Overview of the Celebration

Argonne's Women in Science and Technology (WIST) Program and the Argonne Leadership Computing Facility (ALCF) present the inaugural:

"**Margaret Butler Celebration of Women in Computational Science and Nuclear Engineering**"

About Margaret Butler

Margaret Butler (1924-2013) was a pioneering scientist who spent her career at the forefront of the development of computer science, computational science and nuclear energy. Butler began her career at Argonne in 1948. She was the first woman named a fellow of the American Nuclear Society.

Deeply involved in the mathematics and numerical computations for the design of the Navy's first nuclear submarine reactor, Butler subsequently became part of the logical design team for several early computers at Argonne. She later headed the first operating system used at Argonne for the IBM 704, was leader of the Applications Programming Section in Argonne's Applied Mathematics Division and served as director of the National Energy Software Center from 1972 to 1991.

For additional information about Margaret Butler's career, visit: "The Remarkable Career of a Pioneering Computational Scientist."

Agenda

Building 240, TCS Conference Center
Thursday, June 11, 2015

1:30 p.m. – 1:45 p.m.	**Welcome: WIST Program Initiator and ALCF Representatives** Opening Remarks **Kirsten Laurin-Kovitz** *Program Manager & Principal Mechanical Engineer, Global Security Sciences Division, Women in Science and Technology (WIST) Program Initiator, Argonne National Laboratory* **Michael Papka** *Deputy Associate Laboratory Director, Computing, Environment and Life Sciences, Division Director, Argonne Leadership Computing Facility, Argonne National Laboratory*
1:45 p.m. – 2:15 p.m.	"**The Remarkable Career of Margaret Butler"** Lois Curfman McInnes (MCS), Senior Computational Scientist
2:15 p.m. – 2:30 p.m.	"**Toward a Better Atomistic Description of Intermolecular Interactions in Materials"** Ying Li, 2014 ALCF Margaret Butler Fellowship Recipient
2:30 p.m. – 3:30 p.m.	Keynote Address "**#hpcmatters"** Dona Crawford, Associate Director for Computation, Lawrence Livermore National Laboratory **Abstract**: The extraordinary computing/computational tools at the Department of Energy national laboratories are used to take on epic projects in service to the nation. For over six decades the labs have relentlessly focused on complex, long-term problems that can be advanced through computing. Grounded by 39 years of first-hand experience at Sandia and then Lawrence Livermore, this talk reviews the advancements in computer platforms over the last 60 years and the concomitant application progress.
3:30 p.m. – 5 p.m.	**Poster Session** Research presented by Argonne's computational scientists and nuclear engineers.
5 p.m. – 6:30 p.m.	**Reception at Argonne Guest House**
6:30 p.m. – 8 p.m.	**Dinner and Open Microphone at Argonne Guest House** A reception, dinner and open microphone at the Argonne Guest House will take place. All guests are invited to share perspectives on Butler's research, influence and interactions.

List of posters

Poster #: **0**
Title: Argonne Leadership Computing Facility: Available for Computational Science Research
Authors: Paul C. Messina

The Argonne Leadership Computing Facility provides supercomputing capabilities to the scientific and engineering community to advance fundamental discovery and understanding in a broad range of disciplines.

Supported by the U.S. Department of Energy's Office of Science, Advanced Scientific Computing Research program, the ALCF is one half of the DOE Leadership Computing Facility, which deploys two diverse high-performance computer architectures dedicated to open science.

Available to researchers from universities, industry, and government agencies, the ALCF helps accelerate the pace of discovery and innovation by providing supercomputing resources that are 10 to 100 times more powerful than systems typically available for open scientific research.

Poster #: **1**
Title: Radiological Sealed Source Library: A Nuclear Forensics Tool
Authors: Jodi L. Canaday, David Chamberlain, Martha Finck, Yu Tang, Seema Naik and Kevin Carney

In the event of a terrorist obtaining and possibly detonating a device with radiological material, radiological forensic analysis of the material and source capsule could provide law enforcement with valuable clues to the origin of the material; this information could then provide further leads on where the source or material was obtained.

The concept of nuclear forensic signatures for interdicted nuclear materials is generally understood to include isotopic ratios, trace element impurity ratios, material age and morphological aspects of the material. In contrast, radiological forensic signatures for radiological sealed sources focus more on the physical design and chemical composition of the source capsule and containers, physical markings indicative of an owner or manufacturer, and isotopically determined material age.

Argonne and Idaho National Laboratories have been working since 2003 on understanding signatures that could be used to identify specific source manufacturers. These signatures include source materials of construction, dimensions, weld details, elemental composition, and isotopic abundances of the radioactive material. These signatures have been collected in a library, known as the Radiological Sealed Source Library, which contains more up-to-date information on radioactive source signatures than any other database/library in the world. Details of the Radiological Sealed Source Library will be described.

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Poster #: **2**
Title: Camellia: A Software Framework for Discontinuous Petrov-Galerkin Methods
Authors: Nathan V. Roberts

The discontinuous Petrov-Galerkin (DPG) finite element methodology of Demkowicz and Gopalakrishnan minimizes the solution residual in a user-determinable energy norm and offers a built-in mechanism for evaluating error in the energy norm, among other desirable features. However, the methodology brings with it some additional complexity for researchers who wish to experiment with DPG in their computations. In this poster, we introduce Camellia, a software framework whose central design goal is to enable developers to create efficient hp-adaptive DPG solvers with minimal effort.

Recent efforts have focused on the development of a working prototype Python interface, support for space-time finite elements, and mathematical and computational efforts toward scalability—in particular, the development of scalable preconditioners for the global solve. We have successfully run Camellia solves on ALCF's BG/Q machines on as many as 32,768 MPI ranks.

Poster #: **3**
Title: Fragment Approach to Density Functional Theory Calculations of Large Systems
Authors: Laura E. Ratcliff, Stephan Mohr, Luigi Genovese and Thierry Deutsch

Ab initio electronic structure simulations have been used extensively over the past few decades to improve our understanding of the behavior and properties of materials. In particular, density-functional theory (DFT) has become the method of choice due to its excellent balance between accuracy and efficiency. However, standard implementations of DFT scale cubically with the number of atoms and so algorithms must be designed with reduced scaling in order to allow simulations of realistic (large) systems of technological importance. One such code is BigDFT, which has been designed for massively parallel machines and recently expanded to include a linear-scaling approach. This approach uses an adaptive localized basis set, which is itself represented in an underlying wavelet basis set and thus retains all the benefits of wavelets such as systematic convergence, while also presenting some new advantages. In particular the basis functions can be reused between closely related systems, resulting in further computational savings and facilitating a fragment based approach. This fragment approach is particularly suited to the explicit treatment of solvents and the calculation of charge transport parameters. We will present details of the fragment approach in BigDFT, highlighting an example in each of these two application areas.

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Poster #: 4
Title: Scheduling Simulation-time Analyses for Large-scale Scientific Simulations
Authors: Preeti Malakar and Venkatram Vishwanath

Scientific simulations in various domains like cosmology, climate, and materials are being executed at extreme scale for higher fidelity. Increased computational capability helps in better modeling of the real-world phenomena. Such extreme-scale simulations produce enormous output data which is stored and analyzed to understand the simulated phenomena. However, slower growth in storage bandwidth is a bottleneck in the simulation-analysis pipeline. Traditional post-processing of the stored simulation output leads to increased analysis time due to poor I/O bandwidth. This also increases the time to gain insight from the simulations. Hence, it is essential to perform simulation-time analyses.
Simulation-time analyses are performed during the simulation using the same compute resources, albeit at the cost of minimally increasing the simulation time. However, this significantly reduces the end-to-end simulation-analysis time. Such analyses ought to be scheduled at an optimal frequency so that the total analyses time is within a user-specified threshold. We present the scheduling of simulation-time analysis as a numerical optimization problem to maximize the number of online analyses subject to resource constraints such as I/O and network bandwidth, rate of computation, available memory, etc.
Our optimization-based scheduling recommends the different feasible analyses and their frequencies depending on the threshold on analysis time. It also takes into account the importance of the various analyses that a user may specify. We demonstrate the effectiveness of our approach through two classical simulation codes - LAMMPS and FLASH on the IBM Blue Gene/Q system. Our optimal scheduling results in above 80% usage of the allowed threshold.

Poster #: 5
Title: Accelerating QMCPACK with the SIMD vectorization
Authors: Ye Luo and Anouar Benali

Massively parallel supercomputers have become a great driving force of scientific advance especially in predicting materials properties with sufficient accuracy and confidence. Quantum Monte Carlo (QMC) is one of the most accurate electronic structure methods for ab initio many-body calculations and has the capability to scale to millions of processors.

With the actual trend of supercomputers, clearly oriented towards accelerators and GPUs, the common strategy to achieve performance and energy efficiency is to implement the single instruction multiple data (SIMD) model, also used by the generic CPU with vector units (SSE/AVX on x86 and QPX on Blue Gene/Q). The next supercomputers will see both the number and the size of vector units increase. However, current and, most probably, future compilers are not always able to a generate vectorized code. Scientists are required to adapt their codes to the new hardware feature in order to take fully advantage of the new architectures.

In our application QMCPACK, most of the computation consists of evaluating single electron orbitals represented by cubic B-splines, scaling quadratically with the system size. By vectorizing this part of code using IBM intrinsics, we've obtained a significant improvement compared to the original version (3 folds speedup) and demonstrated the portability of this strategy to future architectures with longer vector units.

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Poster #: 6
Title: Verification Efforts for the Heterogeneous Geometry Neutronics Code PROTEUS
Authors: Emily R. Shemon, Changho Lee and Micheal A. Smith

PROTEUS is a high fidelity, massively parallel neutronics code developed at Argonne National Laboratory under the DOE NEAMS program. PROTEUS calculates the neutron flux and other important physical quantities inside a nuclear reactor. The transition from using a conventional homogenized techniques (legacy neutronics codes) to a high fidelity approach (PROTEUS) for heterogeneous geometry modeling has introduced some challenges, particularly with regards to multigroup cross section generation. Recent progress has been made in verifying PROTEUS against MCNP (Monte Carlo code) reference solutions for heterogeneous geometry. Here we present results and comparisons to MCNP where errors in the multigroup cross sections have been eliminated and the PROTEUS solver itself has been verified.

Poster #: 7
Title: PROTEUS: Comparison to MONJU Start-up Data
Authors: Micheal A. Smith and Emily R. Shemon

PROTEUS is a reactor physics toolset focused on improving nuclear reactor analysis and design through the use of high performance computing. Its intent is to reduce or eliminate considerable engineering approximations and problem simplification taken by existing tools. All of the PROTEUS calculations shown were performed using the Blue Gene/P leadership class computing facility at Argonne National Laboratory.

Poster #: 8
Title: PROTEUS: MC2-3 + SN2ND Modeling of ZPR Experiments
Authors: Micheal A. Smith and Emily R. Shemon

PROTEUS is a reactor physics toolset focused on replacing the existing methodology for nuclear reactor analysis and design. The existing methodology contains considerable engineering approximations and problem simplification which are done to allow predictive capabilities on serial machines, albeit with significant uncertainty bars. Some of these approximations are simply not necessary with modern computing systems, especially with the existence of leadership class computing systems. The initial PROTEUS development has focused on improvements to fast reactor tools where we make extensive use of parallel computing to overcome the challenges associated with introducing more modeling fidelity.

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Poster #: 9
Title: Detection of Weak Gamma Sources in Urban Background Search Survey using Dynamic Quantum Clustering of Spectral Data
Authors: Alexander Heifetz, Frank Moore, Tom Elmer and Sasan Bakhtiari

The challenge of detection and identification of weak gamma sources during urban search surveys consists of performing both saliency and anomaly searches in large volume of data. This is a complex task given that the spectra are measured with low resolution detector under the conditions of highly varying background and with relatively low signal-to-noise (SNR) ratios. Reliable detection and identification of isotopes requires tine-averaging to increase spectral SNR short acquisition interval measurements. However, there is no algorithmic tool to select the size of the averaging window. Incorrect averaging can wash out weak spectral lines of orphan sources. Our method, which is based on data clustering, provides a filter for averaging. Clustering multidimensional data, or equivalently revealing hidden correlations among the many features, is a technique of unsupervised machine learning. As such, clustering is ill-defined. Recently, there has been interest in finding models of physical systems to implement data clustering algorithms. One such system is Schrödinger's equation of Quantum Mechanics, which efficiently solves clustering problem for data represented by Gaussian kernel. This approach forms the basis of Dynamic Quantum Clustering (DQC) technique. We applied DQC to the analysis of noisy gamma spectra measured during search survey with Nai(Tl) detector. Using DQC, we observed that all spectra containing orphan sources 137Cs and 60Co clustered away from the background-only measurements. Spectra in the same cluster could then be averaged to enhance SNR and reveal weak orphan isotopic spectral lines. This would allow for increased accuracy of isotopic identification and lower false alarm rate.

Poster #: 10
Title: Scalable ab initio Dynamics with the Fragment Molecular Orbital Method
Authors: Spencer R. Pruitt, Hiroya Nakata, Olaseni Sode, Yuri Alexeev, Graham Fletcher, Dmitri G. Fedorov, Mark S. Gordon and Greg Voth

The ability to simulate water with accurate methods is important for the study of biological and chemical systems, where on an accurate description of the hydrogen-bonding network in liquid water is crucial. A recent application of the fragment molecular orbital method (FMO) to water clusters has highlighted the importance of three-body interactions in water. The requirement for methods to provide accurate three-body effects in water only emphasizes the need for 3-body analytical gradients as a prerequisite for dynamical simulations.

The scalability of FMO has made it attractive for performing ab initio dynamical simulations. Many recent advances have been made towards this goal, including fully analytic gradients, periodic boundary conditions, constraint algorithms, and a new level of parallelism. However, the current implementation does not allow for "refragmentation" of a system during a simulation. While this does not pose a problem for many systems, the ability to redefine fragments on the fly when modeling chemical reactions is crucial. One example would be any system requiring proton transfer, where the reassignment of a nucleus from one fragment to another is required. The importance of proton transport has been recognized in many disciplines including acid base chemistry, energy storage, and biochemistry.

To address this problem, a new refragmentation scheme called Multi-State Reactive Molecular Dynamics (MS-RMD) has been implemented into the GAMESS program package. This method has been combined with the 3-body analytical gradients, and the new "multi-level" parallelization scheme in GAMESS (GDDI/3), to enhance the stability and scalability of FMO-MD simulation.

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Poster #: **11**
Title: Quantifying Protein-Protein Binding Energy and Entropy using Molecular Dynamics Simulations
Authors: Sunhwan Jo, Wei Jiang and Benoit Roux

Protein-protein interactions (PPIs) represent a critical aspect of a wide range of biological processes, as most proteins need to associate to various binding partners to carry out their functions. While the basic principles of PPIs are generally understood, it is a grand challenge to accurately predict the binding affinity quantitatively for any given complex. Recently, this potential of mean force (PMF)-based methodology was extended to a much larger protein-peptide sys- tem, and we accurately determined the absolute binding free energy between the receptor protein and the ligand peptide. We plan to employ our PMF- based methodology to probe effects of mutations in thermodynamics of protein-protein interaction. Furthermore, thermodynamic decomposition of barstar-barnase protein complex association is attempted to quantify not only to probe the effect of mutation on binding free energy but also on binding entropy.

Poster #: **12**
Title: Preferred Conformations of N-glycan Core Pentasaccharide in Solution and in Glycoproteins
Authors: Sunhwan Jo, Yifei Qi and Wonpil Im

N-linked glycans are on protein surface and have direct and water/ion-mediated interactions with surrounding amino acids. Such contacts could restrict their conformational freedom of N-linked glycans compared to the same glycans free in solution. In this work, we have examined the conformational freedom of the N-glycan core pentasaccharide moiety in solution using standard molecular dynamics (MD) simulations as well as temperature replica-exchange MD simulations. Both simulations yield the comparable conformational variability of the pentasaccharide in solution, indicating the convergence of both simulations. The glycoprotein crystal structures are analyzed to compare the conformational freedom of the N-glycan on the protein surface with the simulation result. Surprisingly, the pentasaccharide free in solution shows more restricted conformational variability than the N-glycan on the protein surface. The interactions between the carbohydrate and the protein side chain appear to be responsible for the increased conformational diversity of the N-glycan on the protein surface. Finally, the transfer entropy analysis of the simulation trajectory also reveals an unexpected causality relationship between intramolecular hydrogen bonds and the conformational states in that the hydrogen bonds play a role in maintaining the conformational states rather than driving the change in glycosidic torsional states.

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Poster #: **13**
Title: Classical Molecular Dynamics van der Waals Force Field Fitting for Organic System
Authors: Ying Li

Classical molecular dynamics (MD) simulations study the movement of atoms and/or molecules with much higher computing efficiency than quantum mechanics (QM) simulations, while keeping reasonable computational complexity by applying the empirical force field. The non-expensive calculation on relatively large-scale atomistic system has been showing the increasingly needs of accurate empirical force field for MD simulations. However, the lack of accurate empirical force field, especially for the long distance intermolecular interactions in organic and biomolecular systems is an urgent issue demanding solutions. We have obtained precise test data set (from HF/6-31G* or MP2/6-31G* level QM results) comparing of van der Waals (vdW) binding energies, i.e. the electrostatic contributions are excluded. The test data set comprises of 1356 different conformations of system having 10 types of organic and/or water molecules. This work illustrates the results of reparameterizing the vdW interactions between organic-organic and organic-water molecules as in Lennard-Jones (12-6, buffered 14-7 and n-m LJ) forms by two different methods: parallel Genetic Algorithm (PGA) and Levenberg-Marquardt Algorithm (LMA) solving nonlinear least square problems. Both methods show their excellences of the results, with different accuracies and different computational expenses. The fitting results show notable improvements over the original CHARMm General Force Field (CGenFF) vdW parameters sets and AMOEBA (Atomic Multipole Optimized Energetics for Biomolecular Applications) vdW parameters sets.

Poster #: **14**
Title: Large-Scale Parallel Visualization of Particle-Based Simulations using Point Sprites and Level-Of-Detail
Authors: Silvio Rizzi, Mark Hereld, Joseph A. Insley, Michael E. Papka, Thomas D. Uram and Venkatram Vishwanath

Recent large-scale particle-based simulations require the most powerful supercomputers and produce vast amounts of data. Computing these very large datasets pushes a supercomputer to its limits, but is also challenging from the points of view of storage, analysis, and visualization. Focusing on the visualization aspects of the problem, one possibility is to map particles into a regular grid for volume rendering, which carries the disadvantages of inefficient use of memory and undesired losses of dynamic range. As an alternative, we propose a method to efficiently visualize these massive particle datasets using direct point rendering techniques with neither loss of dynamic range nor memory overheads. In addition, a hierarchical reorganization of the data is desired to deliver meaningful visual representations of a large number of particles in a limited number of pixels, preserving the locality and clustering of points and also helping achieve interactive frame rates. In this poster, we present a framework for parallel rendering of large-scale particle data sets combining point sprites and z-ordering. The latter is used to create a multi level representation of the data, which helps improving frame rates. Performance and scalability are evaluated on a GPU-based visualization cluster, scaling up to 128 GPUs. Results using particle datasets of up to 32 billion particles are shown.

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Poster #: **15**
Title: Temperature and Irradiation Species Dependence of the Radiation Response of Nanocrystalline Silicon Carbide
Authors: Laura M. Jamison, Kumar Sridharan, Steven Shannon and Izabela Szlufarska

Silicon carbide (SiC) has many properties that make it a desirable candidate material for applications in nuclear energy systems; including low neutron cross-section, chemical stability, and high temperature resistance. Improving the radiation stability of SiC would further enhance its suitability for many of these applications. The possibility of improving the radiation resistance of SiC by reducing the grain size (thus increasing the sink density) is explored in this work. In-situ electron irradiation and Kr ion irradiation was utilized to explore the radiation resistance of nanocrystalline (nc-SiC) and microcrystalline SiC (uc-SiC). The Kr irradiation studies found that radiation resistance decreased with grain refinement, suggesting that an interface-dependent amorphization mechanism is active in SiC. However, under electron irradiation it was found that nc-SiC had improved radiation resistance compared to single crystal SiC. The change in radiation response between the electron and Kr ion irradiations is hypothesized to be due to either the change in ion type, due to a potential change in amorphization mechanism, or a change in temperature. Mechanisms behind the radiation response of SiC in different environments were explored using computational methods, achieved through a collaborative effort. This study explores the possible roles of irradiation species, temperature, and experiment design on the radiation response of SiC.

Poster #: **16**
Title: Modeling Small Platinum Clusters with Quantum Monte Carlo
Authors: William D. Parker, Luke Shulenburger, Anouar Benali, Nichols Romero and Jeff Greeley

Platinum nanoclusters and surfaces catalyze many chemical reactions including the reduction and oxidation of noxious car exhaust components to more inert chemicals such as water. Understanding the catalytic action of platinum requires quantum mechanical modeling of the electrons involved, and quantum Monte Carlo (QMC) methods offer highly accurate, scalable routes to modeling catalysis in high-performance computing environments. However, to scale calculations up to the many-hundred atom systems of nanoclusters and surfaces requires an approximation of dividing electrons into core and valence. Core electrons go into a pseudopotential, which must be carefully tested for accuracy on few-atom systems before scaling up to more massive calculations. To that end, we present QMC calculations of select properties of Pt2, Pt4, and Pt13 molecules, together with those of their singly charged cations and anions. Using both 10-electron and 18-electron pseudopotentials, we compare these values to experiment (where available) and to those of the computationally cheaper but less accurate density-functional theory (DFT) method. Using the 18-electron pseudopotential, QMC and DFT predict values within 5% of experiment for the neutral-ion differences of Pt2, but the QMC value for the Pt2 dissociation energy is within 1% of experiment compared to a 15% deviation by DFT. Within the QMC method, while the neutral molecular properties of Pt2 remain within a few percent of each other between the 10- and 18-electron valences, the charged state properties of the 10-electron pseudopotential vary up to 50% from 18-electron values, indicating the 10-electron representation does not transfer well to charged states in QMC.

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Poster #: **17**
Title: Charting the phase diagram of Quantum Chromodynamics
Authors: Xiao-Yong Jin

Quantum Chromodynamics is the theory of the strong interaction responsible for 99% of the mass of a nucleon due to the binding energy, which confines quarks inside.

Nucleons make up the most of the visible universe today as the dominant matter form. It was different right after the big bang. Experiments at RHIC and LHC can bring temperatures up to a million times hotter than the center of the sun, recreating the environment milliseconds after the big bang, where exists a different form of matter, quark-gluon plasma. So far, we lack theoretical understanding due to the difficulties in calculating strongly interacting gauge theories.

We carry out first principle simulations using the technique of lattice gauge theories, on high performance computing resources of Blue Gene/Q at ANL, K computer at RIKEN AICS, and other GPU and MIC clusters. We aim at exploring the theory of Quantum Chromodynamics at finite temperatures and densities, tracing the phase transitions and critical points, and charting the phase diagram.

We use the Iwasaki gauge action and the non-perturbatively improved clover fermion action on various 4D space-time lattices. We study the system at finite temperatures, both with zero chemical potential, and with finite chemical potentials using the phase quenched fermion action and the reweighting technique to work around the manifestly complex Boltzmann weight. We computed the kurtosis of our observables to study the critical behavior. We also calculated spatial correlation functions to determine the screening masses of various particle states.