and into the intercalation space of electrodes are still poorly understood. Our goal in our research is to take advantage of kinetic isotopic fractionation ^{6}Li and ^{7}Lito advance the understanding of Li ion transport processes in batteries, and ultimately provide a predictive capability of ion mobility so that materials may be selected to optimize the performance of ion-based batteries.

In our research we used: (1) laboratory experiments with battery materials (i.e. electrolytes and Li salts) and (2) computer intensive molecular dynamic simulations of ion migration. In laboratory experiments, small volume glass bulbs containing a solution of Li-bis(oxalato)borate in proplylene carbonate (PC) are immersed in a large volume of pure PC that acts as a sink for Li that diffuses from the bulb. These experiments are run for long periods of time, up to four months, in order to magnify isotopic effects. Molecular dynamics (MD) simulations of $LiPF_6$ in ethylene carbonate (EC) were carried out to predict kinetic isotope effects (KIEs) associated with Li^+ diffusion, electromigration, and solvent exchange kinetics. MD simulations of a periodically-replicated simulation cell containing molecules of EC ($C_3O_3H_4$), Li^+ cations, and PF_6^- anions were carried out using the code LAMMPS and the inter-atomic interaction parameters of Jorn et al. [J. Phys. Chem. C (2013) 117:3747]. An electric field E = 0.05, 0.1, 0.2, or 0.4 V Å^{-1} was applied in the z direction.

Accomplishments

Our simulation results indicate that the diffusivity (D), electromigration velocity, and solvent exchange kinetics (k) of Li^+ in EC all increase with decreasing lithium isotopic mass. The predicted mass-dependence of D and k is consistent with the inverse-power-law relations $D \propto m^{-\beta}$ and $k \propto m^{-\gamma}$, where β and γ are exponents. Our MD simulation results on $D_{Li,MSD}$ and $D_{Li,EM}$ yield $\beta = 0.0035 \pm 0.0007$ and $\beta = 0.021 \pm 0.002$, respectively. The simulation determined value of $D_{Li,MSD}$ (no electric field direction) is in accord with the experimentally determined value of β of 0.0050±0.0008 for Li migration in PC.

In short, the KIE associated with electromigration is much greater than that associated with diffusion, in contradiction with the equality of these KIEs assumed in previous studies [Richter et al., Geochim. Cosmochim. Acta (2006) 70:277]. The ligand exchange rate k_{Li} also has a significant mass dependence ($\gamma = 0.011 \pm 0.001$). The KIEs associated with diffusion, electromigration, and ligand exchange are highly distinct from each other, suggesting that lithium isotopes may provide useful insights into the relative importance of these phenomena in controlling lithium migration rates in Li-ion batteries. In particular, the mass dependence of the ligand exchange rate in the MD simmulations suggests that KIE of Li ion desolvation may prove to be a probe of transport across the interface between the electrode and the electrolyte.

Simultaneous Above- and Below-Ground Terrestrial System Monitoring

Principal Investigator(s): Baptiste Dafflon

Project Description

The field of hydrogeophysics has advanced the ability to use geophysical data to quantify the shallow subsurface over large spatial extents and in a minimally invasive manner. Remote sensing methodologies have also greatly improved in recent years, enabling high resolution estimation of land surface properties, such as topography and vegetation density. The purpose of this project is to develop new methods to combine unmanned aerial vehicle (UAV) technology with ground surface geophysical characterization to perform co-characterization of above and below ground terrestrial processes. Such co-characterization offers a new paradigm for quantifying of many critical zone processes that involve interactions between above- and below-ground processes relevant to carbon cycling, agriculture, energy production and water resources.

The proposed scope takes advantage of and forms a new collaboration between the Earth Sciences and Engineering Divisions at LBNL. The first task is to develop a self contained instrumentation package capable of data acquisition, storage, and independent communication with remotely based controllers. This will enable us to run time-lapse based acquisition with optimal automatization using UAV- and/or pole- based platforms. The second task is to develop infrastructure to reconstruct mosaics and digital surface models (DSM) from above ground datasets, and process such data to a point where they can be meaningfully integrated with below ground datasets. We note that such co-characterization approach does not exist and thus the outcome is expected to make a strong contribution to research in the field of Earth system.

Accomplishments

A significant accomplishment has been to develop a reproducible protocol to acquire multi-spectral images using UAV- and/or pole- based platforms. To this end, a mini-computer has been used to implement an “in house” developed software that enable controlling the camera parameters (using the capability of an open source software (GPhoto2)), data storage and data transfer. This platform can be adapted to many types of different multi-spectral cameras. The approach has been successfully tested for continuous monitoring of landscape properties using a pole-based approach at the Next Generation Ecosystem Experiment (NGEE) site in Barrow, and will be tested using a UAV-based approach as soon as a FAA authorization will be obtained.

A second main accomplishment is the development of an infrastructure that enables (a) geo-referenced mosaic reconstruction, (b) estimation of various spatial metrics (based on pattern recognition and segmentation) and (c) calibration of remote sensing measurements using ‘point’ measurements. Testing this approach to infer DSM and mosaics along a 450x40 m corridor using a kite-based approach at the NGEE-Arctic field site has been successful; comparison with ground control points showed an error of less than -+ 5 cm in x,y and z direction and a spatial resolution of about 2 cm. In addition, an approach has been developed to correct for various light conditions the images acquired using a pole-based approach at the NGEE site. The co-characterization enabled by the above developments has showed amongst others that vegetation greenness index and subsurface bulk electrical conductivity (a proxy for soil moisture) reach a correlation coefficient up to 0.86 at the peak of the growing season. The study has documented the significant co-variability of vegetation and soil moisture in the Arctic ecosystem, and the ability of advanced above-and-below ground sensing approaches to monitor their interactions and feedbacks.

Linking Examination and Computation of Hydrologic Properties of Shales

Principal Investigator(s): Timothy Kneafsey, with Sergi Molins, David Trebotich, Terry Ligocki, and Stefano Cabrini

Project Description

The purpose of this one-year project was to develop and exercise a method to investigate the pore geometry, connectedness, and flow in nanoporous materials including shales and tight sandstones at the meso scale (here tens of nanometers to tens of microns). Pore geometry and connectedness control natural gas (and other fluid) movement at this scale. Included in this project were high-resolution 3-D imaging of the porespace of a large sample (region containing many pores), and simulation of single-phase flow through the porespace of the sample. Previous studies have attempted this, but have been hindered by the scale that the pore geometry could be quantified because the pores are very small (requiring very high resolution), and the porosity is low (requiring quantification over a large region). These studies resulted in a very limited number of very short flow paths which are not adequate for use to describe flow at a larger scale. Our approach was to extend previous studies of tight media to larger scales that approach and exceed the representative elementary volume scale. We also sought to link imaging and computational techniques in order to understand mesoscale emergent processes. We sought to perform high-resolution simulations of flow through the porespace using the Chombo code and the high-performance computing facilities at NERSC.

Data and methods developed during this project will add to the understanding of gas flow in tight rock formations, and to better optimization of gas extraction. In addition, the combination of imaging, image analysis, and simulation will create a digital laboratory to enable the addition of processes and additional realism to gas production from tight formations including the presence of other fluids (e.g. natural brine, natural gas condensate, and hydraulic fracturing fluids) which are only conceptually addressed in other studies.

Accomplishments

We have had several significant accomplishments. First, we obtained several large data sets, which are amongst the largest in the world if not the largest, using the Focused Ion Beam/Scanning Electron Microscope technique. We engaged Tescan USA in support of codeveloping the imaging technique using their newly developed plasma milling tool, based on preliminary work performed using the gallium ion milling tool at the Molecular Foundry. We focused on the structure and porespace of one Marcellus shale sample. This sample was selected because it is from a productive region of the Marcellus, and several other studies have been conducted on nearby samples. A number of data sets were collected at a variety of resolutions in support of this.

Our second significant accomplishment was that we developed methods of addressing and removing image artifacts on a very large number of images, allowing extraction of the porespace for analysis. All FIB-milled samples of heterogeneous samples have artifacts resulting from imperfect beam shape and the nature of sample heterogeneities, and these have previously hindered extraction of porespace.

Third, we successfully simulated single-phase flow through the identified and discretized porespace from one of our largest image sets and are processing our largest image set (196 x 156 x 67 microns at 50 nm resolution) for flow simulation.

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

Principal Investigator(s): Lara M. Kueppers

Project Description

The overarching aim of the proposed research is to improve understanding of the degree to which ecological and land management processes influence the physical Earth system and feedback to climate change. The specific goals of the current proposal are aimed at evaluating and improving models of land-atmosphere interactions and climate change field experiments intended to reveal ecosystem responses to climate change.

Land surface models are used to represent the properties of vegetation and soils that influence weather and climate through their effects on energy, water and greenhouse gas fluxes. Until recently, land management and cropping systems have not been represented well by these models even though crop growth and management practices have potentially large impacts on many aspects of weather and climate. We are using ground based and satellite observations, including from the ARM site and Ameriflux network towers in agricultural regions to validate and improve a coupled atmosphere-land surface model, WRF-CLM. Such model improvements will improve predictions of weather and climate in agricultural regions, and in regions undergoing changing land management. Initial efforts focused on biogeophysics have laid the groundwork for evaluation and improvement of modeled biogeochemistry.

Climate change experiments are used to quantify vegetation responses to altered climate states, and mechanisms underlying the responses. Infrared heating is increasingly used to manipulate temperatures. This method has rarely been evaluated in terms of its effects on winter and early spring conditions, nor have comparisons been drawn across multiple sites with the same treatment implementation. We are using data from existing experiments in the Rocky Mountains to examine snowpack and soil responses to the climate manipulations.

Accomplishments

A key accomplishment in FY14 has been submission of papers describing a regional climate-land surface model that includes dynamic crop growth and irrigation, and its application to assess effects of irrigation decline on heat waves in agricultural regions. The first paper is still in review at *Climate Dynamics*, while the second was rejected by *Geophysical Research Letters* and is in revision for *Environmental Research Letters*. Another analysis was completed to evaluate how irrigation influences land-atmosphere coupling strength. This analysis was presented at the AGU Fall Meeting in December 2014 and is in preparation for a journal submission in FY15. Further progress was made in spinning up an offline version of CLM with crops in the Southern Great Plains – a complex agricultural region with intensive observations.

With Noah Molotch (University of Colorado, Boulder) we revised and submitted a manuscript for publication describing the effects of experimental heating on snow accumulation and melt, and comparing this to a similar site further south and to a snowpack model. The paper was recently accepted for publication pending minor revision at *Forest and Agricultural Meteorology*. We also conducted initial analysis of gap-filled microclimate data from multiple warming experiments for two separate papers; one focused on the relationship between spatial variance in soil temperature and the mean over the growing season, and another describing heating effects on soil microclimate. The first analysis was presented in a poster by PhD candidate Danielle Christiansen at the MtnClim meeting in Utah in October 2014. The second was included in invited talks at Utah State and Penn State Universities in 2014.

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. We believe an ambitious but attainable goal will be to explore such chemistry at the smallest relevant scales, from NOM aggregates and ultimately to single macromolecules. 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. This reduced carbon is important on a mass basis for global carbon cycling, and its' long-term fate is a major outstanding question for predicting the feedbacks associated with global climate change. 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. Vibrational spectroscopy is well suited for investigations of macromolecular behavior and dynamics. Raman scattering was chosen as the central analytical technique because it has good sensitivity to organic matter composition and compatibility with aqueous environments. 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. The results are highly complementary to information obtained by electron and X-ray imaging and spectroscopy.

Accomplishments

Our most significant accomplishment to date has been to show that the naturally occurring iron oxide, magnetite, (Fe_3O_4) can be used as a SERS substrate to probe the interaction of organic molecules with natural mineral surfaces. We believe this development is the first demonstration of SERS behavior in a natural metal oxide and will be broadly useful to the study of NOM dynamics. A manuscript on these results has been prepared by Namhey Lee (the post-doc supported by the project) and is currently under review at Journal of Physical Chemistry Letters. We have also collected preliminary ptychography data on a natural shale sample. While data processing is still underway, we believe that this too is a world unique measurement and will have important implications for our understanding of the nano-scale structure of shale materials. We are in the process of requesting beamtime at the ALS to gain access to the nano-FTIR facility and are optimistic that the results obtain will compliment the ptychography results

Overcoming Technical Constraints to Urban Food Systems: Sustainable Solutions for Energy, Nutrient, Space and Water Demands

Principle Investigators: Rohit Salve, Romy Chakraborty, Roger Sathre, Maryann Villavert

Project description:

There is an increasing interest in urban farming to cope with providing nutritious food in urban areas without further increasing the environmental footprint of agriculture in urban settings. The goal of this project was to initially develop a white paper that explores the feasibility and design options for sustainable urban agricultural systems, to determine the primary energy intensity of various options for urban agriculture, and to identify opportunities to increase sustainability and reduce environmental impacts of urban food systems. The white paper will serve as a foundation for future work by LBNL and others on technological innovations that can be developed and prototyped to enhance the effectiveness, efficiency and scalability of urban farming systems.

Accomplishment:

Urban farm systems are a dynamic assembly of interdependent systems (water, energy, nutrients, space), but there is a fundamental lack of an understanding of how these systems work independently and as a group. Consequently there is only a vague understanding of how commercially and environmentally sustainable urban farming systems can be designed and operated. While there are many innovations around the country in each of the areas described above, for urban farming efforts to be replicable, scalable and cost effective, rigorous scientific knowledge needs to inform their design and implementation. To have impact at scale, technology needs to be developed and tested in partnership with those who would be the on-the-ground urban farmers. We propose a partnership with three cities: Oakland, CA; Toledo, OH; Chicago, IL. The goal would be to develop a rich relationship with existing urban agricultural efforts already going on in these cities and use these relationships to inform ongoing development decisions; test and fine tune new technologies as they are developed, and understand the implementation framework that will support adoption of proposed technologies. Specific tasks that would be conducted in partnership with these places would include:
(a) Initial scan of existing urban agriculture efforts and assets: Each of the proposed cities already has existing urban agricultural efforts. Understanding the scope and scale of these efforts, the innovations that are already being put into play, and the challenges and barriers being experienced will be an important grounding for this work.
(b) Creation and regular engagement of a partner's group in each city. We propose in each city to create a partner's group which would include between 8 to 10 groups involved in urban agricultural efforts. Quarterly meetings with these partner groups would inform larger project decision-making.
(c) Testing of new urban agriculture methods, strategies or tools: As the work evolved these partner groups would serve as the on-the-ground testers of new technologies.

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

Principal Investigator: Jiamin Wan

Project Description

Although CO_2 has been used as an injection fluid for enhanced oil recovery (EOR) for decades, CO_2-EOR remains inefficient. The primary limitation of CO_2-EOR effectiveness has been the low viscosity and high mobility of CO_2 that results in injected CO_2 bypassing oil 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. A variety of surfactants have been designed for generating foams, however, their commercial applications are still lacking. 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

Our most significant accomplishment has been to identify the sources of NSS (abundant and inexpensive), and all has been successfully tested as source materials for NSS extraction (5 samples from different geographic regions). 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 at up to 80 volume% with controllable effective viscosities up to 40 cP, 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.

NANOREPORTER – An RF-Powered, Nanoscale 3D Microelectronic Assembly for Mapping the Functional Connectome of the Brain

Principal Investigator(s): Carl Grace, Peter Denes, John Joseph, and Henrik von der Lippe

Project Description

The purpose of this project is to demonstrate the proof-on-concept feasibility of a < 50 μm / side, self-contained, autonomous, RF-powered sensor / reporter capable of digitizing data at > kHz rates, and fitting into an ensemble of 10^6 similar sensors. This would constitute an enabling technology for the successful mapping of the functional connectome of the brain.

Accomplishments

The budget and effort associated with this project were folded into the LDRD project titled: "Neuro/Nano Technology for Brain Mapping".

In addition to the accomplishments in "Neuro/Nano Technology for Brain Mapping" we conducted a study of various semiconductor process technologies to determine the most appropriate technology for a front-end integrated readout circuit for an electrocorticography sensor. We investigated various tradeoffs involving noise, power dissipation, cost, and long-term availability. The outcomes of this investigation then drove the process selection for the 2D electrocorticography neural amplification integrated circuit described in "Neuro/Nano Technology for Brain Mapping".

SUPERCONDUCTING UNDULATORS FOR LIGHT SOURCES

Principal Investigator(s): Soren Prestemon

Project Description

The purpose of this project is to develop the technology of superconducting undulators for light source applications. The primary goals include a) development of measurement system capable of accurate determination of trajectory wander, b) development of a tuning concept capable of reducing trajectory wander to within tolerance specifications, and c) design and fabrication of a Nb_3Sn undulator demonstrating predicted performance of the technology.
We intend to scale up the field correction/tuning R&D to accommodate full-length devices, a critical development for the application of superconducting undulators to free electron lasers and to storage ring implementations requiring higher-harmonic radiation.

Accomplishments

The project has been successful on all fronts. A summary of accomplishments over the last two years include:

a) The magnetic measurement system has been fully tested on the SLAC ECHO undulator. Our system is based on the well-established pulsed-wire technique, but incorporating significant innovations that enhance the quality of the measurements. The pulsed wire technique is directly applicable to the small-bore, cryogenic environment of the superconducting undulator.
b) The test cryostat fabrication has been completed and the cryostat is currently under commissioning. The cryostat accommodates powering of the main coils as well as the end correction coils and the tuning system.
c) The detailed design of a Nb3Sn prototype has been developed. The design includes optimized ends as well as end correction coils that compensate for nonlinearities arising from varying iron saturation during energization.
d) The core elements of a tuning concept have been developed and tested. The method applies single-turn superconducting loops on poles of the undulator. During the tuning process, the current in each loop can be forced to be either 0 or I_0; all powered loops are in series, i.e. at the same (tunable) current I0. Detailed Monte Carlo simulations have shown that the tuning concept will bring the trajectory wander well within specification for light source applications with a modest number of active powered loops.
e) The tuning system has been further developed to scale it to the level needed for implementation on superconducting undulators for free electron lasers and to storage ring implementations requiring higher-harmonic radiation. The fabrication process includes a number of steps, including photolithography and precision. Each of the steps have been developed with the goal of having a reliable, scalable process compatible with tuning of 1.5m or larger superconducting undulators.

The project has been successful in garnering the interest of SLAC, as the technology has significant implications for the performance of LCLS-II or a future upgrade for the facility, and DOE Basic Energy Sciences, where the technology is recognized as important for all of its future light-source facilities. Some follow-on funding has now been obtained from these sources.

CLINIC-IN-A-BOX

Principal Investigator(s): Shashi Buluswar

Project Description

The purpose of this project is to develop a small suite of highly energy-efficient and low-cost medical devices, in order to enable affordable healthcare in rural Sub-Saharan Africa and South Asia. The specific devices developed as a part of this—identified in LIGTT's "50 Breakthroughs" study—include an infant warmer (to help low-birth-weight or pre-term babies stabilize their temperature in the first 7-10 days of life when they are most vulnerable to hypothermia), and continuing development of a portable solar-powered vaccine refrigerator (aimed at preserving vaccines within the 2-8^{o}C range in which they are effective, per World Health Organization guidelines).

For the infant warmer, the key technical questions that needed to be overcome were the choice of a safe, low-cost phase change material which could maintain the appropriate temperature (37^{o}C) for more about 6 hours; a low-cost, comfortable (enough for a newly-born baby), safe (non-toxic) and sturdy (to withstand temperatures higher that 100^{o}C, and survive many uses) external material; and an overall system design.

For the vaccine refrigerator, the key technical question was the appropriateness of thermo-electric materials to effectively and efficiently transfer heat away from the vaccine chambers.

Accomplishments

Infant warmer: through this effort, we identified options for the necessary phase change material as well as external material. We also worked closely with physicians from Harvard/Boston Children's Hospital and the Ministry of Health in Rwanda to design the overall system. As of Q4 2014, the safety of the technology has already been tested, and they can be produced for <$20, a fraction of what other technologies providing comparable functionality. We will have working prototypes ready for rigorous field testing in in multiple countries, by Q1 2015.

For the vaccine refrigerator, we have developed the essential technical design and prototype to be sent to the World Health Organization (WHO) for approval. We have, however, determined that the current generation of thermoelectrics technology (bismuth telluride) may not provide the efficiency required to operate vaccine refrigerators in hot climates (with average daytime temperatures of 43^{o}C or higher). We expect to have WHO approval for these devices for a temperate zone (average daytime temperature of 32^{o}c) in Q2 2015.

Generative Design Methods for Integration of Energy and Sustainability in Early-Stage Architectural Design

Principal Investigator: Luisa Caldas

Project Description

Early-stage, conceptual architectural design has suffered radical changes in recent years, due to development on powerful modeling tools that allow fast, parametric modeling of complex building geometries, rapid-prototyping of 3D models, and links to diverse performance simulation tools. As parametric design progressively becomes the preferred method for early-stage conceptual design, the use of Generative Design Methods represents the next step in this process, by introducing performance-based optimization into architectural design, namely in terms of low-energy design.
As proofs of concept, this project explored the implementation of Generative Design Methods for optimization at multiple design scales, namely: 1) Design optimization and prototyping of a light redirecting system; main research questions addressed were: a) Currently available methods/tools to use in generative design optimization; b) Reliability and error margins introduced by these methods; c) obstacles for more accurate methods; 2) Whole-building early stage design, for multicriteria lighting, heating and cooling energy optimization.

Accomplishments

Light Redirecting System: The system simulated was built in light-weight aluminum, with a 3M high reflectance film applied on top of louvers (3M D50A Specular Film Protected, with 98.5% visible light reflectance), and a lower face coated in 70% light reflectance white mate paint, to reduce glare to occupants. The double-curvature geometry of the system was optimized using a Genetic Algorithm, with experiments being performed in three stages: Stage 1 – Radiance only (backwards ray tracing, actual geometry simulated); Stage 2 – Radiance + BSDF material (created with Window 7.2); Stage 3 – BSDF + Radiance 3-Phased Method. The second round of experiments focused on Stage 2 and Stage 3 only. Main conclusions drawn were: under direct beam radiation, the difference between the two methods is significant, with the 3-Phase Method performing up to 34% better in simulating the direct solar component. Without a strong direct solar component, the two methods have a closer performance, simulating diffuse light within a closer range, but Radiance+BSDF still has a significant error rate of up to 10%, thus proving unacceptable for this end.
Rapid Prototyping was done initially done using 3D printing, with white plastic coated with 97% reflectance film, and its light transmission measured with the Integrating Sphere at LBNL. A final, industry-grade prototype was designed and budgeted, with an extra thin aluminum profile, 0.020 inches thick, built with 6063 Alloy, T6 temper, and coated with 3M D50A Specular Film Protected, with 98.5% visible light reflectance. A prototype sized for Flexlab, including casting dies, was budgeted at only $1200 by SAPA, but construction was not authorized. Final validation of simulation methods developed against physical measurements was thus not possible. Conclusions regarding product development: for optically complex systems, typical Rapid Prototyping methods do not display the necessary optical accuracy; however, measurements with the goniophotometer require uniform samples, and no larger than one square inch. Thus, for optically complex systems with non-uniform geometry, the only current option is building a full-scale prototype for physical testing. If product development is to be made a priority, new alternatives should be developed to bridge between computer simulations and full scale, expensive and difficult to build prototypes.

Whole Building Analysis with 3D Pareto Multicriteria optimization: building variables under study were: floor stacking patterns, glazing and shading systems characteristics, and shading panes offset, for each orientation, and skylight dimensions. The multi-Objective Metrics and Goals applied were: illuminance levels (Radiance), Cooling Energy Use Intensity (EnergyPlus) and Heating Energy Use Intensity (EnergyPlus). Results suggested that Whole Building Multicriteria Analysis is a fast and effective way of testing complex building alternatives at early design stages, providing useful, operative information for decision making in very short amounts of time, in comparison to standard parametric simulation.

Virtual Grid Integration Laboratory (VirGIL)

Principal Investigator: Sila Kiliccote

Project Description

The large penetration of renewable energy sources requires flexible resources to manage the variability in generation and demand. Increased observability, improved modeling, and more detailed simulation algorithms are necessary to quantify the impact of intermittent generation to the power network, and – at the same time – efficiently plan the operation of the flexible resources. In order to study the interactions of such complex systems, co-simulation platforms are deemed necessary.

The Virtual Grid Integration Laboratory (VirGIL) is a modular co-simulation platform designed to study interactions between demand response strategies, building comfort, communication networks, and power system operation. It combines three different simulation tools (power grid, communication, and buildings) and incorporates functions for the optimal management of both the grid and the flexible resources.

Accomplishments

Significant accomplishments have been achieved during the first year of this project. First, research was conducted to determine the appropriate simulation tools for VirGIL and the interfaces to couple them. The Functional Mockup Interface (FMI) has been selected for coupling the simulation tools. FMI provides a standardized interface, which allows for a very modular co-simulation architecture, where several different modules can be added, exchanged, and tested. FMI enables battery modeling, Electric Vehicle simulation, and advanced optimization functions to be coupled in the future.

DIgSILENT Powerfactory has been selected as the power system simulator. Using a widely used commercial power system simulation platform will help reduce the barriers to the industry for adopting such platforms, investigate and subsequently deploy demand response strategies in their daily operation. Modelica has been selected as the building modeling language. Modelica is an acausal modeling language, which allows for efficient simulation. Given the complexity of the building models and controls, simulation speed and accuracy are important factors. OMNET++, an established open-source network simulator, has been selected as the communication networks simulation tool.

An FMI wrapper was developed for Powerfactory and OMNET++. VirGIL is the first tool worldwide that will connect Powerfactory, and OMNET in a co-simulation environment over FMI. Detailed EnergyPlus models for existing buildings in LBNL campus were converted to RC models through the BRCM toolbox, and then converted to the Modelica language. Model reduction algorithms were used to reduce the model complexity but maintain the accuracy as much as possible. Studies to compare the accuracy have been carried out. All simulation tools are coupled through FMI to a master algorithm, which is implemented in Ptolemy II. To increase VirGIL's simulation speed, novel simulation algorithms, notably the Quantized State Simulation (QSS) algorithm, have been developed in Ptolemy.

The first case study of VirGIL was on the LBNL distribution grid. Real data have been used for the power network and the modeling of Building 71. In the second year, we plan to simulate more complex systems, and extend VirGIL by adding advanced optimization algorithms for power system planning and building operation.

Peel-and-Stick Electricity Metering
Principal Investigator(s): Steven Lanzisera

Project Description

Research shows that electricity sub-metering can lead to a 10%-30% reduction in electricity use in commercial buildings, and it is likely these savings are available in residential and industrial facilities too. The cost to install available electricity metering technology is very high resulting in virtually no market penetration and an inability to achieve the available savings. We aim to demonstrate the core technologies needed for electricity metering technology that has one-tenth the installed cost of today's solutions. This new solution will provide sufficient accuracy and time resolution to enabling the retro- and continuous commissioning as well as distributed resource grid integration activities needed for a low carbon society.

The core technologies behind power meter are voltage and current measurement, and we will demonstrate non-contact measurement of both quantities. A suite of sensors will be installed on the surface of circuit breakers in electrical panels, and this installation can be done with minimal training and without an electrician. The sensors will measure the magnetic and electric fields passing through the face of the breaker thousands of times per second, and a set of inverse electromagnetic algorithms will estimate voltage and current in real-time. Each sensor unit will accurately estimate power under a variety of conditions and also compensate for external error sources automatically and without user driven calibration.

Accomplishments

Our most significant accomplishment is the successful demonstration of accurate voltage, current, and power measurement using a combination of commercially available sensors, custom electronics, and custom electromagnetic and statistical auto-calibration algorithms. We built a proof-of-concept sensor, installed it on various circuit breakers, and demonstrated measurement of voltage, current, and power under laboratory and real-world conditions. We also demonstrated the ability to reliably mitigate the impact of interfering fields from nearby currents.

We have also designed an advanced sensor capable of measuring magnetic field in multiple locations and in multiple directions. This technology is critical for reducing the complexity of the installation, improving interference mitigation, and enabling improved auto-calibration algorithms. The vector fields that are now measurable are useful for key aspects of advanced auto-calibration algorithms that require no reference information.

We are currently applying these results to the design of new sensors and auto-calibration algorithms. The new sensors use a combination of commercially available components and CMOS multi-axis magnetic field sensors. The new algorithms utilize newly identified statistical properties of the primary and interfering signals as well as new inverse electromagnetic analysis techniques.

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

Bryan D. McCloskey, EETD

Project Description

The goal of the first year 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 is envisioned to 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 is now fully operational. 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 three 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, and magnesium corrosion in aqueous electrolyte systems to understand limitations of aqueous Mg-air batteries. Proposals have been submitted to the NSF and JCAP II in an attempt to secure funding for aqueous electrocatalysis research (which the DEMS would be ideally suited to study).

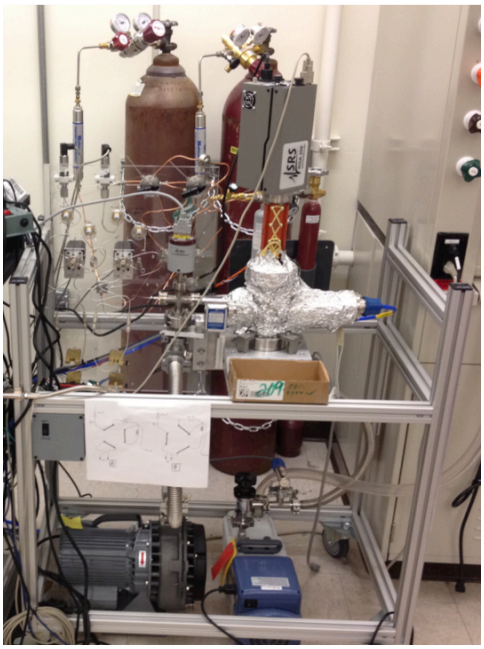


Figure 1: Differential Electrochemical Mass Spectrometer in operation in the McCloskey Lab.

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.

Creating the Vehicle-to-Grid Simulator (V2G-Sim) Platform for Predicting the Impact and Optimally Integrating Plug-in Electric Vehicles on the Electricity Grid

Principal Investigator(s): 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.

This LDRD is developing two versions of V2G-Sim, 1) V2G-Sim Analysis, and 2) V2G-Sim Operations. The V2G-Sim Analysis model couples sub-models for: a) driver behavior, b) automated generation of trip-specific drive cycles (velocity-time profiles), c) vehicle powertrain models of energy usage during a trip, d) vehicle charging, and e) vehicle response to managed charging or V2G algorithms. V2G-Sim Analysis predicts the behavior for individual vehicles/drivers, and then aggregates individual vehicle profiles to generate grid impacts predictions for large numbers of plug-in vehicles (PEVs). With these coupled sub-models, V2G-Sim Analysis provides a platform for scenario analysis of PEV deployment for transmission and distribution infrastructure planning, impacts analysis from various PEV managed charging or V2G algorithms, design of market and pricing structures, etc. V2G-Sim Operations builds upon V2G-Sim Analysis to provide temporally- and spatially-resolved forecasting of PEV charging demands and V2G opportunities allowing an aggregator or integrator to bid PEV services (such as demand response, renewables integration, regulation, etc.) onto an electricity market and operate an electricity grid having many PEVs as a resource within the grid while ensuring each vehicle is sufficiently charged when it needs to be.

Accomplishments:

Some of the key project accomplishments in FY2014 (Oct. 1, 2013 to Sept. 30, 2014) were:

1. A complete functioning prototype of V2G-Sim Analysis was created and sub-models were validated against experimental data.
2. V2G-Sim Analysis was applied in 7 case studies to explore vehicle-grid interactions on a finely resolved temporal and spatial scale, the feasibility for EVs to meet driver needs across the U.S., and to quantify the effects of VGI on battery degradation, etc.
3. Records of invention were filed for V2G-Sim and an end-user application of V2G-Sim for use by vehicle buyers and drivers. The end-user application is called MyGreenCar.
4. 4 publications that applied V2G-Sim were submitted for peer-reviewed journals.
5. Outreach to stakeholders: A website was created for V2G-Sim (http://v2gsim.lbl.gov), press releases were issued, and presentations were made on the methodology behind V2G-Sim and its applications towards transforming transportation and the grid.

INTEGRATED ASSESSMENT CAPABILITY FOR SUSTAINABLE WATER-ENERGY CO-MANAGEMENT

Principal Investigator(s): Michael D. Sohn, William D. Collins

Project Description

An underappreciated aspect of climate change is how uncertainty about expected changes affects climate mitigation and adaptation measures. In the past, energy and water planners counted on a relatively stable assessment of climate, infrastructure and policy baselines. With climate change, planners face new uncertainties and forecasts of greater variability. Infrastructure plans must be revised which might include a new peripheral canal or a more decentralized electricity grid, mitigation measures might be considered, such as incorporating biofuels and improved batteries, and the valuation of water, as a product or as an energy commodity, must be reconsidered. However, the various uses of water are managed through separate processes, and the impact of management objectives for one can result in sub-optimal practices for the other, and will be exacerbated with predictions of greater year-to-year climate variability. Without a coordinated analysis capability, the ability to predict the effectiveness of climate mitigation, adaptation measures, or setting the value of water and energy is severely limited.

In this LDRD, we will develop a computation tool and analysis framework for linked climate-water-energy co-simulation. The LDRD's resulting research will lay the foundation for an overall regional-scale integrated assessment capability. We will (1) develop analysis tools and software to estimate the cost of consuming water to produce energy, and the cost of consuming energy to produce water at regional spatial scales, and decade and multi-decade temporal scales, (2) develop analytical tools to specify the performance requirements of climate models for the aforementioned water-energy capability, (3) develop uncertainty analysis algorithms to map the tradespace between model unknowns (climate, water, & energy), and (4) demonstrate the resulting tools and software by analyzing the effects of climate uncertainty on water-energy management for the American River basin and Sacramento urban region of California.

Accomplishments

We have completed the development of a new model for simulating joint water-energy interactions. We linked two widely used regional planning models (WEAP and LEAP) and applied it to demonstrate the impact of climate variability on water and electricity in an urban area.

We a journal paper submitted to *Climatic Change,* titled "An Integrated Assessment of Water-Energy and Climate Change in Sacramento, California: How Strong is the Nexus?" The paper is one of the first to report on the full integration of basin-scale models that include forecasting of demand and supply of water and energy for residential, commercial, industrial, and agricultural sector users. We have also prepared the draft of a second journal paper, which is under internal review. In these papers we show the relative sensitivity of water and energy supply and demand to temperature and precipitation.

A Novel Nanoscale Chemical Analysis System for Low-Cost Solar Materials

Principal Investigator: Vasileia Zormpa

Project Description

Direct chemical imaging of elemental content and impurities with extreme spatial and depth resolution and specificity is required to understand, predict and minimize processes that adversely affect the macroscale properties of solar and other energy systems. A fundamental lack of key analytical techniques capable of providing this information leaves a pressing need for the development of next-generation nanoscale chemical imaging tools. The objective of this project is to develop a novel ultrafast laser spectroscopy technique based on a two near-field nanoprobe scheme which will overcome current limitations and meet the requirements of a versatile chemical imaging system for detecting and chemically mapping defects in solar energy systems and other energy materials.

This project aims to develop a sensitive femtosecond laser chemical imaging system in which both material excitation and signal detection occurs in the optical near-field vicinity. This chemical imaging system will enable a fundamental understanding of the properties and functionality of new solar material systems at spatio-temporal scales that were previously unattainable.

Accomplishments

In the second year of the project, both ultraviolet and visible femtosecond laser pulses were coupled to the near-field excitation probe to obtain chemical signatures of different material systems including nanoparticles, crystalline, and amorphous materials. We demonstrated near-field visible-range fluorescence originating from ultraviolet femtosecond laser excitation in the optical near-field. Second order diffraction was also observed in the same spectral range, enabling simultaneous femtosecond Rayleigh and femtosecond laser-induced fluorescence signal detection in the near field vicinity with the dual probe near-field system.

We further optimized the near-field excitation and detection processes as a way to improve sensitivity and resolution, and compared the signals from near-field excitation/far-field detection to near-field excitation/near-field detection signals from the same material system (Eu-doped fluorescent nanospheres). Significant improvements in the signal-to-noise ratio were observed in the near-field/near-field configuration, despite the significantly smaller size of excited surface area.

Finally, the potential of generating surface plasmon polaritons from a “femtosecond-laser point source” was explored in the near-field/near-field configuration at a Au/glass interface, and the signal intensity was studied as a function of inter-probe distance using visible femtosecond laser irradiation. These results underline the importance of detecting near-field signals in the near-field vicinity as a way to achieve high sensitivity, high resolution chemical imaging at small spatio-temporal scales.

URBAN SCALE ENERGY GRID MODELING

Principal Investigator: Michael Wetter

Project Description

The purpose of this research is to build and apply to test problems a computational platform for the design, retrofit and operation of urban energy grids that include electrical systems, district heating and cooling systems, and centralized and distributed energy storage. The need for this research arises because an integration of renewable energy beyond 30% poses dynamic challenges on the generation, storage and transmission of energy that are not well understood. Such a platform is also needed to assess economic benefits for the integration of co-generation plants that generate combined heating, cooling and power at the district level in order to decrease the carbon footprint of energy generation.

To address this need, this project will create a flexible computational R&D platform that allows expanding energy and policy analysis from buildings to district energy systems. Questions that this platform enables to address include where to place energy generation and storage, how to set the price structure, how to trade-off incentives for energy-efficiency versus incentives to add generation or storage capacity at buildings, how to integrate waste heat utilization to reduce the carbon footprint of district energy systems and how to upgrade the electricity grid to integrate an increasing fraction of renewable energy while ensuring grid reliability and power quality.

Accomplishments

Significant accomplishments have been made in the development of multi-physics models that describe the interaction between buildings and the electrical grid.

Regarding multi-physics modeling, we completed the development of more than fifty models for analyzing buildings-to-electrical grid integration. The models are now part of the Modelica Buildings library, an equation-based object-oriented library for modeling of dynamic building energy systems. The models can represent DC and AC systems under different assumptions such as quasi-stationary or dynamic-phasorial representation. The electrical models can be connected to thermal models of buildings in order to evaluate the impact of electrical and thermal storages, as well as of building controls, on the distribution grid.

The models have been validated against standard IEEE procedures defined for testing the correctness of electrical network simulation software. The models, the results of the validation and few examples showing the ability to perform building-to-grid simulation studies were presented at the 2014 BauSIM conference in Aachen (Germany). The paper, titled “A Modelica package for building-to-electrical grid integration” won the best paper award.

Using the equation-based modeling parading leads to multiple advantages. It allows to graphically connect components of cyber-physical systems (i.e., building thermal systems, electrical systems, controls and communication systems) that advance in time based on continuous time dynamics, discrete time dynamics, or event-driven dynamics, in order to study building-to-grid integration. These languages also allow accessing the mathematical structure of the entire model. Such information has been used for co-simulation and for solving optimal control problems. For example, we demonstrated how simulation models can be reused to solve optimal control problems by means of computer algebra and numerical methods. The problem investigated was to determine the optimal charge profile of a battery in a small district with multiple buildings and photovoltaic systems that minimizes energy subject to voltage constraints.

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

Project Description

The increasing availability of complete genomic sequences and whole-genome analysis tools has moved the construction of industrial hosts towards rational design by metabolic engineering and systems biology. The current genetic manipulation toolkits available for industrial hosts, however, are desperately sparse and unpolished in comparison to the array of tools available for *E. coli*. The goal of this project is to develop a high throughput 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.*

The original goal of this proposal was to create a secure industrial bacterium by converting all 484 TGA termination codons to TAA in the *C. glutamicum* genome and then reassigning TGA to encode an unnatural amino acid. In our phase I work, we discovered that the recombineering approach alone could not achieve the frequency of allelic replacement needed to complete codon depletion in a reasonable time frame. We concluded that a more efficient genome editing tool would be needed for this project. Recent work on the Clustered Regularly Interspaced Short Palindromic Repeat (CRISPR) adaptive immune system of prokaryotes has led to the identification of a DNA endonuclease called Cas9 whose target sequence specificity is programmed by small spacer RNAs in the CRISPR loci. By editing spacer sequences we can direct Cas9 to cut endogenous DNA targets, thereby forcing cells to repair themselves in a predictably mutagenic manner. Such Cas9 mediated cleavage *in vivo* is more efficient, effective, and potentially multiplexable than any other tools available for genomic engineering.

Accomplishments

Our most significant accomplishment has been to develop a reproducible and efficient protocol for engineering *E. coli* DNA *in vivo*. Our method uses the *Streptococcus pyogenes* CRISPR-Cas9 system in combination with λRed recombineering proteins in *E. coli*. We have created a mobile plasmid with both Cas9 and λRed activities and used it successfully in performing genome editing in all *E. coli* strains in hand. This protocol has been successfully used to modify gene loci in living *E. coli* cells within a 3 weeks time frame. The developed Cas9 toolkit and protocol have already been used in several bioenergy research projects. We have also received requests and started disseminating the toolkit and protocol to general scientific community.

We have also succeeded in developing informatics tools to aid in the design of CRISPR-spacer constructs given a targeted range of genomic sequences. This tool would be handy in the design of Cas9 genome editing at scale.

As we had predicted, our approach provides a significantly faster turnaround time to modify genetic codes than any available tools. 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.

Development of Biosensors for High-Throughput Functional Screening of Biosynthetic Pathways

Principal Investigator(s): Samuel Deutsch

Project Description

The purpose of this project is to develop sensitive and selective biosensors for a diverse set of target chemicals as a way to provide a high-throughput functional screening method for molecule production in microbial cells. Advances in DNA synthesis and combinatorial DNA assembly allow for the construction of thousands of pathway variants by varying both the gene content as well as the expression levels of the pathway components, a technique commonly referred to as pathway refactoring. However, a lack of sufficiently sensitive, selective, and scalable technologies to measure chemical production presents a major bottleneck that limits our ability to fully exploit large-scale synthesis efforts.

We will develop and deploy novel biosensors systems based on both protein and RNA molecules that have been previously shown to respond to the presence of small molecule ligands. In the case of protein-based sensors, we will use synthetic biology approaches to modify the ligand specificity of a known transcription factor (TF). We will screen for ligand-dependent TF function by placing TF binding sites in front of GFP, such that GFP activation should only be observed in the presence of a ligand. We will test the affinity and response of the TF mutant library to a variety of relevant ligands by using several rounds of selection using fluorescence activated cell-sorting (FACS). Samples collected after each round of selection will be sequenced using next-generation sequencing methods and we will seek to understand the relationship between TF ligand affinity and sequence evolution, as this will facilitate more rational engineering approaches.

In the case of the nucleotide sensor, we will develop a system in which cell survival is linked to ligand production by coupling the switch to a chemical selection system used during cell growth. We will then deploy this system to screen a library of 20K pathway variants to select and further characterize high molecule producing *E.coli* strains. Selected strains will be sequenced and we will use modeling approaches to identify the key variables and bottlenecks associated to molecule production.

Accomplishments

During the second year of this proposal we: (i) Continued the characterization of the biosensor developed in year 1, (ii) Constructed a 50K combinatorial library, for which we have selected and sequenced 250 clones. (iii) Transformed the library into the expressing strain that is currently being characterized alkane production by both biosensor-based fluorescence and traditional GC-MS methods. (iv) We have screened the AraC mutant library for response to enzymes. (v) In the case of one library we sequenced the variant pools at different selection stages and identified critical residues for recognition. We identified a high affinity clone, which was subsequently expressed, purified and crystallized for structure determination. (vi) We have deployed a sensor in combination with a refactored combinatorial library for the production of a factor and identified strains producing >20X levels of thiamine relative to the factor in collaboration with Hans Genee at DTU (Denmark).

Function-Based Approaches for Distant-Acting Enhancer Discovery

Principal Investigator: Len Pennacchio

Project Description

The purpose of this project is to develop methodologies to better screen the human and mouse genomes for gene regulatory sequences residing in the 98% of the genome that is noncoding. Such data will provide important functional data on the location of these elusive sequences and aid in annotation the human genome. As whole human genome sequencing is poised to be a routine capability in the clinic, this foundation is essential to link human variation to human disease.

We will develop an unbiased, high-throughput functional assay for identifying and characterizing enhancer gene regulatory elements. These methods will pair pluripotent cell reporter assays and flow cytometry with recent advances in DNA sequencing to allow the parallel functional screening of hundreds to tens of thousands of DNA sequences for enhancer activity. These methods are expected to have a considerable impact on our understanding of transcriptional regulation by allowing for the identification of enhancers that have been thus far intractable to genome-scale identification.

Accomplishments

Over the course of this LDRD funding, we have successfully developed proof of principle for an end-to-end system to screen for gene regulatory sequences in an unbiased manner. This work has been published in ***Nature Methods***, and an additional small project resulting from this work has been reported in *Biology Open*. Briefly, we have shown that we can clone hundreds to thousands of random sequences into a precise location in the mouse genome that is linked to a reporter gene, which is activated when sequences are behaving as enhancers. The targeted cells can be flow sorted to isolate those cells that are actively expressing the reporter gene, and the sequences responsible for this reporter expression can be identified through DNA sequencing. To date, we have used this method to test the embryonic stem cell enhancer activity of more than 0.5Megabases of mouse or human genomic sequence in 1kilobase increments.

To apply this method to a broader range of cell types, a major aim of this proposal, we have coupled the ES cell reporter assays we developed with *in vitro* differentiation and showed that we can accurately identify enhancers active in cardiac and neuronal cell populations. By comparing enhancers active at a specific locus in ES cells to those sites active in cardiomyocytes, we were able to observe the dynamic changes in regulatory architecture during cellular differentiation that likely mimic processes that occurring during mammalian heart development.

During th last year, we explored whether cutting-edge genome editing technologies can allow us to scale this method to assay an even larger number of putative enhancers in a single experiment. Cas9-mediated genome engineering methods indeed lead to higher rates of genome integration of enhancer test sequences, a major bottleneck in increasing the scale of this assay.

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

Principal Investigator: Axel Visel

Project Description

Higher eukaryotic organisms are compartmentalized into many different cell types and organs, tailored to perform specific functions. Plants exhibit especially interesting developmental patterns, as the overall architecture of most plants is indeterminate, i.e. stochastic and environmental effects dictate organ formation and positioning. Plants, as autotrophic systems converting sunlight into biochemical energy, are attractive targets for precision engineering of traits desired for bioenergy and bioindustrial purposes. We proposed to identify and characterize genetic regulatory sequences that dictate when and where genes are expressed within a plant. This promoter set will enable rational design of plant systems following engineering paradigms.

We proposed to identify candidate promoters through an unbiased sequence-based approach. Thousands of randomized nucleic acid sequences ("barcodes") will be attached to a reporter gene under the control of endogenous promoter sequences derived from the *Arabidopsis thaliana* genome. These promoter:barcode sequences will then be incorporated into a plant transformation vector, encoding an antibiotic or herbicide resistance gene, and propagated in a large transfection vector library. The library will be used to transfect *Arabidopsis* plants. Transformed seeds will be selected, and various tissues from these plants (e.g. leaf, stem, flower) will be harvested *en masse*. For example, a single leaf sample will contain representative leaf tissue from several hundred plants. Genomic DNA will then be extracted from each tissue sample, and the promoter:barcode region will be amplified by PCR and sequenced on a next-generation sequencing platform.

Accomplishments

A postdoctoral fellow with experience in molecular biology, functional genomic screens in the *Arabidopsis* model, and computational data analysis was hired to establish the proposed methods, perform molecular biology and plant growth experiments, and execute data analysis.

This project required us to establish infrastructure and protocols to grow and propagate *Arabidopsis* plants, which was previously lacking at the performance site (JGI). During FY2014, we established a plant growth facility, capable of nurturing several thousand individual plants. The equipment was validated to support healthy growth of plants throughout their life cycle, lasting 12 weeks from seed to senescence. Additionally, we have installed an environmentally controlled plant growth chamber, ideal for incubating plants growing on sterile, selective media, an essential component of the transformation-based screen.

We are currently in the process of designing and validating transformation vectors suitable for randomization and coupling to a candidate promoter set. In addition to the promoter reporter vector system described above, this includes a low-expression constitutive promoter, and a C-terminal GFP gene directly downstream of a Gateway cloning site. The presence of this promoter will allow us to identify repressors in addition to activators, as it will give a low, yet detectable amount of activity across all tissue types sampled.

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

Project Overview

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 systematically 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.

PROGRESS TO-DATE

We have now measured the lipids using three independent biochemical methods. Specifically, we measured (1). absolute quantitative TAG measurements by thin-layer chromatography (TLC). Our results demonstrated that PSR1 overexpressing liporotunds cells accumulated more TAG in nutrient repleted condition. (2) transesterification of TAGs to Fatty Acid Methyl Esters (FAMEs) monitored by gas chromatography-mass spectrometry (GC-MS). This data confirmed that TAG accumulation in PSR1 overexpressing liporotunds is indeed higher, with a predominant significant increase in fatty acid component.(3) A detailed lipid composition analysis by liquid chromatography tandem mass spectrometry (LC-MS/MS). The profile provides a refined view of the effects of PSR1 overexpression on lipid metabolism. To ensure the robustness of the method we explored biological significance of methylation in land plants. Methylomes of shoot and root tissues as well as vascular vs. non-vascular tissues were analyzed and manuscript is prepared for submission in the next month. Using this established capability and data, a proposal was submitted to DOE system biology grant call for future funding opportunity.

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 succeeded in obtaining follow-on funding from the National Institute of Health to continue these efforts. 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. We are attempting to apply Cas9 editing to additional bacteria, algae, and plants.

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. During the remainder of this LDRD grant cycle, we plan to synthesize a diverse subset of these computationally identified Cas9 genes, isolate their resulting proteins, and biochemically characterize these proteins in search of Cas9s with a diversity of sequence requirements and sizes.

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 designed and are now fabricating a very high density (10,000 electrode/cm^2 x many cm^2) 2D electrocorticography neural amplification and data acquisition system. To establish infrastructures for enabling discoveries in large neuroscience datasets, and to provide the rapid analysis needed, we have been advancing high-performance computing for both 'off-line' and 'on-line' data analysis. We have: (a) engineered a data storage system based on a specific data format in order to leverage the computing resources of NERSC, (b) developed an algorithm for statistical inference of model parameters from data that gives more accurate and interpretable results than the most commonly used methods in the neuroscience community, (c) applied deep neural networks to 'classify' produced speech from human electrocorticography data, (d) programmed FPGA's to process the neural data collected by the high density system in real-time, and adapted 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 developed a family of fluorescent probes for sodium with a palette of different excitation/emission colors. The reagents show high selectivity for sodium over abundant cellular metals potassium, calcium, and magnesium, and match well with standard microscopy laser lines and filter sets. We have also paired these with upconverting nanocrystals (UCNPs), which absorb in the near infrared and emit in the visible to excite the sodium ion sensors. We have synthesized a series of UCNPs with increased efficiency in activating the fluorescent sodium sensors. 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 UCNPs for deep brain optical imaging and optogenetic stimulation. In a proof of concept imaging experiment, we used near-infrared light to illuminate a 500 micron-thick slice of wild type mouse brain with one surface coated with UCNPs. When the slice was pumped with 980 nm light, we were able to image the newly-designed UCNPs through 500 microns of brain 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.

Multi-Modal Imaging of Microbial Interactions

Manfred Auer, Musahid Ahmed, Bruce Cohen, Trent Northen

Project Description

The purpose of this project was to study model (*Myxococcus xanthus* and *Bacillus subtilis*) microbial communities architectural organization and metabolism using the tools of secondary ion mass spectrometry (SIMS), Nanospray Desorption Electrospray Ionization (nanoDESI) mass spectrometry, Correlative Light and Electron Microscopy (CLEM) and Fluorescence Live Cell Tracking (FLCT) microscopy, as well as high-resolution Transmission Electron Microcopy (TEM). While each of these techniques provides valuable information as a stand-alone technology, the goal of this LDRD was to integrate these different compositional, positional and architectural approaches, and thus to develop a workflow, by which multi-modal information can be acquired from a single sample. From a microbiology point of view we aimed to understand whether the community responds to an external threat in a localized, regional or global manner. Territorial disputes between bacterial species are common in most habitats, and are of great interest to a large number of DOE-relevant topics such as bioremediation, carbon cycling and lignocellulose degradation.

Accomplishments

We have developed the novel technique of correlative ambient environment nanoDESI ion/fluorescence microscopy imaging, and performed correlative fluorescence microscopy/electron microscopy imaging as well as large area 2D electron microscopy imaging, which has allowed us to study in unprecendeted detail the interaction of different species microbial communities. Correlative light and electron microscopy imaging revealed that interterritorial zones are dominated by exopolysaccharides (EPS), as well as by large secreted membrane sheets and outer membrane vesicles (OMVs). Liquid Chromatography Mass Spectrometry (LC/MS) of OMVs identified antimicrobial small molecules (secondary metabolites) in *M. xanthus*, apparently used to fight off the invasion of *B. subtilis*. Using the identified mass signatures specific for *M. xanthus* DZ2 and *B. subtilis* 3610, respectively, as well as the OMV-delivered antibiotics, we were able to show that the interspecies territorial dispute response was a regional response that clearly exceeded the immediate zone of contact clearly showing that the territorial invasion threat was communicated regionally within the M. xanthus biofilm, possibly in a stealth communication mode enabled by the previously identified OM vesicle chains and tubes network.

This project showcased that only the integration of multiple imaging modalities, each of which detect ultrastructural, metabolic/chemical or localization changes of key components, led to an in-depth, comprehensive understanding of microbial processes. Key to this insight was the study of the biological systems at different length and resolution scale levels (including the mesoscale) with different imaging approaches in a correlative integrated manner.

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). Risk assessment is in a similar position: the REACH Act in Europe will require the characterization of 30,000 substances over the next 7 years, a more than 300 fold scale-up compared to the previous 14 years. The cost of testing in vertebrate model systems alone has been estimated above €9.5B. 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.

Specific Aims:

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 a prototype software package that implements a Random Forests model for interaction prioritization in human variation data, and a statistical testing procedure for simultaneously assessing the interactions of multiple genetic variants with multiple genes. We have applied these procedures to a cohort of 91 individuals with genome sequence information and RNA-seq data. We have discovered a number of new *trans* interactions effecting transcript levels in whole blood. We are now exploring phenotypic interactions. We will apply the same method to a larger cohort of ~700, and this is ongoing work.

Aim 2: We have a prototype software package called "Unconstrained Surface Mapping" (USM) that leverages Random Forests models to identify interactions of potentially high order. We have overcome a number of computational challenges, including an NP-Hard counting problem that we overcame with a stochastic (randomized) algorithm. Our algorithm is now scalable to real-world data and we are using it to discovery interactions between transcription factors that govern cell differentiation and organ morphogenesis in the fruit fly.

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 are currently conducting ChIPs of several chromosomal proteins to identify such potential "readers". We have also completed ChIPSeq of H3K27Me3 from Kc cells treated with BPA, and discovered that BPA-induced increases in H3K27Me3 levels only occur at normal genome substrates of EZH2. We are currently testing BPA-specific developmental effects on female larval and pupal tissues based on our results showing higher BPA-induced lethality in female but not male flies.

We have also further characterized 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 are currently investigating the significance of these new H2A-Ub sites and how these chromatin changes are linked to HP1a mobilization, PcG regulation and transcription, using knockdown experiments. 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 an NIH grant to further elucidate the mechanisms of environmental epigenetics.

Modeling Desert Soil Crust Microbial Community Responses To Pulsed Climate Events.
Principal Investigator(s): Trent Northen

Project Description

The overall goal of this project has been to use a tractable environmental soil microbial community, desert biological soil crusts (biocrusts), to provide fundamental insights into bacterial carbon cycling and changes in community structure occurring in response to important environmental parameters, focusing on rainfall and temperature. Thus pioneering approaches and helping to unraveling key mechanistic and dynamic aspects of the biogeochemical carbon (C) cycling in soils. This includes characterizing and modeling the dynamic responses of the soils primary producer *Microcoleus vaginatus*, the metabolites release by this bacterium and investigating possible microbial foodwebs based on these released metabolites. This program is an example of 'team science' and uses integrated biogeochemical, microbiological, genomic, metabolomic and computational approaches to define alterations in carbon cycling and community structure in response to wetting.

Accomplishments:

This year we continued investigation of the targeting of DOC components by biocrust bacteria using liquid chromatography mass spectrometry (LC-MS) analysis. Our work has included analysis of cell pellets, spent media, biocrust soil extracts and biocrust soil water collected over the course of a wetting. To investigate substrate targeting, isolates were grown in rich media composed of biological soil crust extract. LC-MS based comparison of the fresh and spent media identified the profile of uptaken and released metabolites by each of the biocrust isolates. These analyses revealed hundreds of metabolites from biocrust and identified a set of metabolites, including disaccharides, that were uptaken by essentially all studied isolates suggesting a potential competition for these compounds in the soil. Beyond these few metabolites, the individual heterotrophs showed specialization towards specific metabolites. Surprisingly, many of the most abundant oligosaccharides and other metabolites were ignored by these isolates. This observation that soil heterotrophs target specific DOC components is counter to conventional thinking of soil heterotrophs as 'generalists'. Rather it may be that heterotrophs are highly specialized for specific metabolites and DOC composition may play a significant role in determining community structure. Therefore, the observed complexity of soil DOC composition may explain some portion of the tremendous diversity of soil microbes

Development of Protein Localization Atlases at Multiple Scales in Eukaryotes

Damir Sudar, Gary Karpen, Susan Celniker, Roger Hoskins, Erwin Frise

Project Description

The purpose of this project is to develop efficient gene product tagging, automated image acquisition using multiple modalities, visualization-supported image and image-derived data analysis tools, and to integrate these into a high-throughput pipeline to build protein localization atlases, starting with the fruit fly *Drosophila*. A proliferation of genome and transcriptome sequence data has produced comprehensive annotations of the genes, mRNAs and inferred proteins for many different eukaryotic organisms. We are now addressing a new challenge: comprehensive determination of gene and protein functions. Among the most direct clues to the function of an uncharacterized gene are the spatial, temporal and subcellular expression patterns of protein products, and the interactions that a protein makes with other proteins or nucleic acids. This project's ultimate goal is building a *Drosophila* Protein Atlas (DPA) – a comprehensive and quantitative map of subcellular protein localization in tissues and cells in *Drosophila melanogaster*, a key model organism for which we locally have extensive tools and expertise. About 75% of human disease genes have a homolog in the ~14k protein-coding fly genes but have unknown biochemical functions. Thus, the DPA will have enormous value for understanding animal proteomes, including mice and humans.

Accomplishments

We generated panels of 96 previously known tagged proteins and 256 unknown proteins with predicted localizations. The known proteins provided subcellular markers for co-localization experiments and aided development of analysis tools while the unknown proteins were used to test and validate our approach. We developed improved methods to create gene fusion constructs with 8 new cloning vectors with fluorescent protein tags optimized for this project, we sequence verified 812 new constructs, and we developed a high-throughput protocol to transfect these into cultured *Drosophila* S2 cells for live and fixed cell imaging.

For image acquisition we created a multi-modal microscopy pipeline to image subcellular localization of tagged proteins at multiple scales using existing high throughput microscopy platforms and high resolution microscopes, as well as developed a novel open-source platform for automated microscopy, to rapidly image and quantitate protein expression patterns in cell cultures. After imaging and mapping the subcellular localizations of our 96 reference proteins, we selected a marker set of 12 proteins that localize to known subcellular compartments and other interesting patterns that may reveal new compartments. This marker set allows classification of new proteins and constitutes a useful resource for *Drosophila* cell biology.

Proving its power we used the pipeline to co-localize paired proteins tagged with novel GFPs in live S2 cells from tens of thousands of images to validate over 200 protein-protein interactions from the Drosophila Protein Interaction Map and from computational predictions.

For automatic classification of new proteins into compartments identified by the markers we developed and tested two different approaches for supervised learning. We first extracted numerical feature vectors from individual cell images and used support vector machines and random forests in an approach pioneered by the Human Protein Atlas. Next we deployed a convolutional neural network on the pixel values of individual cell images, which, as reported in natural image classification, gave us an increased classification accuracy of about 10% compared to feature vector learning techniques on our image data.

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 novel, graphene-based platform to enable correlative electron microscopy and super-resolution microscopy of wet and live cells. Graphene is an emerging two-dimensional material that is only a single layer of bonded carbon atoms. We are employing 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 even in the hands of experts. The methods involved also create notable difficulties for correlating results with high-resolution fluorescence microscopy. Our approach aims at achieving facile electron microscopy of wet/live cells with minimal sample preparation, and further enabling ready 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 indeed encapsulate and thus protect 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 common electron microscopes operating 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.

We have also succeeded in realizing correlated super-resolution microscopy and electron microscopy of the same cells on our graphene-based platform, and for different subcellular structures, including cytoskeletal filaments and mitochondria. Comparison of the images obtained from the two modes showed excellent correlation/agreement with each other, showing that the graphene protection has been highly efficient in protecting cells and preserving the detailed subcellular structures at the nanometer scale in the vacuum environment of electron microscope.

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 that the combination of strong spin-orbit coupling and symmetry leads to strongly spin-anisotropic magnetic exchange. The building block connected to this property is octahedrally coordinated IrO_6 bonded in a honeycomb lattice, which has the strong spin-orbit coupling (coming from Ir) and the correct symmetry elements (the O_h point group symmetry of the octahedral).

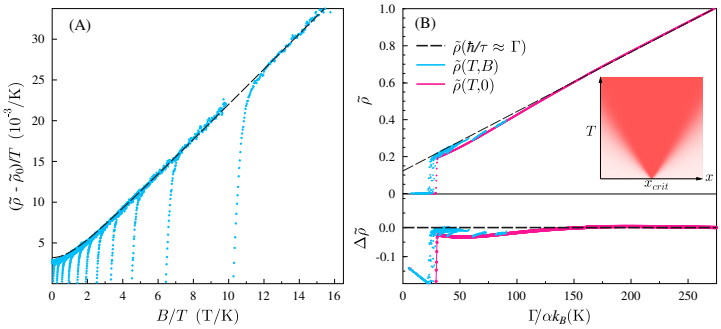


Figure 1: (A) Resistance as function of temperature and magnetic field (blue) falls on a single universal function (black dashed line). (B) Raw data of resistance as a function of field and temperature plotted with respect to a new energy scale that combines magnetic and thermal contributions.

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 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.
3. **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.*
4. **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.

Hard X-Ray Photoemission for Materials Science

Principal Investigator: Charles 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) to probe buried layers and interfaces in multilayer nanostructures with much higher sub-nm depth resolution than has been possible previously. An important element in this is the further improvement and utilization of a unique facility that has been established for HXPS at Beamline 9.3.1 of the ALS, recently chosen as 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 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, and reviewed in publication [3].

Accomplishments

We have carried out studies on several different materials systems, as indicated in the publication list, whose numbers are referenced here in brackets.

- In collaboration with Hellman et al. (LBNL MSD, UCB), and as a continuation of work begun under the previous Magnetic Materials Program, we have used soft x-ray photoelectron microscopy to study the effect of capping materials on interfacial ferromagnetic in FeRh alloys, with these materials of interest for future thermally-assisted magnetic recording [1].
- In a collaboration with Javey et al. (LBNL MSD), we have used soft x-ray photoelectron microscopy to study single-layer transition-metal dichalcogenide semiconductor membrane structures that are very promising for future photovoltaic devices [2]. We have also obtained additional HXPS and SXPS data for these systems that are being analyzed and written up.
- In a collaboration with Stemmer et al. (UCSB), we have also combined HXPS and SXPS, together with SW excitation, in studies of multilayer oxide systems composed of:
  --$SrTiO_3$ and $GdTiO_3$, which are of interest because they exhibit a two-dimensional electron gas (2DEG) at the interface between the two insulating materials that shows in addition ferromagnetic order [8,9], and
  --$BiFeO_3$ and Ca-doped $CeMnO_3$, which again exhibit a 2DEG, but with the property of facile electrostatic switching from conducting to insulating state, has been studied, and the thickness of the 2DEG directly measured [7].
- In a collaboration with Bluhm (LBNL CSD), we have for the first time combined SW excitation with HXPS and ambient-pressure photoemission at up to tens of Torr in the study of solid-liquid films, opening up a exciting range of applications for the technique in energy and environmental studies [4,6].
- In a collaboration with Himpsel (UW Madison), we have 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 [5].

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. We will also investigate NPs, comprised of alloys that undergo rapid phase changes, and possible shape changes, in response to an external stimulus. The key to such adaptive materials is functionalizing NPs with stimuli-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

Carbon Nanotubes: Water-dispersible, acid functionalized and shortened SWCNTs was obtained by acid treatment with somication. The efficient segregation of thefunctionalized SWCNTs at the oil/water interface was induced by dissolving low molecular-weight amine-terminated polystyrene (PS-NH2) in the oil phase. Salt-bridge interactions between carboxylic acid groups of SWCNTs and amine groups of PS drove the assembly of SWCNTs at the interface, monitored by pendant drop tensiometry and laser scanning confocal microscopy. The impact of PS end-group functionality, PS and SWCNT concentrations, and the degree of SWCNT acid modification on the interfacial activity was assessed, and a sharp drop in interfacial tension was observed above a critical SWCNT concentration.

The assembly and mechanical properties of SWCNT is strongly influenced by pH and molecular weight of polymer species. The frequency-dependent elastic and viscous moduli of the resulting films in dilation were characterized by interfacial pendant drop rheology. Structural (fast, minutes) and adsorption/desorption (slow, tens of minutes) relaxations were both noted, and at frequencies intermediate to the two, in a manner almost insensitive to assembly parameters, the films displayed the expected behaviors for 2D critical gels, i.e., at the boundary between fluid and solid. In particular, tan (delta) was frequency-independent over one to two decades of frequency. Power law time behaviors in linear stress relaxation confirmed this interpretation.

Polyfluorenes: Bringing conjugated polyelectrolytes to liquid-liquid interface enables the structuring of liquids having optoelectronic functions. This new class of materials is featured with conjugated backbone and functional side chains, where the side chain provides crucial interfacial activity. Tertiary amine group is used as the pendant dipole molecule on the backbone of polyfluorenes (PFN). The tertiary amine has a pair of electrons, which can be used to initiate weak interactions, like hydrogen bonding, at interface. Complementary to PFN are carboxylic acid functionalized gold nanoparticles were chosen as the pairing material to enable interactions with PFN to further enhance the interfacial function. By controlling the extent of interfacial reactions, e.g. tuning the PH to control the strength of hydrogen bonding, the interfacial properties of the assemblies were changed from a liquid-like to a jammed to a solid, glass-like assembly, that were used to as responsive materials, enabling new functions.

Nanoparticle Surfactants: Furthering our earlier studies on the formation of nanoparticle surfactants at interfaces, the synthesis of a series of well-defined, amine functionalized poly(dimethylsiloxane) was completed, yielding PDMS with molecular weights ranging from 1K to 20K. The interfacial activity and interfacial dynamics were measured by pendant drop tensiometry. Studies are currently underway to probe the responsiveness of the assemblies to changes in pH and temperature.

ENABLING TECHNOLOGIES FOR ADVANCED SEMICONDUCTOR MANUFACTURING RESEARCH

Principal Investigator(s): Patrick Naulleau, Weilun Chao, Eric Gullikson

Project Description

The purpose of this project was to develop new methods, material systems, and processes enabling future breakthroughs in advanced manufacturing techniques in the area of semiconductor devices. In particular, the program was focused on the lithographic patterning component of the semiconductor manufacturing process. Dramatic advances in lithography are what have enabled Moore's Law in the past and continued advancements in this area are crucial to sustaining Moore's Law in the future. E-beam technologies are expected to play an essential role in the future of advanced semiconductor manufacturing. The importance of e-beam is two-fold; first as a direct wafer pattering technology for lower volume production, and second as a mask writing technology for high volume projection extreme ultraviolet (EUV) lithography techniques.

Nanopatterning of EUV masks to achieve specific functionality is further complicated by the fact that EUV masks are comprised of complex material systems of alternating single digit nm layers of high and low-Z materials to achieve high reflectivity at EUV wavelengths. Our goal is to enable new functionalities in these structures such as increased angular bandwidth, through the development of new aperiodic coatings and a deep understanding of the optical properties of the underlying materials and interfaces. We also seek to enable new optical wavefront encoding techniques through the development of etch processes compatible with the complex multilayer structures of EUV masks.

Accomplishments

Our most significant accomplishment has been to develop a new strong phase shift mask design for EUV lithography enabling an improvement in throughput for dense contact hole printing and a relaxation in mask patterning resolution requirements. Additionally a reproducible process for the fabrication of such masks for EUV lithography has been developed. Our method uses a three component nanolayered structure.

After completion of the LDRD project the developed process was used to fabricate a test mask that we are in the process of characterizing in an EUV microscope at the ALS.

As part of the mask process development, ebeam patterning capabilities were refined and these capabilities help lead to new gift funding by Inpria corporation expected in Feb. 2015. The mask development process also required refinement of our nano-layered coating capabilities and characterization which led to a related contract with Applied Materials which kicked off at the end of last year. That project was focused on understanding the impact of roughness on nano-layered structures such as the phase shift mask we developed.

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 to demonstrate that resonant X-ray scattering is an effective probe of the Skyrmion phase in Cu_2OSeO_3. The cubic insulator Cu_2OSeO_3 is a model system for understanding Skyrmions, which are topologically protected, particle-like excitations that emerge as a periodic array of magnetic vortices when the material symmetry is broken under the application of a modest magnetic field. Understanding the origin and dynamics of this novel phase is of tremendous interest for spintronics and related device applications.

A second significant accomplishment has been the first experimental 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. We are in the process of applying similar dynamic X-ray studies to the Cu_2OSeO_3 Skyrmion material.

Exciton Visualization and Engineering in Organic Materials for Energy Conversion
Principal Investigator(s): **Alexander Weber-Bargioni, BiWu Ma, Jeffrey Neaton, Naomi Ginsberg**

Project Description
Our goal is to develop an understanding of excitons and other excited states in photoactive materials with high spatiotemporal resolution, which will lead to breakthroughs in many energy conversion technologies. For example, molecular photovoltaics are promising for solar energy conversion because they are cheap, lightweight, and flexible, and because their properties can be easily tuned via organic synthesis. However, OPVs suffer from low efficiencies. Space- and time-resolved understanding of excited states in these materials will lead to higher efficiencies. Despite more than two decades of past work, the transport and spectroscopic properties of organic materials in photovoltaics - and the nature and dynamics of their excitations - continue to be debated. A major challenge is the lack of knowledge of the interplay between morphology and excited states of these organic semiconductors.
For this LDRD we had proposed to develop and combine new approaches to synthesis, theory, and spectroscopy to, for the first time, spatially map, with nm-resolution, the evolution of excitons - as a function of molecular morphology - in well-defined tailored organic materials as a function of time. We suggested the use of state-of-the-art, materials-specific excited-state theory to interpret the exciton dynamics, study the microscopic origins of their dissociation and degradation processes, and, ultimately, predict molecular moieties and morphologies leading to robust and efficient energy conversion materials.

Accomplishments
In the second year of the LDRD we were able to accomplish three important scientific milestones: 1. Mapping Exciton diffusion length in organic materials, 2. Mapping Foerster Resonant Energy Transfer and its modification through CdSe Quantum Dot assemblies; 3. Actively manipulating Exciton transport from 0 – 2D materials creating the smallest light switch in the world.

Dr. Mauro Melli developed the previous year Localized Excitation Photocurrent Microscopy (LEPCEM) with which he was able to determine exciton diffusion length in P3HT of 25 nm and Rubrene up to 80nm (both are currently summarized as two manuscripts for publication). Together with a collaborating PostDoc Dr. Munechika, Dr. Melli established also the diffusion length of excitons through inorganic nano building block assemblies (CdSe) and determined surprising 70nm diffusion length. Together with the second LDRD postdoc, Dr. Lee, we were able to demonstrate how the resonant energy transfer mediated exciton transport can be modified by dimensionality (monolayer vs 1D assembly), temperature, and applying a local Quantum Confined Stark effect that modifies the energy landscape (currently prepared for publication).

The active manipulation of excitons in 2-D assemblies led to the idea of manipulating resonance energy transfer mediated exciton hopping between PbSe Quantum Dots and Graphene, by gating graphene and changing its optical absorption. The control of individual excited states between individual nano building blocks lead to the smalles light manipulator and switch that can currently be controlled in ambient conditions.

Rational Design Approach to the Formation of Hybrid Framework Materials

Principal Investigator: Omar M. Yaghi

Project Description

Metal-organic frameworks (MOFs) are composed of inorganic secondary building units (SBUs) and organic linkers, which are known to be applicable to the storage of gases, carbon capture, and catalysis, to mention a few. The purpose of this project is to address MOF containing functionalized SBUs that will lead to strategies for the design and synthesis of chemically stable porous materials with various functionalities. Ultimately, our efforts are aimed to create a library with the information to create functionalized SBUs and the needed conditions that led to the formation of given MOFs with the use of these SBUs.

Recently, we were successful in the preparation of two Al-based MOFs, where $Al_8(OH)_8(CO_2)_{16}$ SBUs are connected by tritopic organic linkers. During this year we undertook our efforts on the obtaining of Al-MOFs decorated with various functionalities. To achieve this goal, we explored the synthetic conditions that led to the introduction of new functionality to the Al clusters without losing the crystallinity and porosity. In addition, we have prepared discrete metal-imidazole clusters that can serve as a precursor of the framework material, followed by the synthesis of extended MOF structures. We believe that the two-step synthesis can increase the multiplicity of the framework structures.

Accomplishments

We have been successful in the preparation of a series of MOFs based on the aforementioned Al-based SBU. Through control on the synthetic conditions, we are now able to introduce various functionalities, such as phenyl, naphthalene, NH_2 and COOH groups. The new MOFs are obtained in the form of single-crystals; therefore, the presence of these functionalities was proven by single crystal X-ray diffraction analysis. Furthermore, digestion NMR data showed that the occupancy of these functionalities is greater than 90%. To investigate the effect of functionalities in the pore, we implemented methane adsorption measurements of a series of Al-MOFs. The methane adsorption analysis revealed that the MOFs functionalized with NH_2 and COOH groups showed 50-60% greater uptake at 1 bar and 298 K compared to that of pristine Al-MOF (MOF-520).

We have also prepared new MOF materials using a copper-imidazole cluster as a precursor. The precursor molecules were prepared according to the published procedure, and then these were reacted with zinc ions by a solvothermal method to yield crystalline samples. Atomistic connectivity of the crystalline sample was determined by single crystal X-ray analysis. The Cu and Zn atom ions took square planar and tetrahedral geometries, respectively, and imidazolate linkers are bridging these metal ions. The architectural stability of the new material was confirmed by N_2 isotherm measurements. The profile of the isotherm can be classified into Type I, and the BET surface area is estimated to be 600 m^2/g. This material also showed high water stability due to relatively hydrophobic pore environment. We also revealed that the pore environment can be easily tuned by use of functionality of organic linkers. Indeed, one of the materials showed 3 times greater calculated CO_2/N_2 selectivity ($S_{CO2/N2}$ = 60) compared to the non-functionalized material.

Overall we demonstrated how crystalline porous frameworks with functionalized SBUs are designed and synthesized, and these functionalities are effective to improve the gas uptake and separation properties.

Next Generation Bioimaging
Principal Investigator: David Skinner

Project Description

Exponential data scaling in bioimaging, combined with the data fusion demands of increasingly multi-modal imaging approaches, require new R&D in computational bioimaging solutions. Tools that scale can extend the ways in which scientists can leverage image based data. Bioimaging is leaving an era of images-as-results and entering an era where results come in the form of biological models built on massive gigapixel images and vast image collections. These models require scalable analysis, integration, and dissemination of image data delivered from advanced bioimaging instrumentation. In Big Data bioimaging, images are the feedstock not the end result of the instruments we use to observe biological systems. The NGBI (NextGen Bioimaging) LDRD prototypes Big Data bioimaging methods in the context of biofilms, also known as microbial communities (Auer). Biofilms are of high importance to the Department of Energy, due to their dominance of microbial lifestyle and their significance in microbial mediated processes. Protein expression and its spatial localizations studied by high-throughput automation promise a detailed understanding the proteome. NGBI is co-designing a modular web-based computing and data strategy with these two projects and a plan to extend this capability to other projects in Big Data bioimaging.

Year 2 Accomplishments

- New qualitative understanding of the 3D organization of the Myxococcus xanthus and Desulfovibrio vulgaris RCH1 microbial communities.
- Validation of machine learning data models for random forest classification of Myxococcus xanthus and Desulfovibrio vulgaris RCH1.
- Implementation of RabbitMQ –An advanced message queuing protocol and Taskfarmer –A tool to run multiple tasks in parallel as part of NGBI's software stack to improve performance.
- Increased demand from users particularly in the fields of single-particle EM.
- Deployment of custom-tailored image-processing algorithms and successful integration of a suite of universally used processing software among the biology community into an OMERO-based science gateway using HPC resources from the National Energy Research Scientific Computing Center (NERSC) **URL:** http://ngbi.nersc.gov
- Active participation with the broader bio-imaging community in the development of HPC-enabled tools for bio-imaging processing and analyzes.

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 liaised with scientists from various domains and have obtained key data intensive applications and representative datasets for these applications. We now have a collection of 7 applications and have started analysis of I/O access, memory access and instruction mix.

We have developed a tool to help understand the I/O access pattern of any application, including python applications and closed-source applications. This tool reads trace data and creates simple graphs which show how the file pointer position and cumulative data change over time. Our results show that 1. Some of the data-intensive applications show different I/O access patterns from traditional HPC applications. 2. The time in explicit I/O, i.e. read and write functions, is small for many of our current data intensive applications.

We have also used a tool to help understand the memory access pattern of applications. Our analysis so far includes capturing the memory footprint, average reuse of memory addresses, and distribution of accesses in the full memory address space. Our results show that 1. Some of the data intensive applications (hmmer, sextractor and psfex) have a relatively small memory footprint indicating that all memory accesses can be satisfied from on-package memory (for realistic estimates of next generation on-package memory capacity). 2. These small memory footprint applications have extremely high average reuse of memory addresses, similar to HPL, indicating there is the potential to make extensive use of fast levels of cache. 3. Other data intensive applications (blast and swarp) have low average reuse of data indicating that these applications are less likely to benefit from a deep memory hierarchy. Future analysis of potential concurrency and data reuse as a function of time will show to what extent the applications can hide memory access latency, and motivate whether we can migrate these applications away from nodes with large amount DRAM. 4. All applications analyzed have read/write ratios between 2 and 6 indicating difficulty in replacing DRAM with non-volatile memory with extremely asymmetric read/write latencies.

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

Our most significant accomplishment has been to design a system suitable for studying transfermium nuclei at LBNL. One of the main challenges with developing laser spectroscopy systems for rare nuclei are the expected low efficiencies of <1% for excitation and detection of the nuclei. As such, we have focused on increasing production and efficiency throughout the design. We have developed a new target design that will allow for bombarding the targets with particle-microamp beam intensities – a factor of four increase over current levels. The new targets are currently being produced and will be tested during a beamtime in February 2015.

We have developed a gas chamber to mate to 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. This gas chamber will slow the transfermium nuclei down from 40-50 MeV to thermal velocities with high efficiency. As transfermium nuclei tend to be ionized when they slow down, we have also designed system to attract the ions to a well-defined volume where they can be neutralized, before re-ionization with a two-step resonance-ionization technique.

We are in the process of commissioning the gas catcher and finalizing the design of the neutralization and re-ionization chamber.

Explosive Astrophysics using High Performance Computing
Principal Investigator(s): Daniel Kasen

Project Description

The purpose of this project is to better understand the conditions leading to the creation of the elements in extreme astrophysical environments. Our approach is to use advanced simulation codes on high performance computing systems to model the dynamics, nucleosynthesis, and the radiative transport of supernova explosions and neutron star mergers. Our end-to-end calculations will allow us to predict the composition, energy and geometry of the ejecta, and thereby derive signatures that are directly comparable to observational data. In this way, we will improve our understanding of the physical conditions in explosive astrophysical environments, identify indicators of novel nuclear physics occurring within them, and help clarify the origin of the heavy elements in the Universe.

We simulate the dynamics and radiation transport of explosions using a variety of codes run on modern supercomputers. The smoothed particle hydrodynamics code SNSPH is used to model the dynamics of compact object mergers. In addition, we use the grid based adaptive mesh refinement hydrodynamics code CASTRO to model detonations. The radiation transport problems is addressed using the SEDONA code, an implicit Monte Carlo (MC) transport code which includes modern acceleration and variation reduction techniques, along with our newly developed MC code SEDONA-BOX.

Accomplishments

Our primary computational accomplishment has been the development of a new MC code that uses the BoxLib framework of CASTRO provide a domain decomposed grid. This code permits radiative transfer calculations to be carried out with orders of magnitude better resolution then has been the standard in the field.

Our primary research accomplishments have focused on two different classes of astrophysical explosions: thermonuclear supernovae arising from the merger of two white dwarfs, and radioactive transients from the merger of two neutron stars. Our studies of white dwarf mergers demonstrated that this channel can reproduce observations of a diverse range of thermonuclear supernovae, from those of normal brightness to the most extreme luminosity events. The models also displayed a width-luminosity relation similar to the empirical relation used to calibrate thermonuclear supernovae as standardized candles for cosmology.

Our studies of neutron star mergers clarified the dynamics, nucleosynthesis and radioactively powered transients resulting from these events. We found that heavy elements could be produced and ejected by tidal stripping in the merger itself, as well as in disk winds produced following the merger. We found that the ejected material underwent rapid neutron capture (r-process) to a degree that depended on the neutrino flux, neutron star lifetime, and black hole spin. We demonstrated how observing the colors of the resulting radioactive transients can allow one to quantify the mass and composition of the ejected debris, thereby illuminating the cosmic origin of heavy elements like gold, platinum, and uranium.

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

Principal Investigator(s): Mateusz Ploskon

Project Description

The aim of this LDRD proposal is the exploration of new approaches to detector readout and online data processing, for hadron collider physics experiments with high-intensity beams. We base this study 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 providing efficient, physics-ready information on the trajectories of the particles produced in the hadron/heavy-ion collisions. As part of this R&D effort we will establish physics-based requirements for ITS readout performance, based on a candidate set of observables of heavy flavor production in proton-proton and heavy ion collisions in ALICE. We will explore hardware architectures and software algorithms for both efficient data compression and data selection in silicon-based tracking detectors, guided by the physics requirements. The outcome of this R&D effort will be the identification of hardware design approaches and efficient software algorithms that can be implemented as part of an ITS Upgrade and similar detector systems in other collider detectors.

Accomplishments

We have made significant progress on several items within the LDRD 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. Moreover, 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.

A major achievement was to establish a working environment for massive computing simulations using the High-Performance Computing (HPC) clusters (work done using NERSC computing farms). The lightweight framework combines the conventional computing strategy with the possibility to leverage high capacity and parallelism within the HPC for the future simulation tasks. These developments, utilizing the multi-node and multi-core architecture will provide us with the necessary framework for the studies of the *time-stamp* based digitalization software for the purpose of future detectors. We have started the first tests of the novel setup.

On the hardware side of the project, the main performance benchmarks of the principal elements of the readout system have been identified. The processing chip architecture will be defined within the first quarter of 2015 we will be able to devise (and revise in some cases) the necessary hardware design approaches during the second year of the LDRD funding.

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. Yet, there remains a dearth of information about the *in operando* structure of the protein-material interface. 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. However, there is little information about the protein-material interaction and there is no information on which amino acid residues of cyt *c* are recognized or associated with the material. This project seeks to uncover mechanisms of interaction between these cyt *c* and materials .

Accomplishments

Obtaining adequate amounts of outer membrane decaheme cyts *c* for structural studies is challenging because of intrinsic difficulty of expressing decaheme cyts *c* and their low solubility. This year we overcame these challenges to express and purify two variants of the decaheme cyt *c*, MtrF. First, we expressed a lipidated MtrF with a histidine-tag at its C-terminal. This protein was then purified in the presence of mild detergent using both affinity chromatography and ion exchange chromatography to greater than 90% purity with a net yield of ~1 mg protein/L culture. To eliminate the need for detergent, which will in turn facilitate structural characterization, we also expressed an MtrF variant lacking any lipid modification. To do so, we created a DNA construct containing the MtrB signal sequence, followed by the MtrF coding sequence and a C-terminal histidine-tag. This protein was secreted directly into the culture media, and we successfully purified it to greater than 90% purity at a yield of ~0.5 mg/L culture using a single affinity chromatography step.

We also characterized both the lipidated and non-lipidated MtrF to assess whether they are fully matured decaheme cyts *c*. UV-Vis spectroscopy of these proteins shows the characteristic peaks of c-type cytochromes at 408, 535, and 552 nm. Additionally, Electrospray Ionization Mass Spectrometry shows that the mass of these proteins is equal to the expected mass of decaheme MtrF. Thus, we conclude that these proteins are indeed fully matured MtrF. Lastly, we have established assays to measure the binding affinity of MtrF to inorganic materials. Specifically, we have shown that the fluorescence of MtrF is quenched upon exposure to certain materials. This measurement will allow us to determine the partition coefficient of MtrF for different materials, and thus greatly add to our understanding of the thermodynamics of protein-material binding.

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. Specifically, we aim to develop a flexible, rapid, and inexpensive platform to assay 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. Lastly, we will expand the toolbox of the JGI and offer next-generation microbial characterization to the greater user community to meet DOE missions in energy, environment, and biomanufacturing.

Accomplishments

Our most significant accomplishment has been 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. 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.

To date, we have applied RB-TnSeq to 21 diverse bacteria and generated over 3,000 whole-genome mutant fitness profiles, representing ~9 million gene fitness measurements. We have identified phenotypes for over 20,000 bacterial genes including thousands of genes with no previous known function. We are using these data to predict gene function in diverse species using correlations in mutant fitness across hundreds of diverse growth conditions. In the current year of LDRD funding, we are working to extend the RB-TnSeq to additional, diverse microorganisms relevant to biofuel production, bioremediation, and nutrient cycling including archaea. In addition, we are working to increase the efficiency of transposon mutagenesis in diverse microorganisms by engineering new vector variants. Lastly, we are developing computational tools to enable the microbiology community at large to mine our functional genomic datasets and to globally infer gene function across all sequenced microbial genomes using homology-based methods.

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 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

Our major accomplishment in FY14 was to design and very nearly complete the DNA construction of a refactored (genes recoded; fully synthetic promoter and ribosomal binding-site genetic components) actinorhodin antibiotic pathway (our selected biosynthesis demonstration challenge project). This is an impressive feat, as it constitutes a record-breaking refactored secondary metabolite pathway at 22 genes and 30 kbp in length. [In early FY15, we completed and validated the construction of the refactored actinorhodin pathway, transformed the construct into a modified *Streptomyces coelicolor* host lacking its native actinorhodin pathway, and detected the production of actinorhodin.] Sample preparation and analytical mass spectrometry methods were developed for actinorhodin and other secondary metabolites including violacein, our selected biosynthesis stress-test project target. The completion of the DNA construction of a 60,000-variant refactored violacein pathway combinatorial library is anticipated in the first half of FY15. Significant progress was also made in the development of machine learning algorithms for processing the violacein combinatorial library (and other metabolite) production data, and in the further development of DNA construction process tracking and assistance software.

Simultaneous Inverse Beam Anomalous Diffraction

Principal Investigator(s): James Holton, Ken Frankel

Project Description

We propose to develop a novel technique for determining macromolecular structures by native element (sulfur and phosphorus) phasing. Essentially, first generation XFELs such as the LCLS were designed to solve the "intensity problem" of macromolecular data collection, and by building upon the now proven femtosecond nanocrystallography methods the NGLS may be used to solve the phase problem. By splitting the X-ray beam in two and intersecting the target simultaneously from exactly 180 degree opposing directions the diffracted intensity of Friedel-symmetric pairs of spots may be collected from the same crystal before it is destroyed. The difference between these intensities may then be used for phase determination to 2.5 A resolution.

With this proposal, we seek to address the four major potential stumbling blocks to the success of a SINBAD diffractometer: 1) demonstrate that anomalous differences can be extracted from "still" images at a synchrotron 2) usefulness of the relative anomalous difference (delta-F/F) in anomalous phasing algorithms, which are currently optimized for delta-F standing alone, 3) impact of systematic errors incurred by non-isomorphism between the many crystals that must be combined to make up a complete data set. 4) feasibility of construction, particularly deflecting a 2.5 keV X-ray beam at near 90-degree angles.

Accomplishments

We succeeded in collecting "pseudo-SINBAD" data from our synchrotron beamline after careful re-alignment of the spindle. Collecting back-scattered reflections and extracting anomalous differences form them proved tractable, and indeed easier than expected.

The problems of non-isomorphism and reflecting crystal design proved to be significant, and we have new projects now investigating these two fronts. Non-isomorphism is a problem that must be overcome for any future multi-crystal macromolecular crystallography endeavor to move forward, and this fact is growing in appreciation in the XFEL and synchrotron communities alike. We discovered that ambient humidity can have a dramatic impact on isomorphism, and we are preparing a manuscript on this phenomenon, which suggested apparatus for controlling it.

The design of a high-angle soft-X-ray monochromator also requires further development. This technology is critical for self-seeding in the soft and "tender" X-ray FELs currently under development, so we anticipate significant interest in it. What we learned is that the art of polishing and etching these crystals is absolutely key to preventing severe degradation of the beam emittance at each bounce, but existing manufacturing methods are optimized only for silicon and new etching protocols must be worked out for alternative materials.

We also found that the current status of dynamical theory of reflection is severely lacking in the soft X-ray region, and we re-formulated this theory from first principles. We believe a high-Z and large-cell material is optimal if crystals of sufficient quality can be prepared. Bismuth Telluride is a promising candidate.

OPTIMIZING PLANT-MICROBE INTERACTIONS FOR SUSTAINABLE SUPPLY OF NITROGEN FOR BIOENERGY CROPS

Dominique Loque, Romy Chakraborty, Gary Andersen, Trent Northen, Manfred Auer, Tanja Woyke and Musa Ahmed

Project Description

Nitrogen (N) is an essential component of proteins and consequently a key element for life and cell development. Mineral N is often limited for plants, which consequently reduces plant growth and biomass yield. While this practice has been partly responsible for the 'green revolution,' it has come at high environmental and economic costs. In natural ecosystems, plants have developed strong relationships with microbes to cope with the low availability of essential nutrients such as N. For example, plant rhizospheres contain N2-fixing bacteria that are able to fix atmospheric N2 without the requirement of forming symbiotic association with a host-plant, however several of them depend on plant root exudates for carbon supply. Furthermore, endophytic bacteria colonizing root, stem and leaves of plants with N2-fixing function have been identified in several plants. The aim of this project is to optimize benefits from interactions between plants and free N2-fixing bacteria communities to provide adequate amounts of assimilable N to host-crops. This would reduce fertilizer consumption and carbon footprint of feedstock production, and greatly improve the sustainability of biomass production.

Accomplishments

Several additional N-fixing strains were isolated from plant isolates were phylo-typed based on 16S rDNA analyses. The genome sequences of several diazotrophic strains isolated were obtained through collaboration with JGI. Genomic comparison and extensive phenotypic characterizations were performed with a few of these strains. Most of the endophytes were capable of utilizing a broad range of carbon substrates.

We analyzed the ability of the endophytic diazotrophs to fix atmospheric N2 under varying temperature in-vitro. N2-fixation was followed by the standard acetylene reduction assay. Results indicated that N-fixation occurred optimally under optimal growth conditions. In addition, biochemical and genomic studies revealed that a bacterial strain could produce from a plant exuded compound the plant growth promoting plant hormone. This discovery led us to the engineering a plant to boost bacterial production of the plant hormone (still in progress). Coupled with the ability to provide fixed N2 to the plants, this is an extremely desirable trait that can be utilized for sustainable agriculture of biofuel crops such as Switchgrass.

Plant seedlings when inoculated with endophytic diazotrophs showed enhanced growth. Both above ground shoot and below ground roots increased almost 50% relative to uninoculated controls. We were able to locate fluorescence signal from the strain R1Gly cells bearing the reporter gene gfp localized in the certain plant tissue. This indicated that strains were active inside seedlings, and fixing Nitrogen in-planta.

In order to identify carbon substrates that potentially attract N2-fixing bacteria to plants, diazotrophic isolates were grown in root exudates collected from hydroponically grown plants, and analyzed for substrate uptake/release. Carbon compounds that are consumed by endophytic bacterial strain and carbon compounds that are excreted by this strain have been identified.

Synchrotron X-Ray Footprinting

Principal Investigator(s): Corie Ralston and Musa Ahmed

Project Description

The goal of this project is to establish an x-ray footprinting (XF) program at the Advanced Light Source. XF is a technique that allows determination of protein structure and dynamics in the solution state at the resolution of a single amino acid. With this technique, the probing reagent – hydroxyl radicals – are produced by energetic photons alone, and no extraneous reagents produce additional unwanted protein modifications. After exposure, samples are digested and analyzed with mass spectrometry to determine which amino acids were modified by the hydroxyl radicals; this results in a map of the solvent-accessible areas of a protein, indicating sites of protein-protein or protein-substrate interactions. Since the necessary exposures are on the order of milliseconds, mixing reactions can be performed to give snapshots of protein dynamics or protein-protein interactions as a function of time. The methodology of data collection, buffer calibration, and mass spectrometry analysis for x-ray footprinting has been previously developed and used very successfully at the NSLS over the last decade. Establishment of an XF program at the Advanced Light Source serves two purposes: 1) it allows continued support of projects currently underway at the NSLS beamline X28C (which was formerly the only XF beamline in the country, but was shutdown in September of 2014 for the NSLS upgrade) and 2) it further develops and extends the technique of XF into the sub-millisecond time regime.

Accomplishments

With the previous two years of LDRD funding, an XF program was established at the ALS; experimental feasibility was established using protein and fluorophore standards, and resulted in a publication (Bohon 2014). Further, results from ALS beamline 5.3.1 demonstrated that footprinting can be conducted in the microsecond domain when using a white-light focusing optic from an ALS bend magnet source, representing a significant extension of the technique. These results were published (Gupta 2014). An MOU with the ALS Experimental Systems Group was established, allowing access to beamlines 5.3.1 and 3.2.1 on a regular basis. In addition, permission has been obtained from ALS Management to commission beamline 3.3.1 as a dedicated footprinting beamline at the ALS, and initial top-off calculations of the 3.3.1 aperture show that the beamline can be brought online without further shielding work. In addition, we have established an MOU with the NSLS to support NSLS XF users starting in Oct 2014 using beamlines 5.3.1 and 3.2.1 at the ALS. Several important systems were investigated following establishment of the technique at the ALS, and one example is the orange carotenoid protein (OCP). In cyanobacteria, this 35 kDa protein is involved in a photoprotective mechanism, undergoing a conformational change under high light conditions that results in a cascade of protein–protein interactions to control the blue green algae photo system. XF experiments on OCP at ALS beamline 5.3.1 showed a significant rearrangement of residues on one side of the carotenoid under blue light illumination. The results point to an opening of one domain of the protein during light exposure, allowing access to the carotenoid for interaction with other proteins in the complex. This is a significant contribution to understanding the mechanism of activation for this protein, especially given that the "red" state of OCP has been intractable to crystallization. These results have written up and submitted to Nature.

Computational Methods for X-ray Free-Electron Laser Studies of Solar Energy Converting Biocomplexes

Principal Investigators: Nicholas Sauter, Vittal Yachandra,
Junko Yano, Peter Zwart, Paul Adams, David Skinner

Project Description

The purpose of this project is to understand light-induced water splitting in green plants, algae and cyanobacteria; organisms that are responsible for producing most of the oxygen in the atmosphere. An important application of this knowledge will be in the design of future fuel production schemes based on artificial photosynthesis. The splitting of water, creating oxygen and hydrogen, is accomplished by the protein complex photosystem II, which contains a catalytic center containing four manganese atoms. To drive the reaction to completion, four sunlight photons sequentially oxidize the Mn atoms after which the catalyst returns to the reduced state. Traditional methods for studying structure and function, such as X-ray crystallography, have been hampered by the high sensitivity of the Mn center to probing X-rays, which reduce the metal atoms to the Mn (II) valence state.

We have an unprecedented opportunity to map out the detailed reaction mechanism using X-ray free-electron laser (XFEL) experiments at the Linac Coherent Light Source (LCLS). Photosystem II crystals will be driven through the redox cycle with an optical laser. X-ray probe pulses at LCLS are short enough (50 fs) that all observations can be made before reduction and other damage processes occur. As the probe pulses are extremely intense, the sample becomes fully ionized after the observations are recorded; therefore, a continuous stream of new crystals is required for a full data set. Atomic structure of the protein will be probed by X-ray diffraction, while simultaneously the electronic state of the Mn atoms will be measured by X-ray emission and spectroscopy. The experimental team is a collaboration between many groups at different institutions. This LDRD is specifically targeted at developing the requisite computational methods to handle the large (>100 TB) data sizes, with the involvement of NERSC resources.

Accomplishments

In it's third and final year (FY2014), the project published XFEL-derived crystal structures of photosystem II in the dark-equilibrated state, as well as in three illuminated states along the reaction coordinate. While our published structural data extends to 4.5 Å resolution only, our latest experiments with optimized crystal growth conditions indicate that 2.5 Å data are achievable. We published extensive computational methods for XFEL diffraction experiments applied to structural biology. The unique data collection conditions required us to develop analysis methods to optimally model the crystal orientation and internal physical properties. Our software (*cctbx.xfel*) is general and widely applicable to XFEL-based protein crystallography. In collaboration with Axel Brunger (Stanford University and HHMI) we created procedures for organizing large datasets ($>10^4$ crystals) where the diffraction quality is heterogeneous, explored systematic correction methods for converting the Bragg spots to reduced Fourier coefficients for calculating the electron density map, and contributed to the development of a new microfluidic trap device that will hopefully reduce the amount of sample required for a full dataset. With David Eisenberg (UCLA / HHMI) we developed new algorithms to process very sparse crystal diffraction patterns from small molecules. We've used XFEL diffraction to investigate small peptide fragments that determine the β–sheet protein structure in numerous amyloid diseases, and in particular the mechanism of a single-amino acid mutation causing Parkinson's disease.

Tactical High Throughput Computing:
Improving Interdisciplinary Tools for High Throughput Computing
at NERSC and Beyond

Principal Investigator: Bailey, Stephen

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 independent tasks. For example, users need to apply the same analysis program to many thousands of images or spectra or gene sequences, or run the same simulation with thousands of different input parameters. The traditional batch model of 1 task = 1 script = 1 job becomes impractical for both the batch queue system and the human management of such scripts. At the same time, pre-bundling multiple tasks into a single batch script lacks flexibility, e.g. for processing new data as it arrives. We are developing an alternate model to simplify HTC workflows at NERSC and elsewhere, based upon separating the queue of tasks to perform from the batch jobs that process those tasks. This work will simplify HTC workflows at NERSC, attract new users, and reduce the software development costs for future projects with big data HTC processing requirements.

Accomplishments

In the first year of this LDRD we:

1. performed a comparative study of two options previously developed by our team ("qdo" and "Fireworks") and researched alternatives.
2. implemented significant improvements to both Fireworks and qdo performance:
   - qdo is now 1000x faster to load tasks and 20x faster to pull tasks from the queue
   - Fireworks now scales linearly with number of tasks instead of $O(N^2)$
3. ported qdo to NERSC (Fireworks was already there) and tested it with multiple science use cases.
4. implemented additional qdo features necessary for our scientific work: task dependencies, priorities, and improved robustness.
5. created a prototype web API and user interface for qdo.
6. began work on task parallelism.

Higher Performance CCDs for Next Generation Dark Energy Experiments

Principal Investigator(s): Christopher Bebek

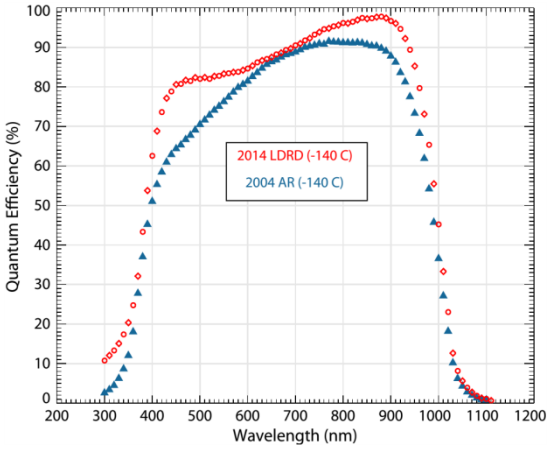
Project Description

We have completed the second 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 recently completed Baryon Oscillation Spectroscopic Survey (BOSS) and its follow-on eBOSS experiment, and the Dark Energy Survey that is in its second year of operation. Future projects such as the Dark Energy Spectroscopic Survey and the Large Synoptic Survey Telescope have adopted the fully depleted CCD technology that was developed at LBNL but further improved performance to meet the science goals is desired.

The areas that we are emphasizing 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 (MSL). The other efforts involve LBNL design work and exploration of advanced fabrication steps with our industrial partner Teledyne DALSA.

Accomplishments

In the first year of the project we submitted a wafer design to Teledyne DALSA, and the CCD wafer fabrication was successful. The second year of the project described here utilized these wafers in the MSL for QE improvement development and for testing the low noise CCD designs. The figure below shows the improvements in QE at both blue and red wavelengths that have been demonstrated. The measured QE on recently-fabricated CCDs is shown by the red symbols, and that is compared to the standard QE shown in the blue symbols. The improvements are due to the use of a thinner backside contact layer and the use of improved anti-reflection coating materials, specifically the use of ZrO_2 in the AR coating.



We also demonstrated improved noise performance. In addition to the use of a direct connection between the CCD sense node and output transistor polysilicon gate electrode that we had described previously, we also explored the use of a thinner gate-insulator layer in the output transistor. This allowed for the use of a smaller gate length in the output transistor, and resulted in a reduction of the noise floor from about 1 e^- rms to about 0.8 e^- rms. We also explored the use of mix-and-match lithography to reduce the size of the sense node to 1×1 μm^2 from 2×2 μm^2. Although this did not result in a noticeable noise improvement, the ability to utilize the finer-line lithography could be useful for future noise improvements. These enhancements were included on both small format CCDs, and on 16-channel CCDs to allow for improved statistics. See the listed publication for more details.

We have also made progress on single-photon detection via impact ionization in a charge-multiplying CCD, with the first demonstration for us of the multiplication of sub-electron light levels with realistic gain values in our p-channel technology.

New Monolithic CMOS Sensors on a Fully Isolated Substrate
Principal Investigator(s): Maurice Garcia-Sciveres

Project Description:

15 Years ago all digital cameras used CCD image sensors. Today they all use CMOS image sensors. This led to widespread interest in the potential for scientific applications. But development of an “ideal” monolithic device, where the sensing function places no restrictions on the electronic circuits and the fill factor is 100%, has so far proven elusive. This LDRD is to design and fabricate a proof of principle, radiation tolerant demonstrator for particle physics and x-ray detection that may finally realize this ambition. This project received end-of-year finding in FY12 and full-year funding in FY13 and FY14. FY14 was the final year.

Accomplishments:

A first prototype chip was designed in FY12 and fabricated in FY13. This chip contains an active pixel matrix. Working devices were received in February 2013 and then tested to validate the design methods used and simulation results. These tests were successful, leading to submission and presentation of results at the International Image Sensor Workshop (IISW) in June 2013. Following this, devices were irradiated in September wiht protons to a maximum dose of 30Mrad. Testing of the irradiated devices took place in FY14. In FY14 devices were also characterized for minimum ionizing particle (MIP) detection efficiency using the SLAC test beam facility. The conclusion from these studies is that the concept works, but cannot achieve the desired 99% detection efficiency for MIP detection. Instead, the MIP efficiency of the tested devices is between 50% and 60%. Irradiaiton did not degrade the performance. To increase efficiency one must reduce capacitance and/or increase the collected charge. A test structure chip was fabricated in FY14 to explore the process parameter space for the charge collection implant to minimize capacitance and maximize breakdown voltage. This characterization was successful, but the results disappointing, showing very little room for improvement. Finally, in FY14, a redesign of the pixel geometry was carried out to reduce the size and therefore the capacitance of the pixel. However, this design was not fabricated. Even with these improvements, simulations show that the efficiency would reach just 80%. A higher substrate resistivity is needed to boost the signal and reach the desired efficeincy (the process used has 2 Ohm-cm substrate). At the conclusion of the LDRD no higher resitivity process with the needed deep implant feature was available.

Post-LDRD Work:

A further SLAC beam test is planned to obtain more detailed efficiency measurements. This is possible thanks to availability of visiting students. A new fabrication process has recently become available with the required implants and with 2 orders of magnitude higher substrate resitivity. We now hope to port the design to this process and fabricate a new test chip. This would be done with programmatic funding, as a device of this type with 99% efficiency is of significant interest for Large Hadron Collider detector upgrades.

Advanced Composites for Next Generation Scientific Instruments

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: A calorimeter was made to measure exothermic energy release during cure of various commercial resins. Neat resin samples were run at varying cure rates to determine a rate that would be safe for cure of appropriately large volumes of resin. Copper is a catalyst and auxiliary samples were cured with chopped SC cable to assess effects on reaction rates. Cure profiles and a new commercial resin were identified with minimal exothermic energy release. **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. Glass transition temperature of the resin is compatible with the highest expected bake out temperature used. **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. This could be used to efficiently cool silicon detectors with heat densities of 0.1 - 0.5 W/cm^2 and dramatically reduce detector mass and complexity, by removing the need for metal pipes carrying liquid coolant. Samples were compared, including: bare tubing, reference aluminum foam at three different porosities, reticulated vitreous carbon foam, and the candidate foam, a CVD coated graphitic carbon. In repeated tests, the CVD material removed 0.3 W/cm^2 at practical flow rates and pressures, proving feasibility for a range of interesting applications. **Resin modification:** an extensive survey was made of candidate non-metallic particle additives for thermal enhancement of structural resins. The goal was to identify a resin modifier which will be practical to use in fabrication of precision detector structures, while significantly improving over the typical thermal performance (1.0 - 1.2 W/m*K) of current modifiers in use. Additives were identified at the micron and nanometer-scale, in platelet, spherical, and fiber geometries, in carbon and ceramic materials. All candidates were mixed with a standard reference structural epoxy resin in ratios covering the full range of practical viscosities. Over 70 unique samples were tested.

Instrumentation for Precision Inspection: Mechanical properties of large composite structures must be measured and hidden defects in laminates identified non-invasively. A variety of 2D and 3D metrology approaches were studied. Key findings include a vibrometric method to find small gaps within a laminate and a fast efficient large area scanning method for precision inspection. A large area multi-purpose test stand which integrates these capabilities is being fabricated.

Next Generation Cosmic Microwave Detector Arrays: Enabling a Factor of 10 – 100 Increase in Array Size

Principal Investigator(s): Adrian Lee, Chris Bebek, Maurice Garcia-Sciveres, Steve Holland, Dan Werthimer.

Project Description

The purpose of this project is to develop detector technology for next-generation Cosmic Microwave Background (CMB) polarimetry experiments. Primordial gravitational waves produced during inflation and gravitational lensing by large-scale structure produce "B-mode" polarization patterns on the sky which have a handedness. A detection of primordial B-modes would be a "smoking gun" for inflation as the origin of the universe and would determine inflation's energy scale. A detailed characterization of the lensed B-modes would also allow us to constrain the sum of the neutrino masses and the evolution of dark energy by cross-correlating with BAO experiments such as DESI. Just last year, experiments such as POLARBEAR detected B-modes from gravitational lensing directly for the first time.

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 discussing a possibility of stage-four CMB experiment (CMB-S4) to definitively characterize B-mode polarization with a 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 proposed to improve their scalability. The five areas that we have chosen to focus on are: Monolithic fabrication of inductors and capacitors for frequency-multiplexed readout, monolithic fabrication of a silicon lenslet array for optical coupling of the detectors, spray application of anti-reflection coatings for silicon lenslet arrays, fully automated wire bonding to the a detector array, and automated electrical inspection of detector array.

Accomplishments

Current CMB experiments using frequency-domain multiplexing use printed circuit boards with thousands of hand-soldered capacitors in the cryogenic readout electronics. We have developed a monolithic technology at LBNL Micro Systems Lab to fabricate superconducting inductors and capacitors on silicon wafers. We achieved resonances with high quality factor, predictable resonance peak location, and high yield. Using lithographic fabrication greatly reduces cost and gives a scalable technology with an order of magnitude increase in multiplexing factor.

We have successfully machined monolithic silicon lenslet arrays from single crystal silicon., which can replace hand-assembed arrays. We have also developed a plasma sprayed ceramic anti-reflection coatings that can replace our current hand-molded coatings.

We have also succeeded in wire bonding to our detector wafers with an automatic wire bonder at LBNL. We are bonding at a 100 micron pitch wire bond, which gives higher connection density and lower cost than the manual wire bonding in current use.

Finally, we have developed automated electrical inspection that can characterize thousands of detectors per wafer automatically and rapidly. Previously each detector was hand tested for electrical continuity.

Transforming Infrared Astronomy with Nanostructure IR Filters

Principal Investigator(s): (Saul Perlmutter and Xiang Zhang)

Project Description

New telescope techniques that can explore objects in deep space with high resolution and sensitivity in near-IR region are highly demanded for the study of properties of dark energy and dark matter over time. However, near-IR observations from the Earth's surface are extremely challenging because of the bright background emitted from the atmosphere. Fortunately, these 300+ OH emission lines are intrinsically very narrow, covering only a small fraction of the total spectrum, and the continuum between the lines is typically as dark as zodiacal light, the background level directly observed from space. Therefore, selectively filtering the OH emission light will enable high sensitive deep space near-IR measurements from the ground.

We are developing **an innovative optical filter system (astrofilter)** for highly sensitive near-IR observation by effectively removing the OH emission lines from the Earth's atmosphere. Different from natural materials, the physical properties of a metamaterial is not primarily dependent on its chemical constituents, but rather upon the structures of the building blocks which are much smaller than light wavelengths. The IR filter design is investigated through numerical simulations and we are exploring effective thin film deposition strategies for large number of layers with controlled roughness and stress. The metamaterial near-IR filter system will be fully compatible with existing telescopes and other instruments because of the large acceptance angle, moderate diameter, and thin filter thickness.

Accomplishments

By tailoring effective optical properties of the nanoscale layered structures, our metamaterial filter system can provide sharp spectral filtering line-width and high transmission of residual signals, which will be otherwise impossible for traditional techniques based on natural materials. Through the design of the nanoscale structures of the filter system and the development of related nanofabrication techniques, we have developed a multilayer algorithm to realize the desired performance. We have also investigated the fabrication process.

Our most significant accomplishment is the design of an integral multilayer-filter system. The system can eliminate a large number of OH emission lines in the spectrum from 1.5~1.8 μm where most of skyline noise comes from. Our approach combines the Needle Optimization and the Tunneling method to search for the global minimum of the merit function. We adopt the scheme of distributed IR filters, and different sub-units are assembled to form an integral filter system with a figure of merit around three. Our method can be generally applicable to a broader bandwidth.

We have also explored proper fabrication process of growing multilayer thin films with controlled thicknesses and surface roughness. Although we have achieved more than 30 layers of Silica and TiO2 thin films with the thickness of each layer monitored *in situ*, we realized that it is very challenging to fabricate the full structure with current state-of-art thin film technologies, which requires the deposition of over 1000 layers with total thickness in the order of millimeters and the roughness of each layer less than 1% of its thickness. We believe this difficulty is resulted from the mathematical limitations of Needle Optimization approach we employed, and a much better mathematical tool must be developed. We are exploring a better design in collaboration with Prof. James A. Sethian, a mathematician to optimize the astrofilter structure with less number of layers and less sensitive to the fabrication errors of surface morphology.

Publications List

AFRD-Schenkel LB13001 Probing Point Defect Dynamics in Solids with Short Ion Beam Pulses

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

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B. B. Godfrey, J.-L. Vay, I. Haber, "Numerical analysis of the pseudo-spectral analytical time-domain PIC algorithm", J. Comput. Phys. 258, 689-704 (2014) http://dx.doi.org/10.1016/j.jcp.2013.10.053

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

David A. Shapiro, Young-Sang Yu, Tolek Tyliszczak, Jordi Cabana, Rich Celestre, Weilun Chao, Konstantin Kaznatcheev, A. L. David Kilcoyne, Filipe Maia, Stefano Marchesini, Y. Shirley Meng , Tony Warwick, Lee Lisheng Yang and Howard A. Padmore, "Chemical Composition Mapping with Nanometre Resolution by Soft X-ray Microscopy", Nature Photonics, 8, 764-769 (2014)

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

C. Steier, et al., "Proposal for a Soft X-ray Diffraction Limited Upgrade of the ALS", Proceedings of the 2014 International Particle Accelerator Conference, 567 (2014), http://accelconf.web.cern.ch/AccelConf/IPAC2014/papers/mopme084.pdf

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ALS-Voronov LB13004 Next Generation Grating for Spectroscopy and Pulse Compression

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CH-Hartwig LB14005 Design of Mesoscale Catalyst Networks

M. Xiao, D. J.; Bloch, E. D.; Mason, J. A.; Queen, W. L.; Hudson, M. R.; Planas, N.; Borycz, J.; Dzubak, A. L.; Verma, P.; Lee, K.; Bonino, F.; Crocellà, V.; Yano, J.; Bordiga, S.; Truhlar, D. G.; Gagliardi, L.; Brown, C. M.; Long, J. R. Nature Chem 2014, 6, 590.

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CH-Head-Gordon (Martin) LB13036 New Algorithms for Performing and Analyzing Large Scale Electronic Structure Calculations

J. Thirman and M. Head-Gordon, "Electrostatic Domination of the Effect of Electron Correlation in Intermolecular Interactions", J. Phys. Chem. Lett. 5, 1380-1385 (2014).

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. (submitted).

CH-Head-Gordon (Teresa) LB14006 Designing Fluctuations and Dynamics of Enzyme Catalytic Networks

Publications

A. Bhowmick and T. Head-Gordon (2015). The role of side chain entropy and mutual information for improving the de novo design of a Kemp Eliminase. Submitted.

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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

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

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

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

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

Publications

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Invited: F. A. Houle and K. R. Wilson, "Stochastic simulations to bridge experiment and theory of complex chemical processes: application to aerosol ageing", 2014 Mesilla Chemistry Workshop on Studies of the Chemical Dynamics of Energy Transfer and Chemical Reaction, Mesilla, NM, February 2-4, 2014

K. R. Wilson, F. A. Houle, W. D. Hinsberg, "Factors Affecting the Uptake and Reactivity of OH with Organic Aerosol", American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle, "Investigating the chemical mechanisms of the functionalization and fragmentation of hydrocarbons in the heterogeneous oxidation by OH using a stochastic kinetics model", American Geophysical Union Fall Meeting, San Francisco, CA, 15-19 December, 2014

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle, "Investigating the chemical mechanisms of the functionalization and fragmentation of hydrocarbons in the heterogeneous oxidation by OH using a stochastic kinetics model", 33rd Annual American Association for Aerosol Research Conference, Orlando, FL, October 20-24, 2014

A. A. Wiegel, K. R. Wilson, W. D. Hinsberg, F. A. Houle ,"Using kinetics modeling to investigate the role of structure and phase on the functionalization and fragmentation of hydrocarbons in the heterogeneous oxidation by OH", 248th National Meeting of the American Chemical Society, San Francisco, CA, August 10-14, 2014

K. R. Wilson, "Multiphase Chemistry of Organic Aerosols," 248th National Meeting of the American Chemical Society, San Francisco, CA, August 10-14, 2014

K. R. Wilson, "Experiments and Simulations of Multiphase Reactive Uptake and the Role of Water and Phase in Controlling Organic Aerosol Transformations," 2014 Telluride Research Conference on "Organic Particles in the Atmosphere: Formation, Properties, Processing, and Impact, Telluride, CO, July 28 - August 1, 2014

K. R. Wilson, "Aerosol Chemistry" Lorentz Center Workshop: Gas/Plasma Liquid Interface: Transport, Chemistry and Fundamental Data, Leiden, Netherlands, August 4-8, 2014

K. R. Wilson, "Probing Molecular Weight Growth and Decomposition of Organic Particles in Planetary Atmospheres Using Vacuum Ultraviolet Photoionization Mass Spectrometry", Photon Tools for Physical Chemistry 2014 Beatenberg, Switzerland, September 28-October 2, 2014

<u>CRD-Buluc LB14008 Graph-based Analysis and Visualization of Multimodal Multi-resolution Large-scale Neuroimaging Data.</u>

S. Murugesan, G.H. Weber, J, Brown, A. Trujillo, K. Bouchard, B. Hamann, W. Seeley "Interactive Visual Analysis of Functional Brain Connectivity", submitted to Eurographics Conference on Visualization (EuroVis).

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

H. Shan, B. Austin, W.A. de Jong, L. Oliker, N. Wright, E. Apra, “Performance Tuning of Fock Matrix and Two-Electron Integral Calculations for NWChem on Leading HPC Platforms”, in High Performance Computing Systems. Performance Modeling, Benchmarking and Simulation, Lecture Notes in Computer Science, 261-280 (2014). http://dx.doi.org/10.1007/978-3-319-10214-6_13

CS-Haranczyk LB12009 An Optimization-based Strategy for Computational Design of Nanoporous Carbon-Zero Materials

R.L. Martin, M. Haranczyk - "Structure Models of Crystalline Porous Polymers: Construction, Characterization and Design" – Crystal Growth and Design 14 (2014) 2431-2440

CS-Oliker LB13007 High-Performance Parallel Graph-Analysis for Key Genomics Computations

Presentations

V. Strnadova, A. Buluç, J. Gonzalez, S. Jegelka, 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'14), November, 2014.

CRD-Saye LB14010 Numerical Methods for Multiple Evolving Interfaces

R. Saye, “High-Order Methods for Computing Distances to Implicitly Defined Surfaces”, Communications in Applied Mathematics and Computational Science, 9(1), pp.107-141, published May 2014, http://dx.doi.org/10.2140/camcos.2014.9.107

R. Saye, “High-Order Quadrature Methods for Implicitly Defined Surfaces and Volumes in Hyperrectangles”, SIAM Journal on Scientific Computing, submitted April 2014, currently under review

CS-Sethian LB12035 Interlinkage of Cross-Disciplinary Mathematical Technologies

Publications

"PbS Nanoparticles Capped with Tetrathiafulvalenetetracarboxylate: Utilizing Energy Level Alignment for Efficient Carrier Transport", M. Scheele, D. Hanifi, D. Zherebetskyy, S.T. Chourou, S. Axnanda, B.J. Rancatore, K. Thorkelsson, T. Xu, Z. Liu, L.-W. Wang, Y. Liu, and A. P. Alivisato, ACS Nano, to appear. http://pubs.acs.org/doi/abs/10.1021/nn406127s

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"Block Copolymer Packing Limits and Interfacial Reconfigurability in the Assembly of Periodic Mesoporous Organosilicas", Andrew W. Wills, David J. Michalak, Peter Ercius, Ethan L. Rosenberg, Rory Runser, Talita Perciano, Daniela Ushizima, Brett A, (submitted to Nano in Sep 2014).

"Coded aperture imaging for fluorescent x-rays", A. Haboub, A. A. MacDowell, S. Marchesini, D. Y. Parkinson, Rev. Sci. Instrum. 85, 063704 (2014).

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"Structure recognition from high resolution images of ceramic composites". D.M. Ushizima, T. Perciano, H. Krishnan, B. Loring, H. Bale, D. Parkinson, and J. Sethian., IEEE International Conference on Big Data, October 2014.

"Toward quantitative structure activity relationship (qsar) models for nanoparticles". K. Odziomek, D.M. Ushizima, M. Haranczyk, and T. Puzyn. American Chemical Society National Meeting - Scientific Excellence Award, August 2014.

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"Challenges and New Developments in Imaging with Large Data Sets", Ushizima, D.M., Bianchi, A.G.C., Krishnam, H., Joint Statistical Meeting (JSM2013), Montreal, Aug 2013 (oral presentation)

<u>CRD-Tull LB13009 SPOT Suite - Towards an End-to-End Solution for Light Source Data</u>

A.Hexemer, D.Kumar, S.Venkatakrishnan, A.Sarje, S.Patton, S.Li, J.Deslippe, C.Tull, E.Dart, F.Liu, T.Russell, E.Gomez, C.Zhu, E.Schaible, P.Stewart, "Fast Analysis of Time-Resolved Scattering Data", Bulletin of the American Physical Society, APS March Meeting 2015, Volume 60, Number 1, March 2, 2015, Accepted.

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CS-Ushizima LB12021 Quantitative Image Analysis for Computational Modeling

Publications

Andrew W. Wills, David J. Michalak, Peter Ercius, Ethan L. Rosenberg, Rory Runser, Talita Perciano, Daniela Ushizima, Brett A, "Block Copolymer Packing Limits and Interfacial Reconfigurability in the Assembly of Periodic Mesoporous Organosilicas", (submitted to Nano in Sep 2014).

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Presentations

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CS-Yang LB12024 Computational Algorithms and Mathematical Software Tools for Material Science and Chemistry

L. Lin, A. Garcia, G. Huhs and C. Yang, SIESTA-PEXSI: Massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization, J. Phys. Condens. Matter 26, 305503, 2014 http://dx.doi.org/10.1088/0953-8984/26/30/305503

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F. Liu, L. Lin, J. Lischner, A. F. Kemper, S. Sharifzadeh, F. Jornada, D. Vigil-Fowler, J. Deslippe, C. Yang, J. Neaton and S. G. Louie, Numerical integration for ab initio many-electron self energy calculations within the GW approximation, submitted

M. Jacquelin, L. Lin and C. Yang, PSelInv – A distributed memory parallel algorithm for selected inversion : the symmetric case, submitted

A. Damle, L. Lin and L. Ying, Compressed representation of Kohn-Sham orbitals via selected columns of the density matrix, submitted

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CS-Yang LB13010 Computational Approaches to Understanding Ultrafast Science

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PH-Haber LB14023 Advanced Composites for Next Generation Scientific Instruments

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