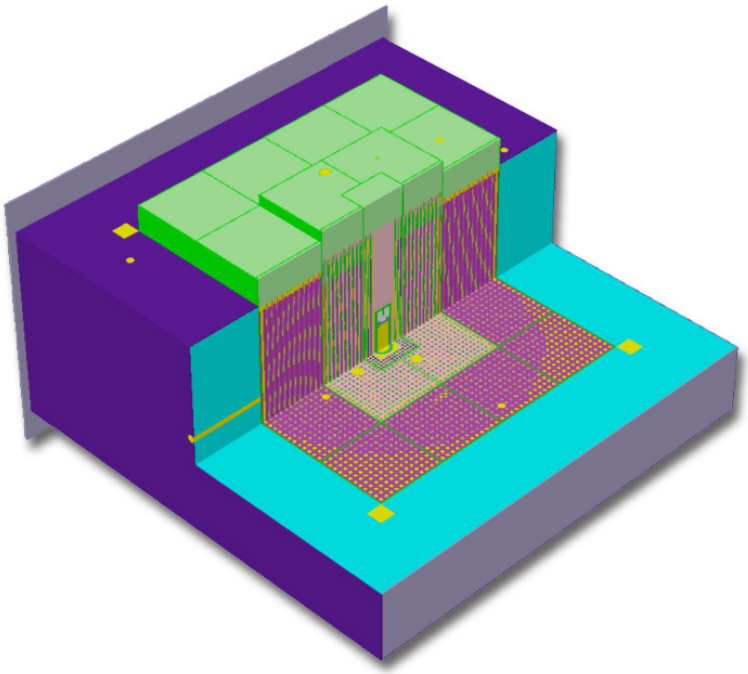
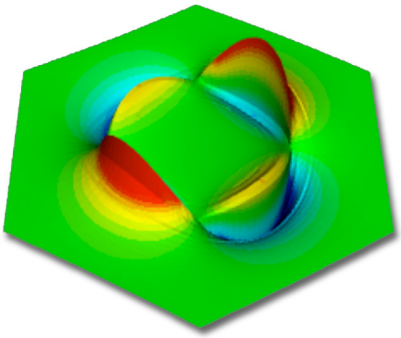
Argonne NATIONAL LABORATORY

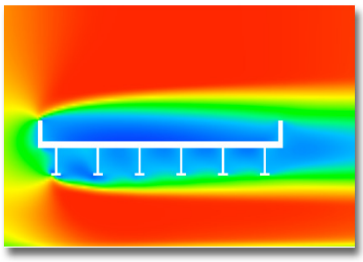
ANL-10/03

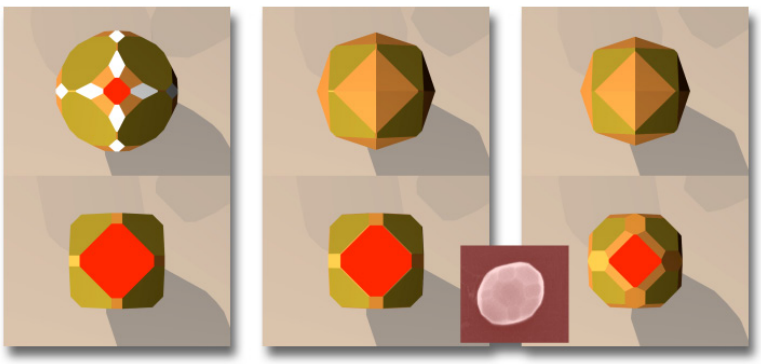
Argonne's Laboratory Computing Resource Center

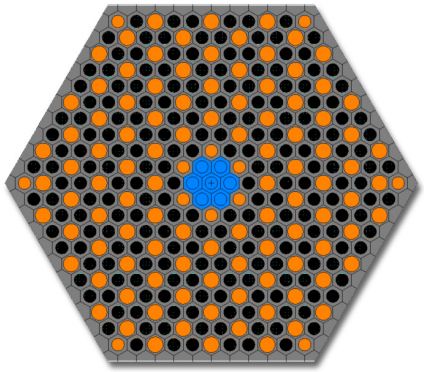
2008 Annual Report











Argonne Laboratory Computing Resource Center

FY2008 Report

Now in its sixth year of operation, the Laboratory Computing Resource Center has become an integral component of science and engineering research at Argonne, supporting a diverse portfolio of projects for the U.S. Department of Energy and other sponsors. The LCRC's ongoing mission is to enable and promote computational science and engineering across the Laboratory, primarily by operating computing facilities and supporting high-performance computing application use and development. This report describes the scientific activities, computing facilities, and usage of LCRC operation in 2008 and the broad impact on programs across the Laboratory.

The LCRC computing facility, Jazz, is available to the entire Laboratory community. In addition, the LCRC staff provides training in high-performance computing and guidance on application usage, code porting, and algorithm development. All Argonne personnel and collaborators are encouraged to take advantage of this computing resource and to provide input into the vision and plans for computing and computational analysis at Argonne.

The LCRC Allocations Committee makes decisions on individual project allocations for Jazz. Committee members are appointed by the Associate Laboratory Directors and span a range of computational disciplines.

For further information about the LCRC and Jazz, please see the LCRC Web site at http://www.lcrc.anl.gov/, or send e-mail to support@lcrc.anl.gov.

Ray Bair
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Executive Summary

Argonne National Laboratory founded the Laboratory Computing Resource Center (LCRC) in the spring of 2002 to help meet pressing program needs for computational modeling, simulation, and analysis. The guiding mission is to provide critical computing resources that accelerate the development of high-performance computing expertise, applications, and computations to meet the Laboratory's challenging science and engineering missions. LCRC includes both a mid-range supercomputer and expert staff to support researchers and administer the systems.

The 350-node LCRC cluster, named "Jazz," began production service in April 2003 and has been a research work horse ever since. Hosting a wealth of software tools and applications and achieving high availability year after year, researchers can count on Jazz to achieve project milestones and enable breakthroughs. Over the years, many projects have achieved results that would have been unobtainable without such a computing resource. In fiscal year 2008, there were 55 active projects representing a wide cross-section of Laboratory research, including work in chemistry, biosciences, climate, computer science, transportation, environmental science, accelerator science, materials science, mathematics, nanoscience, high-energy physics, nuclear engineering, and nuclear physics.

The LCRC continues to foster growth in the computational science and engineering capability at the Laboratory. LCRC staff provides expert assistance to help researchers solve computing problems and get the most out of the computer. The wealth of compilers, libraries, and tools available on Jazz facilitate development of many kinds of science and engineering applications. The available selection of popular community and commercial applications supports rapid model construction and analysis. Jazz is a platform for developing one's first parallel computing code, a dependable resource for mid-range supercomputing, and a tool for developing and testing applications that target much larger supercomputers.

Finally, recognizing that Jazz is oversubscribed and that much better technology is now available, LCRC has developed a plan to acquire the next generation of LCRC computing resources in 2009.

The Laboratory Computing Resource Center

The Laboratory Computing Resource Center was established in 2002, based largely on the recommendation of Argonne's Computational Science Advisory Committee. The driving mission of the LCRC is to enable and promote computational science and engineering across the Laboratory, primarily by operating computing facilities and supporting application use and development. The Computing, Environment and Life Sciences Directorate operates the LCRC on behalf of the Laboratory. The long-term goal of the LCRC is to develop a vigorous computational science and engineering community at Argonne. Therefore, in addition to supporting Jazz, the LCRC provides consulting services to the Argonne computational research community. These services include training in computation techniques from the fundamentals to advanced topics, assistance with code performance analysis, guidance with algorithm development, and general help and advice.

Cluster Configuration

Jazz is a "Beowulf" cluster, built largely from commodity components. The cluster has, however, been tuned for Argonne-specific use, with diverse tools installed to support parallel computing and project management. Documentation has also been added for user support. The Jazz system configuration includes the following.

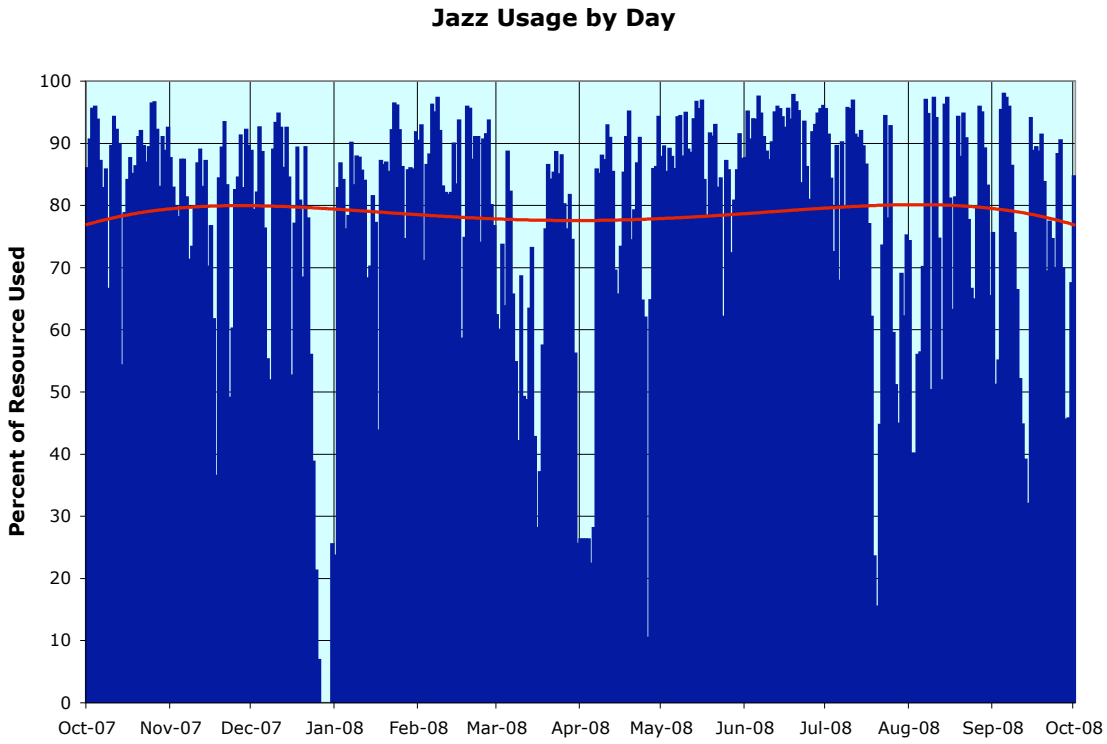
- 350 computing nodes, each with a 2.4 GHz Pentium IV processor and an 80 gigabyte (GB) local scratch disk; half the nodes have 2 GB of memory and half have 1 GB
- 14 terabyte (TB) home file system, and 10 TB global working disk
- Myrinet 2000 and gigabit Ethernet network fabrics to all nodes
- 4 front end nodes for user login and 8 system management nodes

Cluster Usage

The usage of Jazz was high throughout most of fiscal year 2008, with usage averaging 80% and peaking over 90% at times. The maximum sustainable usage on Jazz is about 85% over long periods, given that some nodes go idle when the smallest computation waiting to run is requesting more nodes than are available. Reservations for very large computations (e.g., over 200 nodes) create additional holes as nodes are held open for a while until the large computation has sufficient resources to begin.

Jazz supports a wide mix of computations, from long runs with a few nodes to short runs with many nodes, with many variations between. On a project-by-project basis, usage varies considerably over time. Projects often start slow, then ramp up, then increase and decrease in cycles as the project progresses, with interruptions for analysis, manuscript preparation, conferences, and vacations. This usage pattern also causes fluctuations in the overall utilization of Jazz.

The chart below plots the daily usage on Jazz for the fiscal year. On this chart, 100% means that all 350 nodes on Jazz were used continuously for the day. With a few exceptions for extended maintenance, usage was high throughout the year.

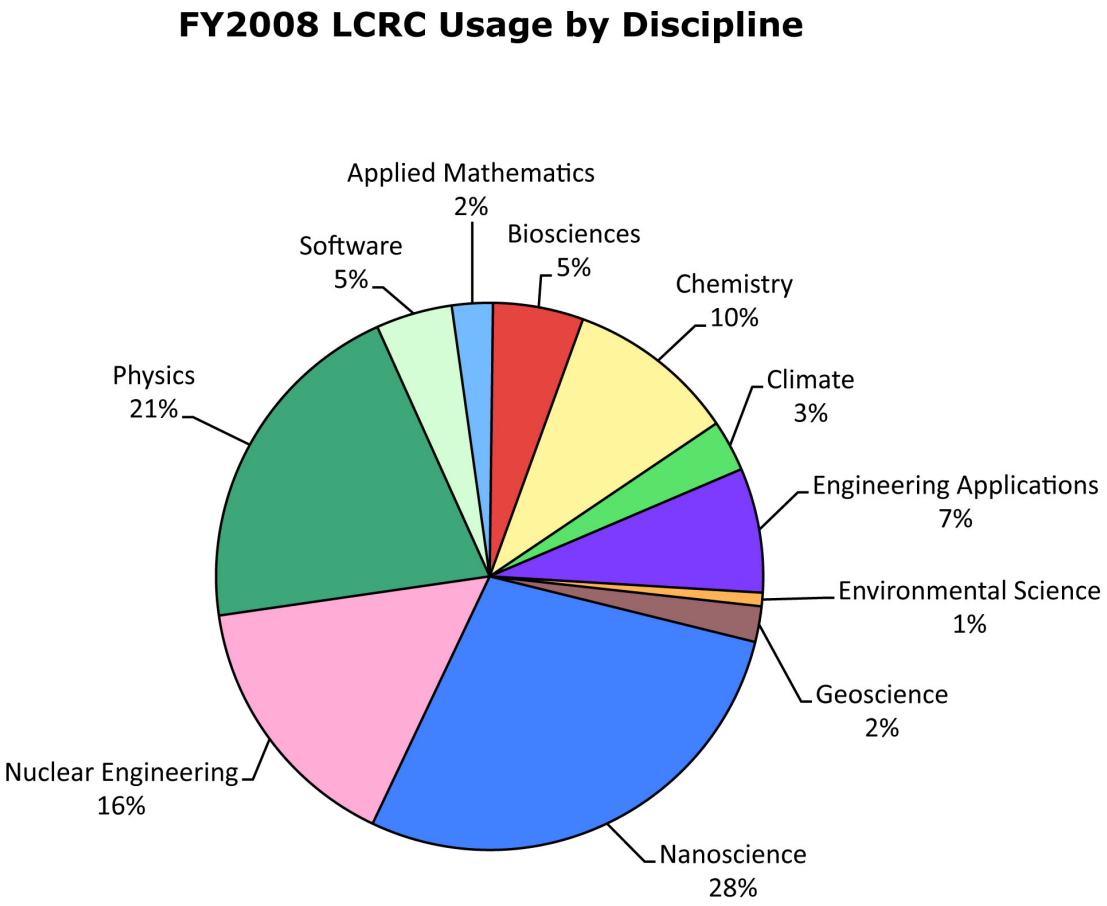


Users and Projects

LCRC resources are available to all Argonne personnel. Non-Argonne collaborators working with an Argonne principal investigator are also welcome. All such personnel who would like to use the Jazz system may sign up for an account on the LCRC Web site, www.lcrc.anl.gov. New users are granted an initial allocation of 1,000 computing hours on the system to become familiar with the Jazz system and evaluate its applicability to their work. Researchers can also request larger project allocations via the Web site. Aside from the startup efforts, all computer time is allocated to projects, rather than individuals, where a project is focused on a specific technical activity or avenue of investigation. A project usually has several scientists or engineers working on it, and a person may be active on more than one project. All project requests are judged on the basis of scientific merit by the LCRC Allocations Committee, composed of scientists from across the Laboratory, appointed by the Associate Laboratory Directors.

Usage by Discipline

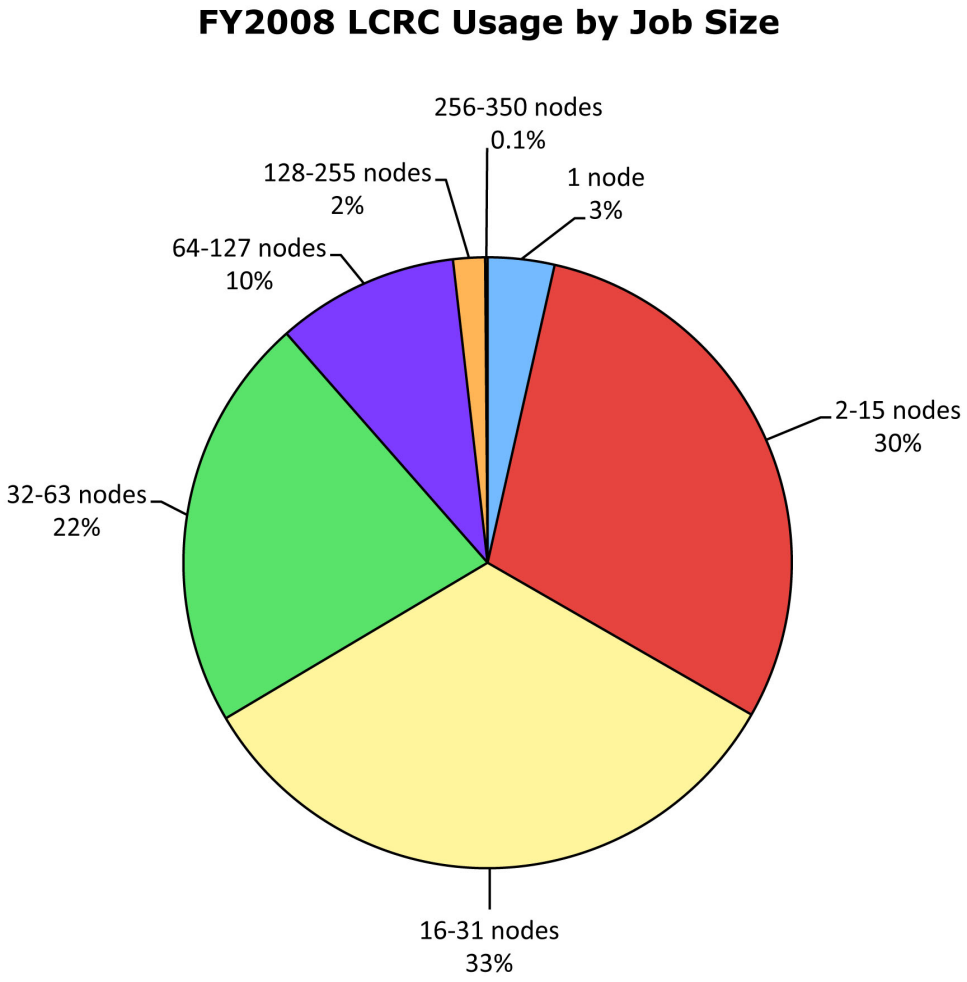
Jazz supports research in a wide range of disciplines, and usage varies from year to year. The chart below shows what fraction of the Jazz resource (number of node hours) was used by projects in each discipline during fiscal year 2008. There were multiple projects in each of the disciplines that used the most time: nanoscience, nuclear engineering, and physics.



Job Size Characteristics

Jazz is configured to support parallel computing work of many types, with jobs using a handful of nodes to hundreds of nodes. The number of nodes that a particular application can use effectively depends on many factors, including the computational approach taken, the problem size, and the ratio of computational effort to interprocessor communications required. Jazz is also a multiuser system, and it is almost entirely space-shared, rather than time-shared. Each large job gets a set of computational nodes dedicated to it for the duration of the computation. At any time, several jobs will be running, each using a part of the system.

Data about the number of computing nodes that jobs used provides an interesting view of how the system is being utilized and the degree of scalability or parallelism commonly utilized on Jazz. The chart below shows the amount of computing time used by jobs of various sizes in FY2008. Over 50% of the computing time was used for jobs that employed 16–63 processors, and about 12% of the time for 64–350 processor jobs.



On a system such as Jazz that is heavily used, job turnaround is related to the number of nodes requested. That puts a practical bound on the turnaround for very large jobs. To compensate, users may reserve a portion of the system for a specific period during a night or weekend to carry out large computations or to meet an urgent computing need. All users are notified in advance of these reservations.

Scientific and Engineering Applications

The LCRC has become an essential resource for a wide range of projects in many Argonne divisions, from production runs to exploratory modeling and simulation research to high-performance algorithm and application development. In 2008 there were 55 active projects from more than 15 divisions/departments that use Jazz for research in science and engineering. In addition, creation of the LCRC has provided an important catalyst for establishing a high-performance computing community in the Laboratory, building relationships that enable cross-disciplinary efforts and developing computational science skills in many mission areas. LCRC staff continue to help build this community by assisting researchers who are getting started with new parallel codes or expanding the range of their codes to address larger, more complex problems. Sharing experience in parallelizing codes can save huge amounts of time and effort. The LCRC also provides a launching point for researchers who gain experience on Jazz and then move up to larger systems at national centers like the new Argonne Leadership Computing Facility (ALCF).

Most of the projects using the LCRC fall into three broad, overlapping categories:

Strategic. Jazz is a critical resource for most all of the Laboratory directed research and development (LDRD) strategic initiatives as well as completion of programmatic work in strategic areas. In other cases, Jazz is the testing ground for the concepts that will make up future LDRD and programmatic proposals.

Production. An important component of LCRC's mission is to provide a fast and reliable resource for the Laboratory's production modeling and simulation activities. Some of these production codes are still under development; others are fully mature. Often Jazz is the largest resource available to a research group; for other production applications, Jazz fills the need for quick turnaround on mid-range runs, where larger runs are done on systems bigger than Jazz at NERSC, ALCF, or other national centers. Also, parallel versions of a number of commercial science and engineering codes are available on Jazz, for example, for production computational fluid dynamics, finite element, and quantum chemistry computations.

Exploratory. Some Jazz projects are investigating approaches and algorithms for next-generation computations, developing prototype applications with new capabilities, and evaluating software performance, accuracy, or programming models. While large parallel computing resources offer tremendous power, frequent access to parallel computers is essential to develop effective algorithms and codes. Challenges include strategies for dividing the problem into many pieces, optimization of the kernels of computation, and management of the massive flow of results to storage. Other projects on Jazz are exploring new designs or models of complex phenomena, forging new paths to extend the range of existing applications, or starting a parallel programming project from scratch and drawing on the experience of the LCRC staff.

In the following sections, we present examples of research performed with Jazz throughout 2008. The examples span both the basic and applied missions of the Laboratory and touch most of our strategic initiatives. These examples highlight the science and engineering advances being made, tackling important problems in nanosciences, physics, biosciences, nuclear engineering, climate, and many other disciplines. The research also encompasses a wide range of computational techniques, including agent-based simulations, computational fluid dynamics, Monte Carlo solvers, and "first principles" solutions.

Atmospheric Chemistry and Transport

PIs: Veerabhadra Kotamarthi and Beth Drewniak (Environmental Science)

The scientific aim of this modeling activity is to further scientific understanding of the chemistry and distribution of oxidants in urban and rural air masses. We focus on such key unresolved processes as (a) the importance to oxidant chemistry of rapid surface reactions cycling NOx and HOx reservoir species to NOx and HOx; (b) different HC lumping schemes and their effect on the NOy and HOx partitioning as it relates to the formation of oxidants; and (c) oxygenated hydrocarbons and their impact on determining the urban and rural boundary layer oxidant levels.

Three-dimensional models of the atmospheric dynamics, chemistry, and transport are used to evaluate the impacts of energy-related and biogenic emissions on urban, regional, and global-scale environments. These include MM5, a mesoscale meteorological model to simulate the dynamics of the regional-scale atmosphere; CMAQ, a regional-scale transport and chemistry model for atmospheric trace gases and aerosols; SMOKE, a model for generating gridded emissions from EPA provided emission inventory; CALMET/CALPUFF, for simulating dispersion of selected number of puffs in the atmosphere; MOZART4, a global-scale chemistry transport model for mercury transport and deposition; and GEIOD-CHEM, a global-scale chemistry transport model for trace gases and aerosols. We have ported and successfully tested these models on the Jazz cluster and completed a number of preliminary calculations.

During the past year we have used MOZART to evaluate the impact of mercury transport from China on the United States. Since elemental mercury can transport long distances, local mercury concentrations can be influenced by transcontinental transport and the impact of growing anthropogenic emissions from sources in Asia is a concern in the U.S. We evaluated three scenarios to determine the sensitivity of mercury concentrations to emissions from China. We found concentrations of mercury in the U.S. were up to 7% higher when emissions from China were included. The largest increases in mercury occurred during the spring and summer months. Jazz was used to run multiple-year simulations of the global chemical transport model with full chemistry. Atmospheric elemental mercury has a lifetime of approximately 1.5 years, and this required that we run the model to about 4 years in order to get a steady-state distribution of mercury in the model. We computed three different cases of mercury distributions requiring close to 20 years of model years. We also made several test runs with mercury chemistry included in the model.

Our results show that long-range transcontinental transport of mercury has a non-negligible impact on mercury concentrations and deposition in the United States. The transport of mercury into the U.S. from outside its borders is thus a significant issue for policy development.

Publications and Presentations:

B. A. Drewniak, V. R. Kotamarthi, D. Streets, M. Kim, and K. Crist, "Estimates of Mercury Flux into the United States from Non-Local and Global Sources: Results from a 3-D CTM Simulation," Atmos. Chem. Phys. Discuss., 8, 19861-19890, 2008.

Bridge Hydraulics

PI: Tanju Sofu (Nuclear Engineering)

Bridges provide a critical component of the nation's transportation network. Evaluation of bridge stability after flooding events, including structural response of the bridge itself and the erosion of the riverbed surrounding bridge support structures, is critical for highway safety. Traditionally such evaluations have relied heavily on scaled experiments to provide measurements for flow field and structural response. However, the availability of parallel computers and analysis capabilities of commercially available software provide an opportunity to shift the focus of these evaluations to the domain of computational fluid dynamics (CFD).

Efforts in 2008 focused on assessing hydrodynamic loads on bridge decks under various flood conditions (Fig. 1). We investigated the applicability of commercial CFD codes such as Fluent and Star-CD for predicting these phenomena, and we determined the agreement between the code predictions and experimental data for various modeling options. We also evaluated the scalability of these simulations to large numbers of processors, particularly for the simulation of full-scale bridge deck interactions, and we evaluated the computational efficiency and accuracy of various codes.

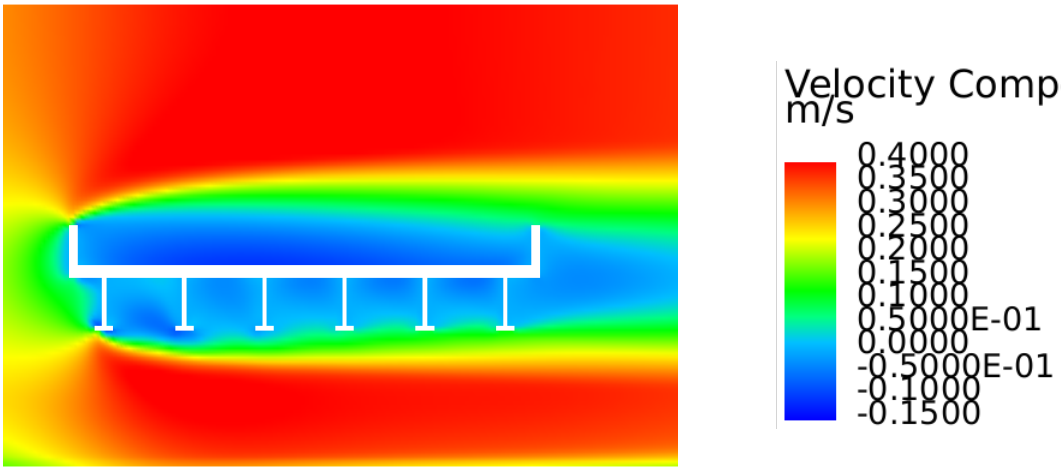


Figure 1. *Six-girder bridge deck model (top) and calculated flow field under the free surface (bottom). The free-surface simulations are performed with a time-dependent solution scheme, and, for most configurations, a steady solution is reached within a few minutes (as simulated real time). However, with the time step size limited by the Courant number for flow, the free-surface simulations require significant computation time depending on the size of the model and the number of processors used. Most calculations are performed by using a symmetric segment of a bridge deck model (shown in yellow) on 4-16 processors, requiring 5-10 hours computation time.*

Publications and Presentations:

T. Sofu and K. Kerenyi, "Innovative Solutions: Advanced Technologies and Equipment to Resolve Hydraulic Issues: Computational Fluid Dynamics for Bridge Hydraulics," 2008 National Hydraulic Engineering Conference, Partnering for Progress in a Changing Environment, Portland, Maine, August 25-29, 2008.

Funding: This project is funded by the U.S. Department of Transportation.

Spatio-Temporal Chaos of a Fluid Layer

PIs: Mark Paul and Paul Fischer (Mathematics and Computer Science)

This work is a computational effort to push as deeply as is currently possible toward a quantitative understanding of how complex dynamics (i.e., spatio-temporal chaos) arise in spatially extended nonequilibrium systems at the frontiers of numerous science and technological problems. We are exploring Rayleigh-Benard convection, which is a horizontal layer of fluid warmed uniformly from below and cooled uniformly from above. We are also studying Faraday waves, which are the surface waves that form on a shallow fluid layer when oscillated in a gravitational field. In both cases we are performing numerical simulations for experimentally realistic conditions using a highly optimized spectral element code.

For Rayleigh-Benard convection we explored the relationship between the spectrum of Lyapunov perturbation vectors and the pattern of the fluid convection. We have found that different Lyapunov perturbation vectors yield different information regarding the pattern dynamics. Overall, spatially localized defect events tend to contribute most to the growth of perturbations.

For the Faraday waves we have successfully simulated two-dimensional waves in a shallow layer with periodic sidewall boundary conditions. For these calculations we use an arbitrary Lagrangian-Eulerian formulation of the spectral element code. The 2D calculations marked an important step in establishing that these difficult calculations can be performed. We are currently running simulations to explore the possibility of a drift in the waves as predicted by theory. We are also planning to run three-dimensional simulations.

We have also gained an understanding of rotating Rayleigh-Benard convection for relatively large rotation rates, well above the Kuppers-Lortz instability. Unexpected square patterns have been reported in experiments in this parameter regime. These square patterns had not yet been understood theoretically. We are able to replicate the experiments if the centrifugal and Coriolis forces are both included. But, we have determined that the square patterns are not a result of Coriolis force.

We also have begun to explore the upper bounds on Rayleigh number for our simulations (10^7 and beyond), with small-aspect ratio (diameter/depth = 1-3) Rayleigh-Benard convection. Researchers have reported experimental results showing thermal plumes carried by a mean wind at such high Rayleigh numbers. This mean wind would reorient itself aperiodically. We have confirmed the presence of a mean wind with our simulations and have found the orientation of the mean wind to drift (no reorientations have yet been found). These results shed new insight on the fundamental nature of the complex dynamics that occur in experimentally accessible fluid systems. Our findings can be used to improve our understanding of more complex real-world systems such as the dynamics of the weather and climate, and the sloshing problems that occur in many technological applications.

Publications and Presentations:

P. L. Mutyaba, T. Kimmel and J. D. Scheel, "Patterns in Rayleigh-Benard Convection for High Rotation Rates," American Physical Society Division of Fluid Dynamics Meeting, Salt Lake City, UT (2007).

N. O'Connor, E. Knobloch, P. F. Fischer, and M. R. Paul, "Numerical Simulations of Viscous Faraday Waves," American Physical Society Division of Fluid Dynamics Meeting, Salt Lake City, UT, 2007.

Nicholas O'Connor, "The Spatiotemporal Dynamics of a Shallow Fluid Layer," Master's thesis, Virginia Tech, Spring 2008.

A. Duggleby and M. R. Paul, "Exploring Extensive Chaos in Rayleigh-Benard Convection Using Fractal and Karhunen-Loeve Dimensions," 22nd International Conference on Theoretical and Applied Mechanics, Adelaide, Australia, August 25-29, 2008.

Grants:
Cottrel College Science Award #7968, PI: Janet Scheel, Numerical Simulations of Turbulent Thermal Convection: Investigations of the Large-Scale Circulation and Its Reorientations

NSF CAREER Award NSF CBET-0747727, PI: Mark Paul, Spatiotemporal Chaos in Fluid Convection: New Physical Insights from Numerics.

NSF SGER CTS-0604376, Award, PI: Mark Paul, Symmetry-Breaking Bifurcations in an Oscillating Fluid Layer

High-Energy Collider Physics

PIs: Edmond Berger (High-Energy Physics) and Zack Sullivan (Illinois Institute of Technology)

Supersymmetry is the leading candidate for new high energy physics that extends beyond the Standard Model FOR particle physics. This theory predicts the existence of a significant number of new particles that should be observed at the CERN Large Hadron Collider (LHC). Uncertainties in the current estimates of the supersymmetry processes themselves, and the Standard Model backgrounds to many signatures of new physics, range from tens of percent to order-of-magnitude estimates. Significantly improved understanding of the Standard Model backgrounds is vital for establishing a discovery.

A "golden signature" for supersymmetry is the observation of 3 leptons plus missing energy coming from the decay of the supersymmetry states chargino and neutralino. Experimental analyses and data triggers are designed assuming that the Standard Model backgrounds to this channel are modest. Our results predict both the overall magnitude and the expected population in phase space of both the supersymmetry signal and the dominant Standard Model backgrounds.

Some Standard Model backgrounds are huge, such as the background associated with a Z boson plus a bottom quark final state. We find that a potentially useful discriminant is the amount of "missing energy" produced. This missing energy is the energy carried away by essentially noninteracting final state particles, such as neutrinos. Nevertheless, the overall magnitude of the background is so large in our estimations that "tails" of the background extend well into the signal region. Hence, we had to devise more complex, multivariable analysis strategies. We discussed our findings with experimenters involved in the search for supersymmetry in two major collaborations at the LHC. Coupled with previous work on two-lepton final states, our new results confirm that the class of previously ignored heavy-flavor hadron decays will pose a serious

challenge to the analysis of a wide range of experimental signatures. Given the complexity of the simulations, a major experimental effort will be required to understand what measures can be developed to quantitatively control the uncertainties (see Fig. 2).

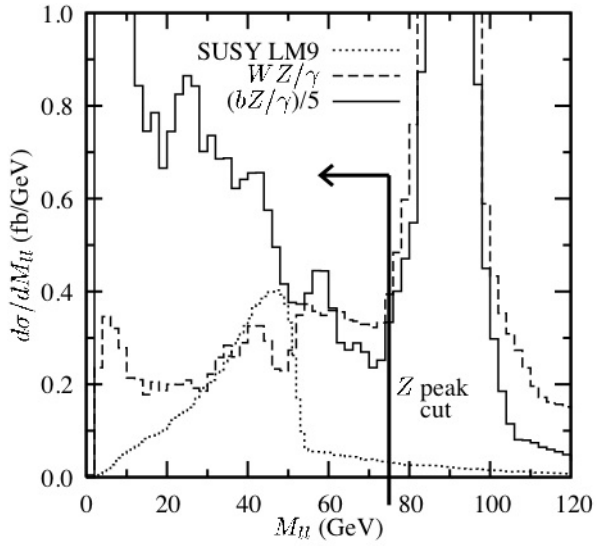


Figure 2. *Calculated invariant mass of the opposite-sign same-flavor (OSSF) lepton pairs for the supersymmetry point LM9 (dotted) and various Standard Model backgrounds.*

Publications and Presentations:
E. L. Berger and Z. Sullivan, "Trilepton Production at the LHC - Standard Model Sources and Beyond," Phys. Rev. D78, 034030 (2008)

Search for the Onset of Color Transparency

PIs: Kawtar Hafidi and Lamiaa El Fassi ((Physics))

According to QCD, point colorless systems, such as those produced in exclusive processes at high Q^2 have small transverse sizes. Therefore, they are expected to travel through nuclear matter experiencing very little attenuation. This phenomenon is known as color transparency (CT). An analogous mechanism is well known in QED: the interaction cross-section of an electric dipole is proportional to its square size. As a result, the cross section vanishes for objects with small electric dipole moments. Since color in QCD is equivalent to the charge in QED, the cross section of a color-neutral dipole –- as formed by a pair of oppositely colored quarks, for instance – is also predicted to vanish for small sized hadrons.

The main goal of the E02-110 experiment is to search for the onset of CT in the incoherent diffractive ρ^0 electro and photoproduction on deuterium, carbon and copper. In this process, the virtual photon fluctuates into a (q q-bar) pair, which travels through the nuclear medium evolving from its small initial state with a transverse size proportional to 1/Q, to a "normal size" vector meson detected in the final state. Therefore, by increasing the value of Q^2 one can squeeze the

size of the produced (q q-bar) wave packet. The experiment was performed with the CEBAF Large Acceptance Spectrometer. The data was taken with both 4 and 5 GeV electron beams incident on 2 cm liquid deuterium target and a solid target (0.4 mm thick Fe and 1.72 mm thick C) simultaneously to reduce systematic uncertainties. In these measurements we are interested in the scattered electron and the two pions from the ρ^0 decay in the low t region below 0.5 GeV. Although the two targets are very close to each other compared to the distance where the CLAS detector is sitting, the acceptance correction was found to be important for our reaction of interest. To ensure that this correction was reliable, we simulated hundreds of millions of events for different targets and beam energies. The effect of the acceptance correction can reach up to 30% in the low Q^2 bin, as shown in Figure 3. The present analyses are now being reviewed by CLAS collaboration.

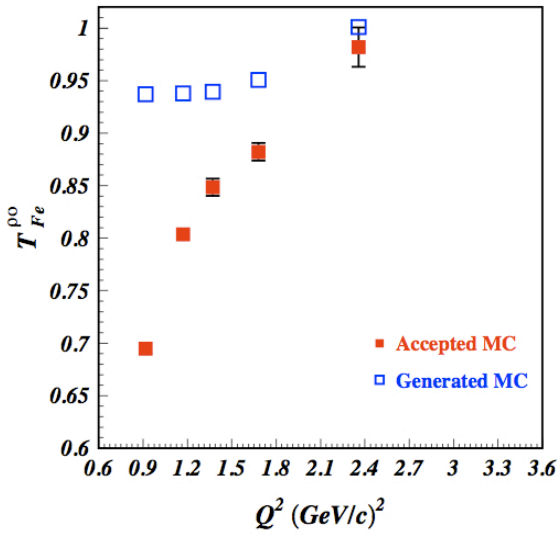


Figure 3. *The nuclear transparency ratio from the Monte Carlo. Empty squares represent generated events, and the full squares are the accepted ones.*

Computational Nanoscience

PI: Peter Zapol (Chemical Sciences and Engineering, Materials Science, Center for Nanoscale Materials)

Metal nanoparticles are currently receiving a lot of attention because of their suitability for advanced fuel cell applications. Our work focuses on noble metal nanoparticles in oxygen atmosphere; specifically, we are examining the effects of various adsorption configurations on the equilibrium shape under different annealing conditions. We also include the influence of oxide support in the study. The ability to create nanoparticle arrays of a uniform size, shape, and orientation is important for both model catalyst studies and improvement of real systems. Knowledge of the surface and interface energies determined by the first-principles calculations results in prediction of equilibrium shapes for supported crystals; Pt on SrTiO3 (STO) was chosen for this study.

We developed a thermodynamic model to describe the shape of nanoparticles. This model enables us to predict the stability of metal nanoparticles. Parameters of the model are determined by density functional calculations, used to accurately determine surface and interface energies. These calculations involved generalized gradient approximation and projected augmented wave potentials, as implemented in the Vienna ab initio simulation package VASP. We investigated the effect on the surface energies of oxygen adsorption (at different coverage) on several low-index surfaces. These calculations are very demanding because large surface cells and thick slabs are needed to get meaningful results.

During the past year we predicted equilibrium Pt particle shapes under different temperatures and oxygen pressures, investigated the effects of surface reconstructions on a supported particle shape, and experimentally verified the findings. We also compared the optimized structures with experimental results. These studies help experimentalists to understand the properties of metal nanoparticles and tune synthesis conditions for particular applications (see Fig. 4).

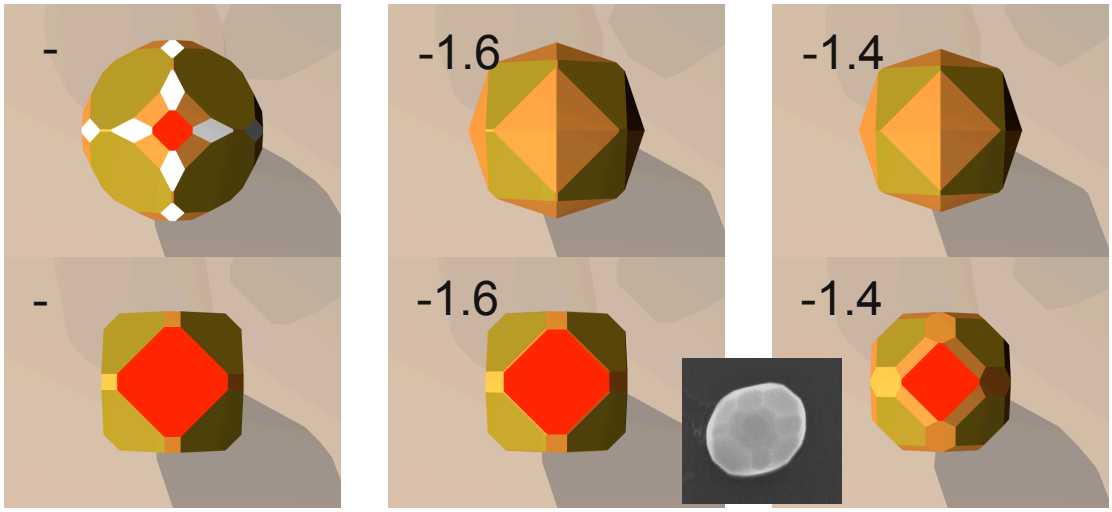


Figure 4. *Calculated equilibrium particle shape at different values of oxygen chemical potential (in eV). Top row: no reconstruction; bottom row with Pt(110)-(2x1) missing row reconstruction, and the Pt(100)-hex reconstruction. Inset: experimental SEM image of 100 nm Pt particle supported on SrTiO3 (100) surface.*

Publications and Presentations:

P. Zapol, "Functional Nanomaterials from First Principles," Argonne MSD Colloquium, February 2008.

Density Functional Theory Calculations of Electrocatalytic and Nanocatalytic Phenomena

PI: Jeffrey Greeley (Center for Nanoscale Materials)

This work has focused on developing first principles-based electronic structure models of catalytic reactions in both electrochemical systems and on subnanometer metal clusters. Electrocatalysis lies at the heart of a large number of chemical and physical processes, with applications ranging from fuel cells to petrochemical processing to corrosion science. Although electrocatalysis has been experimentally studied for many years, the use of computational techniques to analyze electrocatalytic processes is a relatively recent development. These techniques, which generally involve the application of simple, yet powerful, thermodynamic corrections to standard density functional theory calculations, permit the treatment of electrochemical systems with only modestly more computational effort than is required for standard electronic structure analyses. The present research has used these techniques to analyze both ethanol electrooxidation on platinum catalysts and the production of hydrogen from methanol on subnanometer palladium clusters.

Two major topics of catalytic significance were examined during 2008. The first focused on the electrooxidation of ethanol on both smooth and stepped single crystal platinum surfaces. Although ethanol is widely used as a gasoline additive for internal combustion engines, a more efficient strategy to extract energy from this molecule would be to convert it directly to electricity in a low-temperature fuel cell. No existing fuel cell catalysts, however, are able to process ethanol with sufficient efficiency; and to develop improved catalysts, it is essential to first understand the fundamental reaction steps that occur on platinum, one of the best ethanol electrooxidation catalysts identified to date. To this end, we performed extensive first-principles calculations on both smooth Pt(111) surfaces and stepped Pt(211) surfaces to understand how ethanol will decompose and be oxidized in acidic fuel cell environments. The calculations indicate that ethanol electrooxidation on Pt(111) is a highly activated process until an electrode potential of at least 0.25 V vs. SHE is reached; at higher potentials, the ethanol is rapidly dehydrogenated to form CH_3CO, CH_2CO, and other products. However, on Pt(111), these dehydrogenated products are too stable to decompose further; neither C-C bond cleavage, nor reaction of the intermediates with water to form acetic acid or other partially oxidized products is thermodynamically or kinetically favorable. On Pt(211) steps, however, we have found that reaction of dehydrogenated intermediates with water to yield acetic acid is a much more energetically favorable process; we conclude, therefore, that experimentally observed acetic acid formation from ethanol must occur on these highly undercoordinated surface features.

The second area of inquiry has focused more on nonaqueous heterogeneous catalysis. We analyzed the production of hydrogen and other products from the partial oxidation of methanol on subnanometer Pd clusters; we modeled subnanometer clusters using four and eight palladium atoms. We performed a detailed analysis of the energetics and thermodynamics by calculating binding energies and reaction barriers associated with all possible adsorbates and coadsorbates. These calculations enabled us to develop a detailed picture of these complex reaction pathways at the atomic level. Two insights have emerged from this analysis. First, we found that carbon monoxide is significantly more stable on both Pd_4 and Pd_8 than any other intermediate in the reaction network; it is therefore highly likely that, at room temperature, CO will poison the surface of the catalyst, and much higher temperatures will be required to remove CO and H_2 from the Pd clusters. Second, we found that most energetic quantities (reaction energies and activation barriers) are not substantially different between Pd_4 and Pd_8. This result implies that, although

methanol decomposition may proceed differently on subnanometer clusters compared to bulk Pd surfaces, there are no significant differences in reactivity *between* Pd clusters of different sizes.

The first component of the project (ethanol electrooxidation) has contributed significantly to the interpretation of experimental electrochemical results in the literature, and it is possible that continued work in this area will, ultimately, lead to the design of improved catalytic materials for low-temperature, ethanol-based fuel cells. The work on the reaction of methanol on subnanometer Pd clusters has produced intriguing predictions about the expected chemistry of these systems and will be used to guide experimental efforts in this area (Fig. 5).

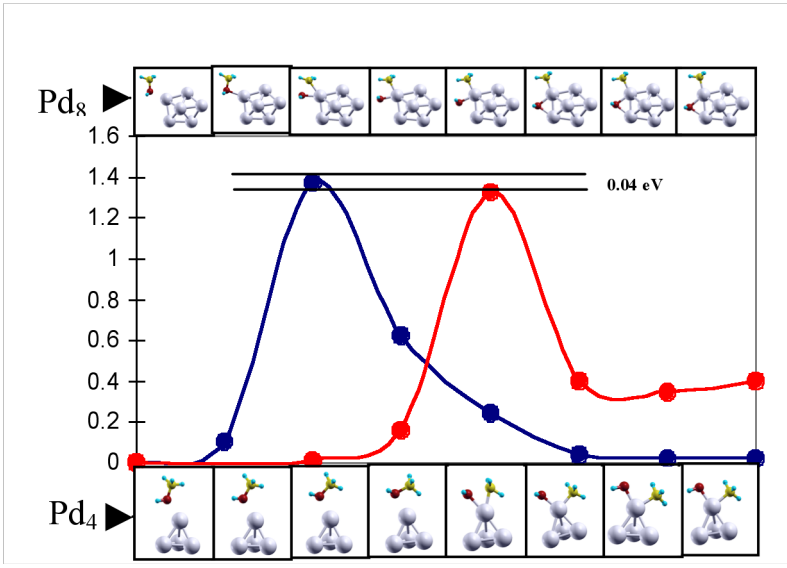


Figure 5. *Breaking of a C-O bond in methanol on Pd_4 and Pd_8 clusters. Although the length of the reaction pathway is different between the two clusters, the reaction barriers are nearly identical. Similar results for many other bond-breaking and bond-forming steps lead to the conclusion that methanol reactivity is similar on subnanometer clusters of different sizes.*

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P. Strasser, S. Koh, and J. Greeley, Phys. Chem. Chem. Phys., in press.

D. Strmcnik, D. Tripkovic, D. van der Vliet, K.C Chang, V. Komanicky, H. You, J. Greeley, V. Stamenkovic, and N. M. Markovic, "Unique Activity of Platinum Adislands in the CO Electrooxidation Reaction," J. Am. Chem. Soc., 130, no. 46 (2008) 15332-15339.

S. Vajda, M. Pellin, L. A. Curtiss, J. Greeley, C. Marshall, G. Ballentine, J. Elam, S. Mucherie, P. Redfern, and P. Zapol, Preprint, 2008.

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Kinetics of Enzymatic DNA Repair

PIs: Aaron Dinner (Department of Chemistry, University of Chicago) and Stuart Rice (Office of the Director)

Research on molecular recognition has focused largely on structural properties of molecules such as arrangements of functional groups. Examples of how nature uses collective dynamics to enhance specificity are now emerging and leading to a shift from a static to a dynamic perspective. Interpretation and rational design of experiments to probe these novel mechanisms require relating systems-level events to atomic-level ones and their associated changes in free energies. Computational tools for this purpose are being developed and applied to a paradigmatic system, the human protein O6-alkylguanine-DNA alkyltransferase (AGT).

AGT repairs modified guanine and thymine DNA bases by flipping nucleotides into its active site and transferring alkyl groups irreversibly to cysteine. Extensive biochemical and structural data available make it ideal for computational investigations. We have recently introduced means for efficiently characterizing collective dynamics automatically and initiating transition path sampling simulations. These methods are now being applied to AGT to understand the dynamics of sliding along DNA to compare directly with single-molecule experiments. The length of trajectories and the size of the system necessitate simulation in parallel.

Earlier simulations had revealed that the protein AGT flips damaged nucleotides for repair by a two-step process and had provided us with explicit pathways for each step and statistically meaningful descriptions of these pathways; key coordinates were identified to characterize the system. In 2008, we obtained free energy projections onto the key coordinates and diffusion tensors in these collective variables. These calculations enabled us to estimate the rates for nucleotide flipping and compare them with data from single-molecule experiments performed in collaboration with researchers at the University of Chicago. The studies revealed that DNA repair proteins can rapidly scan DNA sequences by partially flipping each base and then using kinetics to filter damaged bases from undamaged bases. This novel mechanism resolves the conundrum of how DNA repair proteins rapidly slide on DNA while still performing their function, which has been of substantial interest to the field.

We implemented a protocol for obtaining quantitative structure-property relationships in CHARMM. It comprises an artificial neural network for elucidating input-output relationships and a genetic algorithm for selecting between different input combinations to maximize the quality of the fit for a limited number of descriptors. This tool, which is useful also for drug design, was used to identify the key dynamic coordinates mentioned above. We also introduced an umbrella sampling method for obtaining nonequilibrium steady-state probability distributions projected onto an arbitrary number of coordinates that characterize a system (order parameters). We adapted the method to enable restricted sampling in the vicinity of a path in a many-dimensional space of collective coordinates. For the study of transitions between stable states, the adapted algorithm results in improved scaling with the number of collective coordinates and the ability to progressively refine the regions of enforced sampling. We have demonstrated the algorithm by applying it to a two-dimensional model of driven Brownian motion and a coarse-grained model for nucleation under shear. This work has the potential to open up a much larger range of application to path sampling than currently possible, which would have major impact on the study of systems far from equilibrium (Fig. 6).

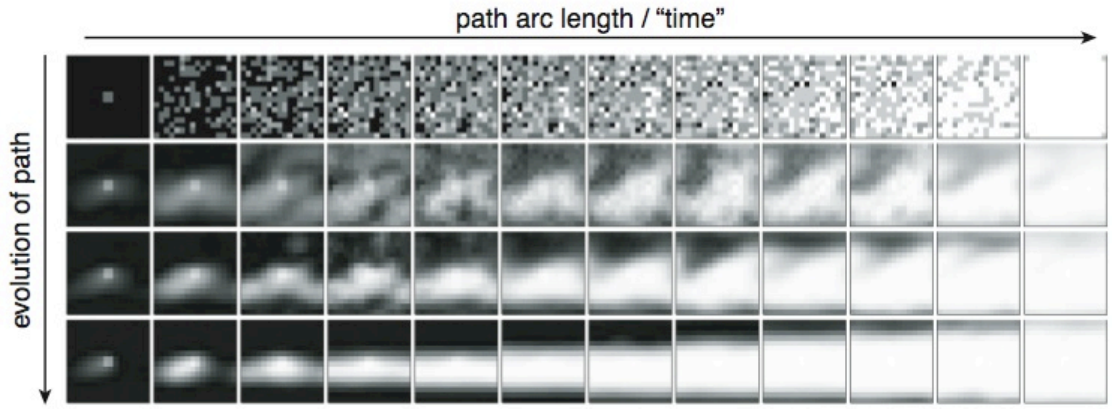

Figure 6. *Evolution of a path for a coarse-grained model of nucleation under shear. The brightness of each square is proportional to the density in that region. Each row comprises one path, and there are successive four snapshots. One can see that an initial linear interpolation in the space naturally approaches a nucleation mechanism in which there is a cluster of density that grows outward. Such a process could not be studied previously since the time for nucleation is prohibitively long in direct simulations.*

Publications and Presentations:

J. Hu, A. Ma, and A. R. Dinner, "A Two-Step Nucleotide-Flipping Mechanism Enables Kinetic Discrimination of DNA Lesions by AGT," Proc. Natl. Acad. Sci. USA, 105, 4615-4620, 2008.

A. R. Dinner, "Automated Analysis of Path Sampling Simulations Reveals a Mechanism for DNA Damage Detection," Gordon Research Conference on Computational Chemistry, Mt. Holyoke College, South Hadley, Massachusetts, July 2008.

A. R. Dinner, "Automated Analysis of Path Sampling Simulations Reveals a Two-Step Nucleotide-Flipping Mechanism for a DNA Repair Protein," Searching for Reaction Coordinates, Telluride, Colorado, June 2008.

A. R. Dinner, "Automated Analysis of Path Sampling Simulations Reveals a Two-Step Nucleotide-Flipping Mechanism for a DNA Repair Protein," Searching for Reaction Coordinates, American Chemical Society National Meeting, New Orleans, Louisiana, April 2008.

A. R. Dinner, "Automated Analysis of Path Sampling Simulations Reveals a Two-Step Nucleotide-Flipping Mechanism for a DNA Repair Protein," Mechanistic Analysis of Biological Systems with Novel Computational Models, Telluride, Colorado, March 2008.

A. R. Dinner, "Automated Analysis of Path Sampling Simulations Reveals a Two-Step Nucleotide-Flipping Mechanism for a DNA Repair Protein," Metastability and Rare Events, Erwin Schrodinger Institute, Vienna, Austria, February 2008.

A. R. Dinner, "Umbrella Sampling for Non-Equilibrium Processes," Condensed Phase Dynamics, Telluride, Colorado, July 2008.

A. R. Dinner, "Umbrella Sampling for Non-Equilibrium Processes," Metastability and Rare Events, Erwin Schrodinger Institute, Vienna, Austria, February 2008

Meson and Baryon Observables via Dyson-Schwinger Equations

PIs: Andreas Krassnigg and Craig Roberts (Physics)

This project deals with a nonperturbative continuum approach to QCD, the fundamental theory of the strong interaction between quarks and gluons. This approach uses coupled integral equations to calculate the basic building blocks, the Green functions – the propagators and vertices, of the theory.

A typical solution in our approach yields functions that describe quarks and hadrons on a common basis (in practice with the same quark-gluon interaction) such that the symmetries of the underlying theory are respected and their manifestations visible in the numerical results. This can be used to both illustrate exact results of the theory and identify unknown patterns. By describing quarks (the constituents) and hadrons as quark-antiquark or three-quark bound-states on the same footing, we can begin to reliably address one of the key questions of modern physics, namely, the mechanism behind confinement (this property means that no single quark or gluon has ever reached a detector).

The project's main directions are twofold. On the one hand, we investigate mesons and their excitations in order to study the long-range part of the strong interaction. This part of the interaction is not accessible with perturbative methods and requires a nonperturbative framework. On the other hand, we investigate the structure of nucleons by calculating properties such as their electroweak and strong form factors. These are key elements in our understanding of the nucleon and its structure. A manifestly Poincaré covariant approach such as ours is ideal to compute form factors and is essential on the domain of high momentum transfer that is probed with modern accelerators.

Meson Structure. In 2008 the meson code was restructured: Instead of using a 2D grid, the solution is now stored on a 1D complex contour, which reduces storage requirements, speeds the computation, and, together with a proper numerical setup, is now precise enough to compute properties of systems of bottom quarks. Moreover, the code was restructured to further optimize the speed of the computations. Using the Bethe-Salpeter equation, we completed a study of the full mass range for mesons from the chiral limit up to bottom in the rainbow-ladder truncation of QCD's Dyson-Schwinger equations. The meson mass spectrum, consisting of 8 states with J=0,1, including states with exotic quantum numbers for each quark mass, was tested with regard to the states' dependence on the long-range part of the strong interaction between the quark and the antiquark in the meson. Over the whole range, the pattern is the same: pseudoscalar and vector mesons show little or no dependence, while differences for others are large. The latter is even more pronounced in radial excitations, whose properties were also calculated. The interpretation is that, in addition to radial excitations, scalar and axial-vector mesons are also ideal candidates to study the long-range part of the strong interaction. While our results indicate that mesons with exotic quantum numbers also fall in this category, corrections to the present truncation will have to be included in the analysis to allow for robust statements. The meson calculations have shown that the Bethe-Salpeter-equation approach in our present form can be used to describe meson properties from the chiral limit of massless quarks up to and beyond the bottom-quark mass. Such a unified approach is important for a comprehensive understanding of meson physics, which is the medium-term goal of our studies (Fig. 7).

Nucleon Structure. We made further modifications to the nucleon code and therewith achieved a further order-of-magnitude increase in speed. This enabled us to use 10^8 adaptive Monte-Carlo sample points in evaluating the two-loop integrals that contribute to the nucleon's

electromagnetic form factors. The improved accuracy enabled a calculation of the current-quark-mass-dependence of the nucleon's magnetic moments. We used a Poincaré covariant Faddeev equation model for the dressed-quark core of the nucleon, augmented by a nucleon-photon vertex which automatically fulfills the Ward-Takahashi identity for on-shell nucleons and a rudimentary estimate of the contribution from pseudoscalar meson loops, to obtain insight into the response of the nucleons' static electromagnetic properties to changes in current-quark mass. Our results for the moments can assist in constraining the allowed temporal variation of the current-quark mass via, for example, experiments with atomic clocks and various astrophysical measurements. Our results also suggest that observables dependent on the nucleons' magnetic and charge radii might provide a useful means by which to place limits on the allowed variation in nature's fundamental parameters. It is notable, for example, that the calculated energy levels and transition frequencies in hydrogen and deuterium, which are some of the most precise theoretical predictions in physics, are quite sensitive to the value of the proton's charge radius. Moreover, all hyperfine transition frequencies in atomic clocks and astrophysics react to a change in nucleonic charge and magnetization distributions: the former alters electronic wave functions and the latter changes the hyperfine interaction Hamiltonian. As a byproduct of this study, we arrived at an improved understanding of diquark correlations. Within the nucleon they are usually far from being on-shell, and hence it is a poor approximation to represent, for example, the active magnetic properties of the axial-vector correlations by on-shell values. Our computations focus on various form factors of the nucleon. We aim to identify and isolate contributions from the quark core of the nucleon and quantify effects owing to pseudoscalar meson degrees of freedom. In this way we will connect the nonperturbative and perturbative domains of quantum chromodynamics.

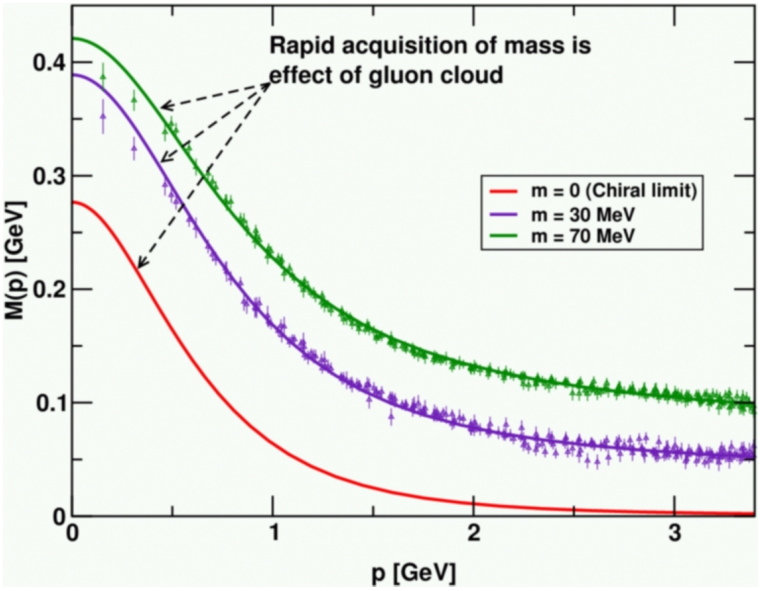

Figure 7. *Dressed-quark mass function, M(p): solid curves – DSE results; "data" – numerical simulations of unquenched lattice-QCD. In this figure one observes the current-quark of perturbative QCD evolving into a constituent-quark as its momentum becomes smaller. The constituent-quark mass arises from a cloud of low-momentum gluons attaching themselves to the current-quark. This is dynamical chiral symmetry breaking: an essentially nonperturbative effect that generates a quark mass "from nothing"; namely, it occurs even when the quark in the Standard Model Lagrangian is massless.*

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I. C. Cloet, A. Krassnigg, and C. D. Roberts, "Dynamics, Symmetries and Hadron Properties," Preprint, 2008.

M.S. Bhagwat, I.C. Cloet, C.D. Roberts, "Covariance, Dynamics and Symmetries, and Hadron Form Factors," Preprint, 2008.

C. D. Roberts, "Hadron Properties and Dyson-Schwinger Equations," Prog. Part.Nucl. Phys. 61:50-65, 2008.

I. C. Cloet, G. Eichmann, V. V. Flambaum, C. D. Roberts, M. S. Bhagwat, and A. Holl, "Current Quark Mass Dependence of Nucleon Magnetic Moments and Radii," Few Body Syst. 42:91-113, 2008.

C. D. Roberts, "Calculation of Parton Distribution Functions," invited talk given at the Workshop on Nonperturbative Aspects of Field Theories, Instituto de Fisica y Matematicas, Universidad Michoacana, Morelia, Michoacan, Mexico, November 5-6, 2007.

C. D. Roberts, "Hadron Physics and DSE Perspective," invited talk given at the XI Mexican Workshop on Particles and Fields, Tuxtla Gutierrez, Chiapas, Mexico, November 7-12, 2007.

C. D. Roberts, "Covariance, Dynamics and Symmetries, and Hadron Form Factors," Medium Energy Physics seminar given at Pittsburgh and CMU, Pittsburgh, April 17, 2008.

C. D. Roberts, "Gluing Together Constituent Quarks," seminar given at the Institute for Nuclear Structure and Astrophysics, University of Notre Dame, April 21, 2008.

C. D. Roberts, "Form Factors: A Dyson-Schwinger Equation Perspective," invited talk given at the Workshop on Hadron Electromagnetic Form Factors, ECT*, Trento, Italy, May 12-23, 2008.

C. D. Roberts, "Hadron Form Factors," invited talk given at the 2008 Annual Users' Group Meeting, JLab, Newport News, VA, June 16-18, 2008.

C. D. Roberts, "Modern Hadron Physics," Lecture Series (Zhongshan Forum) given at the Physics Department, Nanjing University, Nanjing, China, June 24-26, 2008.

C. D. Roberts, "Hadron Form Factors & DSEs," invited talk given at Light Cone 2008: Relativistic Nuclear and Particle Physics, European Physical Society Mulhouse, France, July 7-11, 2008.

C. D. Roberts, "Dyson-Schwinger Equations and QCD," Lecture Series given at the 25th Students Workshop on Electromagnetic Interactions, Bosen (Saar) Germany, August 31 - September 5, 2008.

C. D. Roberts, "Hadron Form Factors," Argonne Physics Division Seminar, Sept. 15, 2008.

I. C. Cloet, "Nucleon and Delta Form Factors in Covariant Quark-Diquark Theories," invited talk given at the Workshop on Hadron Electromagnetic Form Factors, ECT*, Trento, Italy, May 12-23, 2008.

A. Krassnigg, “The Bethe-Salpeter Equation Applied to Meson Studies in QCD,” seminar given at the Theoretical Physics Department of the University of Zagreb, Zagreb, Croatia, November 16, 2007.

A. Krassnigg, “Bethe-Salpeter Equation Studies of Mesons: Recent Progress and Challenges,” invited talk given at the Workshop on Non-Perturbative Functional Methods in Quantum Field Theory, Heviz, Hungary, January 24, 2008.

A. Krassnigg, “Meson Spectroscopy from the Bethe-Salpeter Equation,” talk given at the 415th Wilhelm & Else Heraeus Seminar Quarks and Hadrons in Strong QCD, Schloss Rheinfels, St. Goar, Germany, March 17, 2008.

A. Krassnigg, “Mesons from QCD,” seminar given at the Department of Physics, Kent State University, Kent, Ohio, April 3, 2008.

A. Krassnigg, “Toward a Complete Study of Mesons with the Bethe-Salpeter Equation,” seminar given at Physics Division, Argonne, April 8, 2008.

A. Krassnigg, “A Bethe-Salpeter-Equation View of Pion Electromagnetic Properties,” invited talk given at the Workshop on Hadron Electromagnetic Form Factors, ECT*, Trento, Italy, May 12-23, 2008.

A. Krassnigg, “Excited Mesons in a Bethe-Salpeter Approach,” talk given at Confinement8 (Quark Confinement and the Hadron Spectrum), Mainz, Germany, September 3, 2008.

A. Krassnigg, “Light and Heavy Mesons from a Bethe-Salpeter-Equation Study,” talk given at the Symposium Approaches to Quantum Chromodynamics, Oberwoelz, Austria, September 9, 2008.

Grants:
A. Krassnigg: FWF (Austrian Research Fund) project P20496 (duration 3 years, project sum 292.000 Euro), Meson Resonances in a Dyson-Schwinger Approach

Computational Electromagnetics

PI: Misun Min (Mathematics and Computer Science)

We develop algorithms and software for solving computational nanoscience problems and accelerator modeling on high-performance architectures. Highly accurate, fast numerical algorithms and design of scalable code are essential for solving surface-enhanced scattering features near the metal surface at nanoscale and wake field calculations for accelerating components. Such problems are relevant to many aspects of nanoscience technology and accelerator design. We have implemented a high-performance electromagetics code, NekCEM, which is based on high-order methods using spectral elements.

During 2008 we built 3D nanohole and bowtie meshes and carried out time-averaged electric field calculations for various sizes of periodicities in the square and hexagonal lattice at nanoscale. We also implemented a moving window mesh in parallel. One can reduce the full domain simulation time proportional to moving window length for wake field and wake potential

calculations for accelerating components. Figure 8 shows simulations of various nanostructures in 3D. Our study shows that the high-order numerical code NekCEM represents the material surface accurately and resolve the electromagnetic field efficiently using fewer grid points per wavelength than conventional methods (conventional methods do not capture reasonable profiles even using large number of grids due to slow convergence and errors with non material-conforming grids).

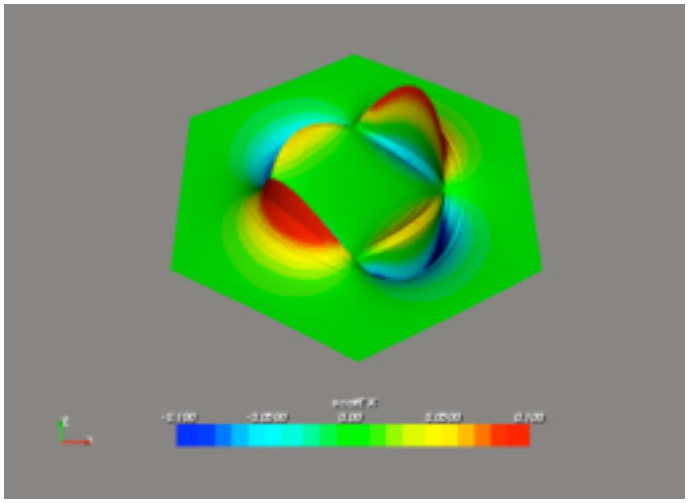


Figure 8. *Electric field profile for 3D nanohole simulations on a unit-cell for hex-lattice (left); Electric field z-component on x-z plane (right).*

We carried out convergence and performance tests for NekCEM on Jazz. Figure 9 shows that the computational cost is not dependent on the approximation order N but increases linearly proportional to the total number of grids. The errors drop dramatically with higher approximation order N for a fixed amount of grid points.

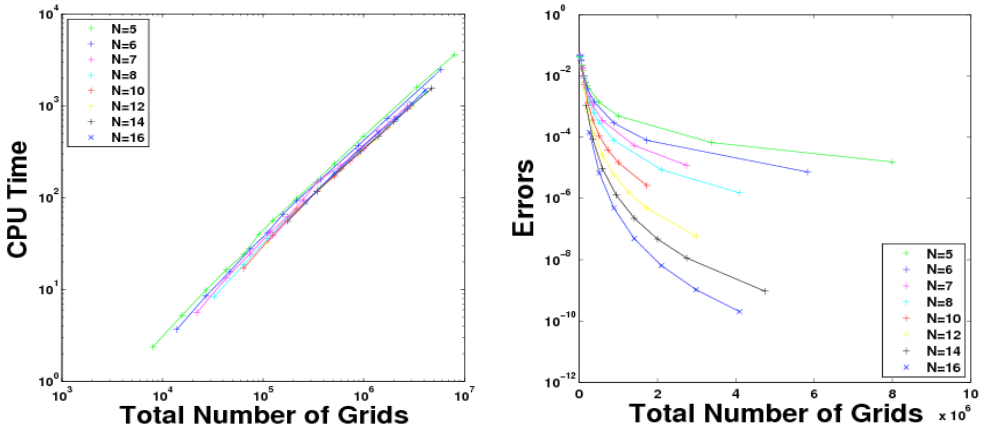


Figure 9. *Convergence and performance tests on Jazz with 32 processors. Left: CPU time; right: accuracies for approximation order N=5-16 with total number of grids.*

Grant:
Misun Min, "New Framework for Electromagnetic Simulations on Exascale Supercomputers," LDRD Strategic grant for 2009.

Earth System Modeling Framework

PIs: Jay Larson and Rob Jacob (Mathematics and Computer Science)

The goal of the Earth System Modeling Framework (ESMF) project is to build high-performance, flexible software infrastructure to increase ease of use, performance portability, interoperability, and reuse in climate, numerical weather prediction, data assimilation, and other Earth science applications. We are aiming to create a framework usable by individual researchers as well as major operational and research centers.

The ESMF hierarchical, component-based architecture facilitates the systematic construction of complex climate and weather applications and the interoperability of model components. ESMF also offers application developers an extensive toolkit for standard modeling functions such as grid transformations, data communication, logging, and calendar management.

This year we delivered new grid structures, including unstructured meshes and observational data streams. These were integrated into the framework so that data fields can be built on either of these, as well as logically rectangular grids. We also delivered an online, parallel regridding capability that can perform grid-grid, grid-mesh, and mesh-mesh transformations. Performance of the sparse matrix multiply was assessed to 16,000 processors. We used Jazz to run exhaustive nightly unit and system tests and examples, taking advantage of the assortment of Jazz compilers. These tests were instrumental in ensuring that the ESMF software was robust and portable. We also used Jazz as a development platform.

ESMF is in production use at NASA GMAO, NRL, and NCEP, and is in the process of being evaluated and adopted by many other groups across the country, including the U.S. Air Force Weather Agency, U.S. Army, the Community Climate System Model (CCSM), GFDL, MIT, and the Weather Research and Forecast (WRF) model. Widespread use of ESMF represents a paradigm shift in the way weather and climate models are constructed. Through increased code interoperability, community building, and standard tools, ESMF is beginning to make model development easier and to facilitate new, multi-agency science collaborations. The end result is an Earth science community better equipped to explore basic research issues and better equipped to answer questions about the impacts of Earth science on society.

Publications and Presentations:
Reports are available at http://www.esmf.ucar.edu/metrics/performance

S. Klasky, J. Loftstead, and M. Vouk, "End to End Scientific Data Management Framework for Petascale Science," JST Telecon, September 23, 2008. (Download PowerPoint file)
http://www.esmf.ucar.edu/presentations/pres_0809_klasky.ppt

P. Li, "Preparing for the Petascale: ESMF Scalability Benchmark," 7th Annual ESMF Community Meeting, Ft. Lauderdale, FL, May 28-30, 2008 (Download PDF)
http://www.esmf.ucar.edu/presentations/pres_0805_peggy.pdf

S. Murphy, "Application of RDF-OWL in the ESG Ontology," GO-ESSP Meeting, Seattle, WA, September 18, 2008. (Download PowerPoint file)
http://www.esmf.ucar.edu/presentations/pres_0809_go_essp_murphy.ppt

R. Dunlap, "The Earth System Curator: Metadata Infrastructure for Climate Modeling," 2008 SIParCS Final Presentation, Boulder, CO, August 4, 2008. (Download PowerPoint file) http://www.esmf.ucar.edu/presentations/pres_0808_rocky.ppt

S. Murphy, "Curator," NCAR ASP Dynamical Cores Summer Colloquium, Boulder, CO, June 1-13, 2008. (Download PowerPoint file) http://www.esmf.ucar.edu/presentations/pres_0806_dycore_workshop.ppt

S. Murphy, "Metadata Support for Model Intercomparison Projects," 13th Annual CCSM Workshop, Breckenridge, CO, June 17-19, 2008. (Download PowerPoint file) http://www.esmf.ucar.edu/presentations/pres_0806_curator_at_ccsm.ppt

S. Murphy, "Documenting and Comparing Models Using Earth System Curator," 7th Annual ESMF Community Meeting, Ft. Lauderdale, FL, May 28-30, 2008 (Download PowerPoint file) http://www.esmf.ucar.edu/presentations/pres_0805_curator_at_esmf.ppt

S. Murphy, "ESMF Usability and Training," BEI Meeting, Boulder, CO, May 7, 2008 (Download PowerPoint file) http://www.esmf.ucar.edu/presentations/pres_0805_bei_train.ppt

D. Neckels, "Parallel Rendezvous Regridding in ESMF," SIAM Parallel Processing, Atlanta, GA, March 12, 2008 (Download PDF) http://www.esmf.ucar.edu/presentations/pres_0803_neckels.pdf

G. Theurich, "ESMP Development Update," ESMF Core Team, May 28-30, 2008 (Download PDF) http://www.esmf.ucar.edu/presentations/pres_0805_gerhard.pdf

G. Theurich, "Direct Coupling in ESMF," April 3, 2008 (Download PDF) http://www.esmf.ucar.edu/presentations/pres_0804_directcoupling.pdf

Computed Tomography

PI: Eugene Koehl (Nuclear Engineering)

The Non-Destructive Evaluation group of the Nuclear Engineering Division, System Technologies and Diagnostics department, uses x-ray imaging technology to investigate the internal structural and flaw morphology of metal and nonmetal components. The components may comprise metals or earthen elements such as those found in archaeological artifacts, metal-ceramic matrix, ceramic or carbon, and their fiber composites such as those found in aircraft wings and fuel cells, or a mixture of low- and high-density metals such as those found in low-enrichment fuel plates. Many of these components are under development and in use in aerospace, power generation, and transportation industries. We are seeking to develop, refine, and expand our tomographic image reconstruction capabilities to (1) operate on massive datasets obtained from 16-bit, large area, flat-plate detectors; (2) operate on data from 16-bit, high-resolution, linear x-ray detector arrays comprising thousands of elements arranged in a single row; (3) identify and reduce software bottlenecks and improve code efficiency; (4) apply lessons

learned to in-house systems; and (5) obtain volumetric imaging in near real time (e.g., 8-inch diameter volume at 200 micron resolution, reconstructed and displayed within 15 minutes).

The goal of the FastCTdev project is to render and display the details of a 10-inch, 3D volume dataset with 150–175 micron resolution from a series of 2D x-ray projections within 30 minutes of acquisition. We have been working on imaging higher-density (greater the 3–4 g/cc) materials. The project supports the development of nondestructive and analytical techniques employed in the examination of rare archeological and hard to obtain geological samples, and one-of-a-kind prototype engineering designs. The Jazz cluster is the only system to which we have access that can accommodate and manipulate the very large datasets that make up the output of our x-ray CT systems. In some cases these datasets exceed 20 GB. In most cases, the Jazz system provides near real-time visualization of these complex components. In others, it reduces to hours or days what would have required weeks to months to compute on stand-alone, single-, and multiprocessor workstations.

Publications and Presentations:
The Jazz system has been used to display data from a prototype aluminum casting processes, Eurasian archeological and American geological samples, NASA shuttle components for the "Back To Flight" program in 2005 (STS-114), military body and vehicle armor, turbine blades and rotors and combustor liners for stationary and mobile power systems, and prototype fuel cells. The results from these efforts are proprietary to the companies developing the sample fabrication process. Images have not been released to the public domain.

Fast Ocean Atmosphere Model

PI: Rob Jacob (Mathematics and Computer Science)

The goal of the FOAM project is to maintain a fully coupled climate model that puts an emphasis on high throughput as measured in simulated years per day. Like most climate models, FOAM is composed of separately developed pieces, many developed by other groups. The atmosphere model, PCCM3, contains two numerical methods: a spectral transform scheme for the dry dynamics and a semi-Lagrangian transport scheme for moisture. Both methods have been parallelized with a two-dimensional decomposition of the horizontal dimension. The physics, which refers to all the parameterizations of factors such as radiation and convection, is done entirely within a vertical column and so parallelizes trivially with the dynamics. The ocean model, Om3, uses a finite-difference method with explicit subcycled time stepping. It also has a 2D parallel data decomposition and does the small amount of ocean physics in columns.
The other pieces of FOAM include a land model (which contains no dynamics and can be thought of as an extension of the atmosphere column physics) and a sea ice model. The pieces are integrated into a single system with a special-purpose coupler.

Using lower resolution and simplified physics FOAM can simulate 100 years of interaction between the atmosphere, ocean, land surface and sea ice in one day using 64 processors of Jazz.

We are using FOAM to understand the processes that control the climate on geologic time scales. On that time scale, the level of CO2 in the atmosphere is controlled by volcanism (the source) and silicate weathering (the sink). We use FOAM to find the mean precipitation and river runoff for various times in the Earth's history. The output from FOAM becomes the forcing for a model called GEOCLIM that can calculate the atmosphere's CO2 concentration in response to this forcing. In a paper published in G-cubed, we have showed that the break up of the Pangea supercontinent triggers an increase in continental runoff, resulting in enhanced atmospheric CO_2 consumption through silicate weathering. As a result, atmospheric CO_2 falls from values above 3000 ppmv during the Triassic, down to rather low levels during the Cretaceous (~400 ppmv), resulting in a decrease in global mean annual continental temperatures from about 20°C to 10°C.

We found that accounting for the climatic role of the continental vegetation dynamics (albedo change, water cycle, and surface roughness modulations) strongly affects the reconstructed geological climate. Indeed the calculated partial pressure of atmospheric CO_2 over the Mesozoic is twice the value calculated when assuming a uniform constant vegetation. This increase in CO_2 is triggered by a global cooling of the continents, itself triggered by a general increase in continental albedo owing to the development of desert surfaces. This cooling reduces the CO_2 consumption through silicate weathering, and hence results in a compensating increase in the atmospheric CO_2 pressure.

Jazz was used to develop and test this new model that includes vegetation effects.
In 2008, thanks to a collaborative work through a shared student between the University of Chicago and the French Research Agency, we developed and used FOAM with a new interactive component: land vegetation, simulated by the LPJ model. All tests of this new coupling were performed on the Jazz computational facilities.

This study demonstrates that the impact of land plants on climate and hence on atmospheric CO_2 is as important as their geochemical effect through the enhancement of chemical weathering of the continental surface. Our simulations also define a climatic baseline for the Mesozoic, around which exceptionally cool and warm events can be identified (see Fig. 10).

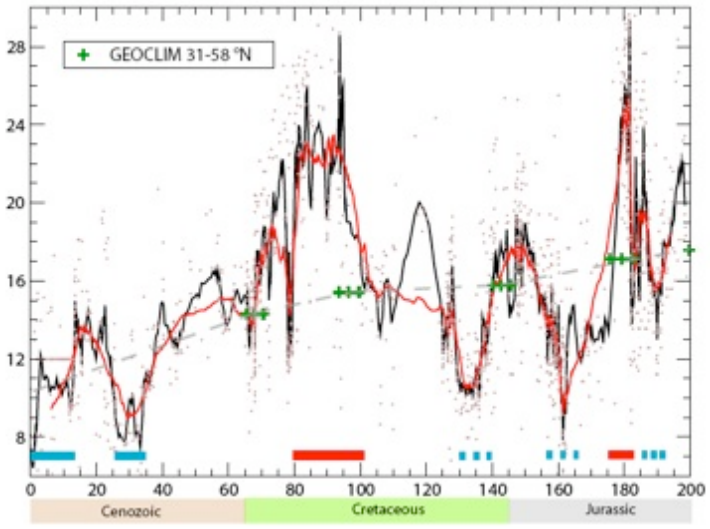


Figure 10. *Northern mid-latitudes sea surface temperature estimates from the 18O database published by Prokoph et al. (2008) using the palaeothermometer of Kim and O'Neil (1997) and a sea water 18O of -1. The brown points are the original data, the black curve represents a 2 Myr time-window running average*

and the red curve represents a 5 Myr time-window running average. Green crosses show the temperature of the northern mid-latitudes as simulated by GEOCLIM-FOAM-LPJ.

Publications and Presentations:

Y. Goddéris, Y. Donnadieu, C. De Vargas, R. Pierrehumbert, G. Dromart, and B. van de Schootbrugge, "Causal or Casual Link between the Rise of Nanoplankton Calcification and the Tectonically-driven Massive Decrease in Late Triassic Atmospheric CO_2," Earth and Planetary Science Letters, 267, 247-255, 2008.

Y. Goddéris, Y. Donnadieu, M. Tombozafi, and C. Dessert, "Shield Effect on Continental Weathering: Implication for Climatic Evolution of the Earth at the Geological Timescale," *Geoderma*, **145**, 439-448, 2008.

G. Lehir, Y. Donnadieu**,** Y. Goddéris, R. T. Pierrehumbert, M. Macouin, G. P. Halverson, A. Nédélec, and G. Ramstein, "The Snowball Earth Aftermath: Exploring the Limits of Continental Weathering Processes," Earth and Planetary Science Letters, accepted.

Y. Donnadieu, Y. Goddéris, and N. Bouttes, "Exploring the Climatic Impact of the Continental Vegetation on the Mezosoic Atmospheric CO_2 and Climate History," Clim. Past Discuss., 4, 1021-1045, 2008.

Advanced Plasma Applications

PIs: Tatyana Sizyuk and Vitali Morozov (Mathematics and Computer Science)

Next-generation lithography devices require the production of extreme ultraviolet (EUV) photons. The photons can be generated by several methods: discharge-produced plasma (DPP), laser-produced plasma (LPP), and synchrotron radiation. In order to meet the Intel Lithography Roadmap goals for high-volume manufacturing and SEMATECH's EUV Source Program goal, the EUV source must have power exceeding 200 W at a wavelength of 13.5 nm. The conversion efficiency of the EUV radiation is important in the successful development of the source. Many factors influence the efficiency, such as the plasma material, form and size of the radiated area, and amount of debris generated. Only computer modeling can generate a complete picture of EUV devices in a reasonable time and cost. To this end we have developed the HEIGHTS computer package to simulate the full cycle of plasma evolution in LPP and DPP devices. In our simulations we investigated parameters of laser-prepared plasma for the optimal discharge stage performance. Laser heating stage of hybrid device should prepare low-temperature homogeneous plasma for an effective start of the discharge and optimum pinching as a result (Fig. 11).

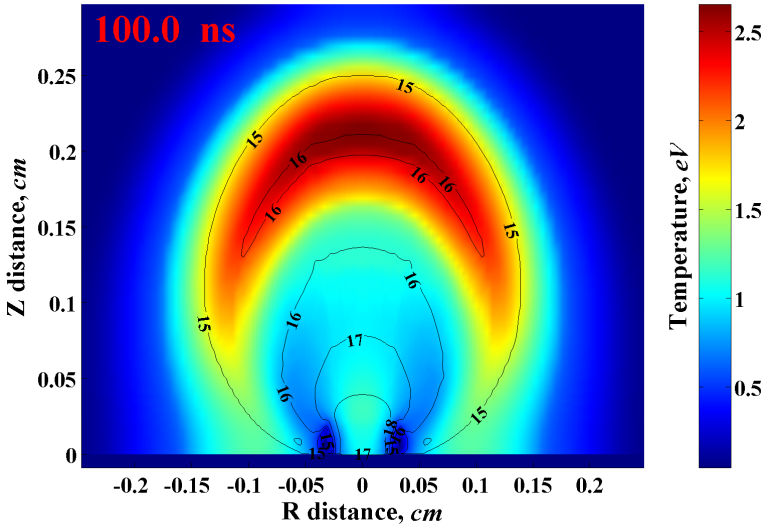


Figure 11. *Typical plasma electron density and temperature directly before the discharge start.*

We also carried out numerical experiments of self-confined plasma in a hollow beam configuration (Fig. 12).

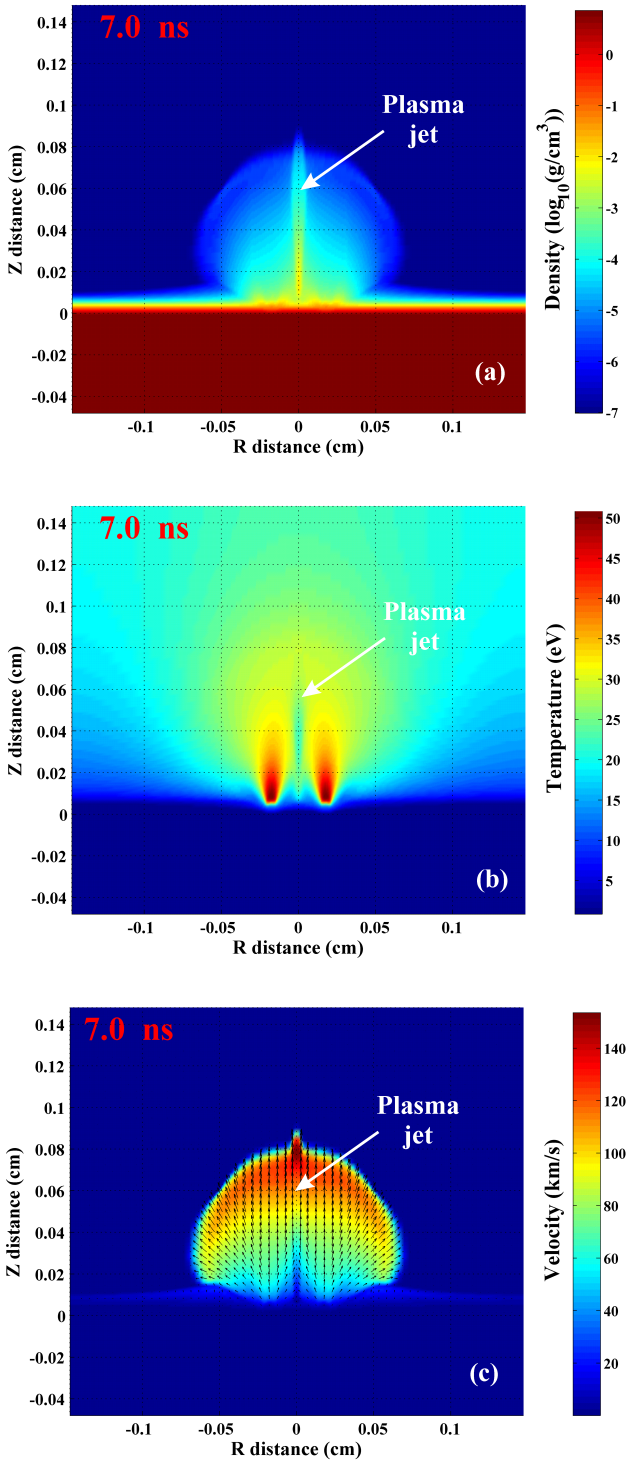


Figure 12. *Tin plasma distributions at 7.0 ns in z-r plane for hollow laser beam (laser energy, 300 mJ; wavelength, 1064 nm; ξ = 0.7): density (top), temperature (middle), and velocity (bottom).*

Publications and Presentations:
V. Sizyuk, A. Hassanein, and T. Sizyuk, "Hollow Laser Self-Confined Plasma for Extreme Ultraviolet Lithography and Other Applications," Laser and Particle Beams, 25, no. 2, pp. 143-154, 2007.

A. Hassanein, V. Sizyuk and T. Sizyuk, "Multidimensional Simulation and Optimization of Hybrid Laser and Discharge Plasma Devices for EUV Lithography," in Proc. SPIE. Emerging Lithographic Technologies XII, San Jose, CA, vol. 6921, p. 692113-1, SPIE, Bellingham, WA, 2008.

Validation of Neutronics Tools for Advanced Burner Reactor Design

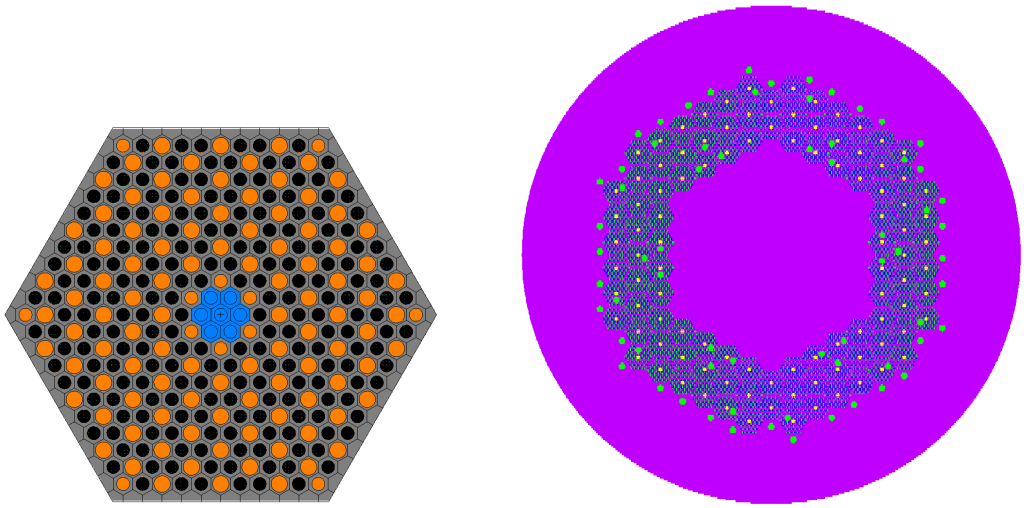
PI: Taek K. Kim (Nuclear Engineering)

The very high-temperature gas-cooled reactor (VHTR) is an important element in DOE's program to revitalize nuclear power in the U.S. suite of energy generation options. Current plans are to build the first VHTR, so-called the Next Generation Nuclear Plant (NGNP), in the near future. Under the NGNP program researchers have been developing computational tools. To ensure confidence in the NGNP design, we are validating these new computational tools.

As a first step, we developed the prismatic fuel assembly and whole core models for the Monte Carlo code MCNP5 and the Monte Carlo depletion code MONTEBURN. Using these codes, we performed runs on Jazz. Figure 13 shows the assembly and core models for the MCNP5 calculations. In Table 1, the results of the lattice codes, DRAGON and WIMS (considered the lattice code systems in the NGNP program) were compared with the MCNP5 results, which are considered as the reference solutions. The results of lattice code show about 0.5% difference from the reference solutions as the result of strong double heterogeneity effects and the base cross-section libraries used by the MCNP5 and lattice codes.

Table 1 Comparison of Deterministic and Monte Carlo Results

	Assembly Types (Fuel type)		
	New NGNP (UCO)	Old NGNP (UCO)	GT-MHR (TRU)
Eigenvalue			
MCNP5	1.54400 ± 0.00118	1.53280 ± 0.00082	1.25838 ± 0.00040
DRAGON		1.54393	1.26794
WIMS8/9	1.53796	1.52993	1.25326
Double heterogeneity effect			
MCNP5	2.8%	2.3%	13.1%
DRAGON		2.9%	13.1%
WIMS8	2.7%	2.7%	12.9%



Assembly model Whole core model

Figure 13. *Assembly and whole core models.*

CO Hydrogenation with Co Carbonyl Catalysts

PIs: Randall Meyer (University of Illinois at Chicago), Jerry Rathke and Robert Klingler (Chemical Sciences and Engineering)

The rapid depletion of oil necessitates the discovery and development of new ways to make other potential energy sources viable. One such process is the Fischer-Tropsch catalytic process to take syn-gas, a mixture of CO and hydrogen produced from coal, to make higher molecular weight hydrocarbons of greater value such as those used for diesel fuels. Unfortunately, the mechanisms and surface intermediates of Fischer-Tropsch catalysis are not well understood. Therefore, as a first step to develop improved Fischer Tropsch catalysts with a high selectivity to particular products, we have chosen to examine a homogeneous analog, $HCo(CO)_4$. If the reaction pathways for the homogeneous catalyst can be precisely identified and if the factors that influence the catalyst's selectivity can be understood, then this knowledge can be used to aid in the design of new heterogeneous Fischer-Tropsch catalysts.

The primary aim of our work is to test various hypotheses for the mechanisms in an effort to understand how to improve selectivity of these catalysts. During the past year, we identified transition states for the isomerization of the formaldehyde intermediate into either the methoxy intermediate or the hydromethyl intermediate. The barrier for hydroxymethyl formation was found to be 0.73 eV, whereas the barrier to the methoxy intermediate, which results in methyl formate production, was found to be only 0.32 eV (Fig. 14).

Calculations of vibrational frequencies of all molecules and intermediates in the cycle allow us also to take our results from density functional theory and develop a free energy diagram in additional to a simple zero Kelvin internal energy diagram. The calculations have definitively identified the overall reaction barrier to CO hydrogenation with good agreement with experiment. Furthermore, the results explain why methyl formate formation is favored when the reaction is operated in supercritical CO or CO_2. The calculations give some guidance as to the rate-limiting step in the process and therefore some path for catalyst improvement.

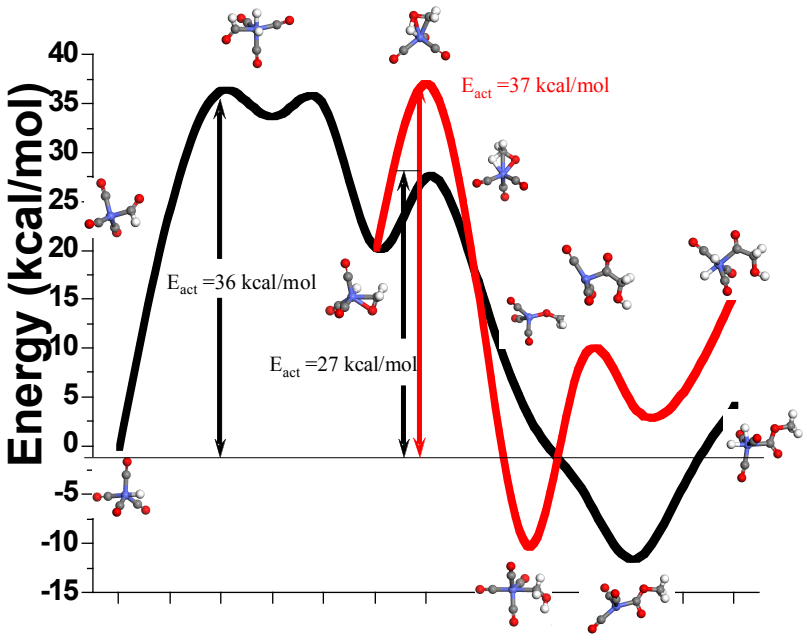


Figure 14. *Potential energy diagram showing formation of the methoxy and hydroxymethyl intermediates. The overall barrier for the methoxy route, which leads to methyl formate production, is favored over the hydroxymethyl intermediate, which leads to ethylene glycol.*

Publications and Presentations:
R. Meyer, R. J. Klingler, and J. Rathke, "A Combined Theoretical and Experimental Study of CO Hydrogenation with $HCo(CO)_4$ Catalysts," presented at the AIChE (American Institute of Chemical Engineers) annual meeting, Salt Lake City, UT, November 4-9, 2007.

End-to-End Simulation of the ILC Positron Source

PI: Wanming Liu (High Energy Physics)

The International Linear Collider (ILC) is the highest-priority project for the world high-energy physics communities. One of the key components of ILC is the positron source. A leading candidate positron source is a gamma-ray-based scheme; however, no detailed study of the

positron source has been done. The purpose of our research is to develop a complete model for the ILC positron source and a commissioning strategy for the ILC.

During the short time of this project in 2008 before the U.S. budget was reduced, we were able to obtain new results regarding the emittance evolution of drive electron beams passing through the ILC undulators. The results show that the emittance of drive electron beams gets damped instead of growing as a result of radiation of photons. We also confirmed the theory behind this damping effect.

Publications and Presentations:
Wei Gai, "Emittance Growth of the Drive Beam through Undulator and Effects of Mis-alignments," presented at the ILC Positron Source Collaboration Meeting at DESY, Zeuthen

Lattice Quantum Chromodynamics

PI: Donald Sinclair (High Energy Physics)

We are studying quantum chromodynamics (QCD), the accepted theory of the strong (nuclear) interactions, at finite temperature and baryon-number density. This describes the hot dense nuclear matter produced at relativistic heavy-ion colliders at BNL, CERN, and GSI. In particular, we study the transition from nuclear matter to a quark-gluon plasma. In the regime probed by these high-energy heavy-ion machines, the most interesting feature of the phase diagram proposed by the community is a critical endpoint where the transition changes from a smooth (although abrupt) crossover to a first-order phase transition. Theoretically such simulations give information about the phase diagram for QCD at finite temperature and density. They also help in our understanding of the dynamics of QCD, including confinement and chiral symmetry breaking.

We are using lattice QCD simulations to study the crossover from nuclear matter to a quark-gluon plasma. At finite baryon-number density there is a sign problem that prevents direct simulations. To avoid this, we have adopted the phase-quenched approximation, which uses only the magnitude of the complex fermion determinant. Model calculations suggest that such an approximation preserves the interesting physics for small densities. In addition, we are using our simulation techniques to obtain the equation-of-state of nuclear matter, which is needed for the description of the evolution of the final state after a relativistic heavy-ion collision.

Using Jazz, we have been able to demonstrate as incorrect the suggestion that the critical endpoint for three quark flavours is directly connected with a similar critical point observed at zero density when the quark mass is varied. Our simulations appear to rule out a critical endpoint for low density (quark-number chemical potential less than half the pion mass). These conclusions are in accord with those obtained by others, using analytic continuation methods. Thee results mean that the critical endpoint is outside of the range of the highest energy heavy-ion colliders (RHIC and the heavy-ion program at the LHC), and is more likely to be seen at lower energy machines (GSI/SIS and possible lower energy runs at RHIC).

We are now performing more extensive simulations to obtain the equation-of-state for hot nuclear matter, Jazz is being used to calculate the zero temperature subtractions required for the calculation of the pressure; we use other high-performance computers to concentrate on the finite temperature and density simulations and on the application of reweighting techniques. Jazz has been particularly helpful as DOE and NSF supercomputer centers give precedence to applications requiring large numbers of processors (typically > 1000).

Publications and Presentations:

J. B. Kogut and D. K. Sinclair, "Lattice QCD at Finite Temperature and Density in the Phase-Quenched Approximation," Phys. Rev. D77, 114503 (2008), [arXiv:0712.2625 [hep-lat]].

D. K. Sinclair and J. B. Kogut, "Phase Quenched Lattice QCD at Finite Density and Temperature," PoS LAT2007, 225 (2007) [arXiv:0709.2367 [hep-lat]].

"QCD in Extreme Conditions," presented an invited talk at the Laboratori Nazionali di Frascati dell' INFN, Frascati, Italy, August 6-8, 2007.

Grants:

1. ERCAP grant for allocation at NERSC

2. NRAC grant for allocations at NSF supercomputing centers (NCSA, PSC)

3. JTI grant (with Roberts, Wagner, and Zachos of Argonne and Harvey, Kutasov, and Wagner of Chicago)

Monte Carlo Characterization of Accelerator-Driven Subcritical Facilities

PI: Yousry Gohar (Nuclear Engineering)

Accelerator-driven subcritical assemblies are under consideration for incinerating nuclear waste from nuclear power reactors. Consequently, studies and experiments are performed to define its kinetics parameters. MUSE and YALINA are example for such experiments. The MUSE experiments were carried out at the MASURCA facility (Cadarache, France), where a fast subcritical core has been driven by an external neutron source from (deuterium-deuterium) or (deuterium-tritium) reactions. The goals were to validate the computational tools and to investigate methods and techniques for measuring the kinetic parameters of subcritical assemblies. The YALINA-booster experiments have similar neutron sources driving its subcritical assembly. However, the YALINA subcritical assembly has fast and thermal zones with a thermal absorber zone in-between. The coupling between the two zones is done only with fast neutrons. The geometrical model used for performing the analyses is shown in Figure 15. In this work, the experimental results from the YALINA facility of Belarus are compared with the Monte Carlo results using – for the first time – a high-fidelity computational method.

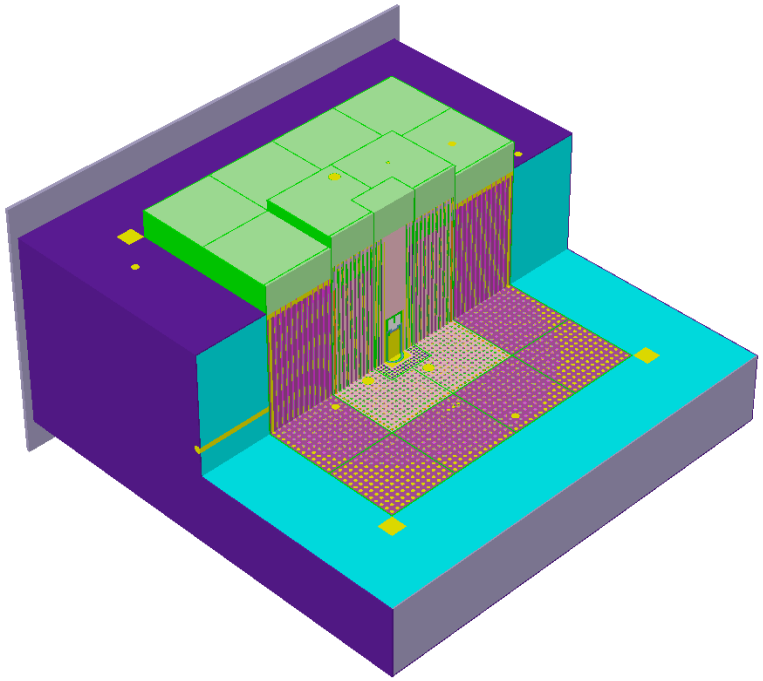


Figure 15. *YALINA-booster geometrical model.*

One of the most reliable experimental methods for measuring the kinetic parameters of a subcritical assembly is the Sjöstrand method applied to the reaction rate generated from a pulsed neutron source. The Sjöstrand method requires the time period of the neutron source to be much shorter than the delayed neutron precursor half-life (the shortest half-life of the precursor families is 179 ms for ^{235}U) and much longer than the prompt neutron lifetime (~0.1 ms). Under these conditions, prompt fission neutrons contribute only to their pulse in which they are generated, whereas delayed neutrons contribute to the pulse in which they are generated and many successive pulses. The delayed neutrons from a specific pulse contribute for about 200-300 seconds after the pulse since the longest decay half-life of the precursor families is 54.51 seconds for ^{235}U.

To date, the published results for simulating the detector response in the subcritical assembly from a pulsed neutron source neglect the effect of the delayed neutrons from the previous pulses. In these simulations, the detector response is calculated due to a single neutron pulse, and these simulations cannot predict the detector response due to repeated neutron pulse operation. In the present work, a new computational method was developed to simulate the repeated neuron pulse operation so the Sjöstrand method measurements can be compared with the analytical results as a function of time for the first time ever. The method is based on the simulation of a single pulse over a long time period till the delayed neutron contribution to the detector is vanished. The obtained detector response is superimposed to itself simulating the repeated pulse operation with respect to the time until the asymptotic level of the reaction rate, set by the delayed neutrons, is achieved. The detector reaction rate as answer to a single pulse can be calculated with great accuracy by the MCNP/MCNPX computer codes without any geometry homogenization of the facility.

This new simulation method predicts correctly the experimental results using the Sjöstrand method, and it can be extended to simulate accurately the kinetics measurements using other experimental methods. In fact, this method can also be applied to a modulated or random pulsed neutron source. The pulse superimposition can be done with different frequencies and amplitudes. Consequently, the pulse superimposition method can also validate analytical theories from general reactor physics for evaluating the kinetics parameters. The results are shown in Figure 16, where excellent agreement was obtained.

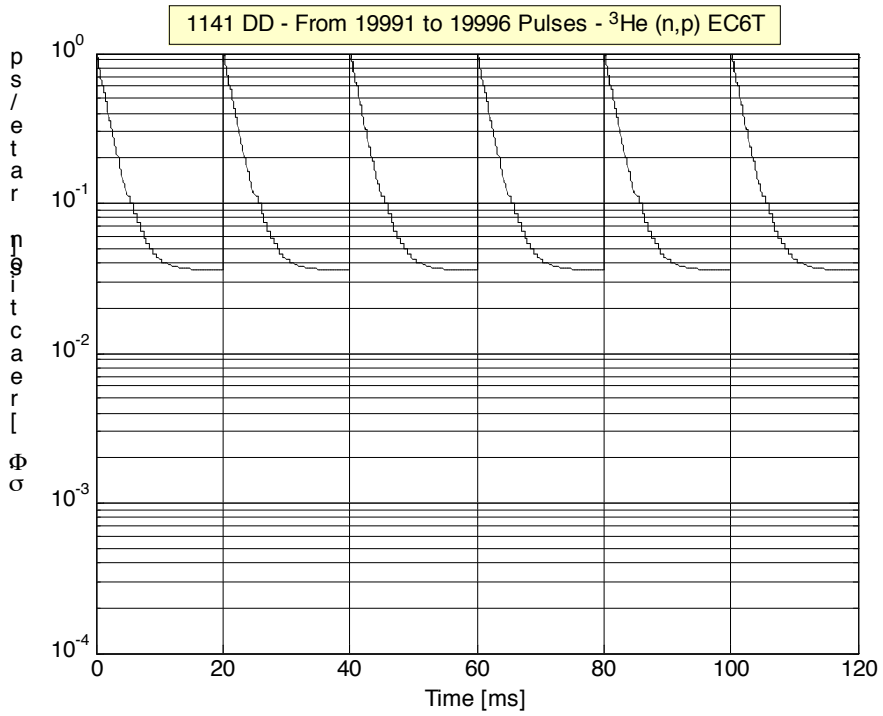


Figure 16. *^{3}He(n,p) reaction rate calculated for 6 successive deuterium-deuterium neutron pulses starting from pulse number 19991 for the YALINA-booster configuration.*

Publications and Presentations:

Alberto Talamo, Yousry Gohar, Filip Kondev, Hanna Kiyavitskaya, Ivan Serafimovich, Victor Bournos, Yury Fokov, Christina Routkovskaya, "Modeling of the YALINA Booster Facility by the Monte Carlo Code MONK," Eighth International Topical Meeting on Nuclear Applications and Utilization of Accelerators (AccApp07), Pocatello, Idaho, Sept. 30 - August 2, 2007.

Alberto Talamo and Yousry Gohar, "MONTE CARLO Modeling and Analyses of YALINA-Booster Subcritical Assembly Part I: Analytical Models and Main Neutronics Parameters," Argonne National Laboratory Report, ANL-NE-08/13, March 2008.

Alberto Talamo, Yousry Gohar, Filip Kondev, Gerardo Aliberti, Hanna Kiyavitskaya, Victor Bournos, Yury Fokov, Christina Routkovskaya, Ivan Serafimovich, "Monte Carlo Analyses Of The Source Multiplication Factor Of The YALINA Booster Facility," International Conference on the Physics of Reactors, PHYSOR'08, Interlaken, Switzerland, September 14–19, 2008.

Alberto Abánades, Gerardo Aliberti, Victor Bornos, Mario Carta, Yousry Gohar, Jerzy Janczyszyn, Anna Kiyavitskaya, José Maiorino, Cheolho Pyeon, Alexander Stanculescu, Alberto Talamo, Yury Titarenko, Wolfram Westmeier, IAEA coordinated research project (CRP) on "Analytical and experimental benchmark analyses of accelerator driven systems," International Conference on the Physics of Reactors, PHYSOR'08, Interlaken, Switzerland, September 14–19, 2008.

G. Aliberti, Y. Gohar, F. Kondev, A. Talamo, H. Kiyavitskaya, V. Bournos, Y. Fokov, C. Routkovskaya, and I. Serafimovich, "YALINA-Thermal Experiment Analysis with the Deterministic Code System ERANOS," American Nuclear Society Annual Meeting 2008-11.

Alberto Talamo, Y. Gohar, F. Kondev, Gerardo Aliberti, Anna Kiyavitskaya, Victor Bournos, Yury Fokov, Christina Routkovskaya, Ivan Serafimovicj, "Comparison of MCNP/MCNPX Results with Experimental Data of YALINA-Booster Facility," American Nuclear Society Annual Meeting 2008-11.

Multimethod Linear Solvers in Terascale PDE-Based Simulations

PIs: Boyana Norris and Lois Curfman McInnes (Mathematics and Computer Science)

Many large-scale scientific simulations involve the parallel solution of time-dependent or nonlinear partial differential equations. Overall simulation time is often dominated by the parallel solution of large-scale, sparse linear systems. Typically, application developers select a particular algorithm to solve a given linear system and keep this algorithm fixed throughout the simulation. However, it is difficult to select a priori the most effective algorithm for a given application. Moreover, for long-running applications in which the numerical properties of the linear systems change as the simulation progresses, a single algorithm may not be best throughout the entire simulation.

We are thus exploring polyalgorithmic multimethod linear solvers in the context of several parallel applications, including flow in a driven cavity, compressible Euler flow, radiation transport, and edge plasma simulations to potentially improve the execution time and reliability of linear system solution. We are investigating an adaptive, polyalgorithmic approach, where the solution method is selected dynamically to match the attributes of the linear systems as they change during the course of a simulation.

This year we have focused primarily on designing and developing initial versions of computational quality-of-service (CQoS) tools, a key component technology initiative within the SciDAC Center for Technology for Advanced Scientific Component Software. These tools support the automatic composition, substitution, and dynamic reconfiguration of components to suite a particular computational purpose and environment. The two main facets of CQoS tools are (1) measurement and analysis infrastructure and (2) control infrastructure for dynamic component replacement and domain-specific decision making. We plan to use these tools to facilitate broader and more comprehensive parallel experimental runs on Jazz for multimethod solvers research.

We are also developing capabilities for monitoring, checkpointing, and gathering of data that may be managed through two types of databases. The first is created and destroyed during runtime and stores performance data for code segments of interest, as well as various application-specific performance events in the currently running application instance. The second database is persistent and contains performance data from various applications and different instances of the same application. This database can also contain performance information derived through offline analysis of raw data.

Publications and Presentations:

B. Norris, H. Johansson, L. McInnes, and J. Ray, "Component Infrastructure for Managing Performance Data and Runtime Adaptation of Parallel Applications," in Proc. PARA08 (9th International Workshop on State-of-the-Art in Scientific and Parallel Computing), Trondheim, Norway, May 13-16, 2008.

L. Li, L. C. McInnes, and B. Norris, "Database Components for Support of Computational Quality of Service for Scientific CCA Applications," SIAM Conference on Parallel Processing for Scientific Computing (SIAM-PP08), Atlanta, GA, March 12-14, 2008.

V. Bui, B. Norris, S. Bhownick, L. Li, and L. C. McInnes, "Toward Dynamic Selection of Parallel Linear Solvers Based on Performance and Power Considerations," poster, SIAM Conference on Parallel Processing for Scientific Computing (SIAM-PP08), Atlanta, GA, March 12-14, 2008.

V. Bui, "A Component Infrastructure for Performance and Power Modeling of Parallel Scientific Applications," presentation at the University of Houston, 2008.

Computational Nanocatalysis

PI: Peter Zapol (Materials Science, Chemistry, Center for Nanomaterials)

Nanostructured membrane catalysts based on anodized aluminum oxide (AAO) hold promise for improving catalyst performance and stability. AAO has tunable pore diameters as small as 30 nm, which can be further shrunk to only a few nanometers by atomic layer deposition (ALD) of amorphous Al_2O_3 layers with precise control of stoichiometry and thickness. The surface structure of these alumina films is of great interest because they serve as a support for highly dispersed catalytically active species such as VOx clusters. Vibrational frequency of V=O bonds in these species permit identification of catalytically active species on the surfaces.

The surface structures of hydroxylated amorphous Al_2O_3 obtained from atomistic molecular dynamics simulations and of θ-alumina were used as models of catalytic supports for VOx species. Based on density functional calculations of structures of vanadium oxide monomers on a dehydrated surface of θ-alumina, we have found that the measured frequencies match well with calculated stretching frequencies for tridendate, bidendate, and molecular structures. The free energies calculated for these three structures as a function of temperature suggest that all three

could exist on the surface. The calculated free energies of hydrated and dehydrated surfaces indicate a crossover from hydrated to dehydrated at around 600 K at 10^{-6} atm pressure, consistent with the experimental observation of isolated OH stretching frequencies at high temperatures.

Magnesium oxide also presents interest as a catalytic support for metal particles. Despite considerable research, various important questions remain unanswered regarding adsorption mechanism, saturation coverage, and the chemical nature of the adsorbate and desorption kinetics. To complement the experimental investigations in this project, we have carried out quantum chemical calculations of water formation on MgO (111) surfaces. We have modeled hydrogen-, OH- and O-terminated MgO surface using applied DFT method. Binding energies of OH, H and H_2O and coverage dependence of binding energy were also calculated on MgO surfaces.

A detailed picture of reaction pathways at microscopic level was obtained from reaction barrier calculations using nudged elastic band (NEB) method. Each NEB calculation requires from 2000 to 4000 node-hours on Jazz, which is 6-10 time more than one adsorption geometry calculation of, for example, OH/MgO(111). Several reaction pathways are possible for making H_2O on MgO depending on the coverage of OH and H. We have considered most of these cases and performed NEB calculations for diffusion of H or OH on MgO to form H_2O, which gives rise to a number of reaction pathways. The detailed analysis provides the structural information on MgO surface, gives adsorption mechanism for various adsorbate coverages, and elucidates the role of surface morphology (Fig. 17).

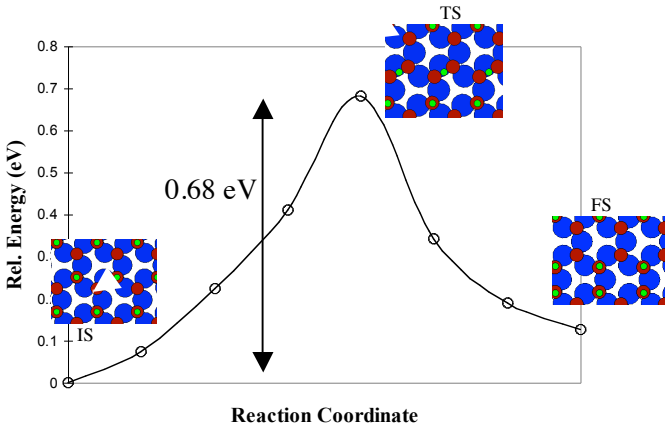


Figure 17. *Calculated barrier for hydrogen diffusion on √3×√3 MgO(111) as a first step in water formation reaction on MgO. Blue solid circles represent Mg, red - O and green H - atoms.*

Computational Nanophotonics

PI: Stephen Gray (Chemical Sciences and Engineering)

In our studies in computational nanophotonics this past year we showed how a light energy can be efficiently coupled in a layered structure containing a thin metal film. For certain thicknesses of the layer underneath the metal film the corresponding energy excitation, called a surface plasmon polariton, can be guided very long distances. Such a result is of relevance to the collection and transport of solar energy (Fig. 18).

We also initiated two projects on surface-enhanced Raman scattering. In these projects the aim is to optimize the system configuration to achieve controllable electromagnetic hot spots that can lead to enhanced spectroscopic responses from molecules that are near these spots. Such systems are of relevance to chemical and biological sensing.

To aid in the above activities, we developed a three-dimensional finite-difference time-domain code, called Forms. The central novelty of the code is in its flexible interface, which lets users define injected signals, materials and their distributions, and virtual measurements on the simulated systems functionally, by providing Scheme expressions, or by loading pre-defined, and where possible precompiled, configurations from the code's library. The code, the basic framework of which was designed in Chombo and derived from an earlier two-dimensional production code, called Shapes, runs in parallel on the Jazz cluster under MPI. Extension of the Chombo framework to three-dimensions required development of new classes for face and edge centered data – only face-centered data are supported by the Chombo package and even this incompletely. Additional semantic extensions were developed and implemented to let users manipulate Scheme data and Scheme-level computations in parallel.

The results of the calculations could benefit research on solar energy and chemical sensors. We are actively working with experimentalists at Argonne, Northwestern University, and UIUC on these projects.

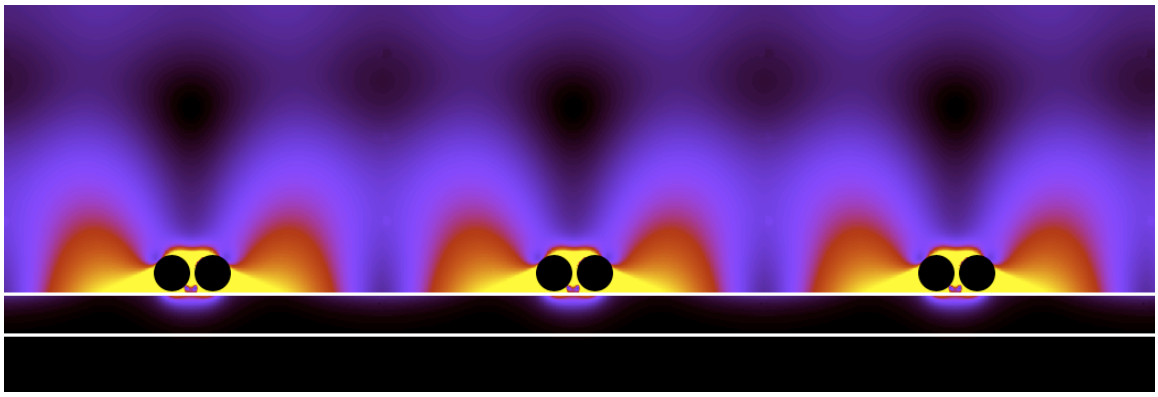


Figure 18. *Electric field intensities for a periodic array of 40 nm diameter gold spheres (black circles) above a silver film. Results show excitation of surface plasmon polaritons on the silver film coupling into local surface plasmons of the spheres, giving rise to high fields around the nanoparticles for increased SERS activity. [Yellow indicates intensities greater than 20 V^2 / m^2, with a maximum intensity of nearly 10000 V^2 / m^2 between the spheres. The incident intensity was 1 V^2 / m^2.]*

Publications and Presentations:
J. M. Montgomery and S. K. Gray, "Exciting surface plasmon polariton propagtion lengths via coupling to asymmetric waveguide structures," Phys. Rev. B 77, 125407 (2008).

Neocortex Simulations

PIs: Mark Hereld, (Mathematics and Computer Science) and Rick Stevens (Computing, Environment, and Life Sciences)

Epilepsy, a neurological disease characterized by repeated seizures with no direct external cause, is the third most commonly diagnosed neurological disease. In EEG recordings of epileptic patients, seizures are often seen to initiate from a specific area of the brain (the focus) and spread, so the epileptic focus is generally suspected of possessing abnormal neurons, abnormal connectivity between neurons, or both. Furthermore, seizure foci often exhibit seizure-like behavior that does not spread, implying that conditions need to be right in order for full clinical seizures to occur.

Ideally, one would like to record from many cells simultaneously in vivo to create a picture of how seizures start and spread from the focus, much as current EEG records possess upwards of 128 channels. Unfortunately, current in vitro experimental recording techniques are time-consuming and are generally limited to a handful of simultaneous recording sites or cells; they thereby provide an incomplete picture of the process at best. In vivo experiments are even more challenging.

To overcome some of these limitations, we are investigating seizure generation in a scalable computational model of neocortex. The cells and connectivity included in the model are, of course, simplifications of reality, but they preserve what we consider the essential elements – multiple inhibitory and excitatory cell types, Hodgkin-Huxley based ion channels, and several types of inter-neuron connections that vary in their topology and signaling speed. The model helps address a number of open questions in the field: Are seizures more of a cellular (ion channels) or network (connectivity) phenomenon? How small can a focus be? What conditions govern whether seizurelike behavior propagates or dies out? The model can provide insight into these questions because it is more easily manipulated than real neurons in an experimental setup.

In 2008, we continued to focus on identifying mechanisms for seizure initiation. Our model scripts were reorganized to more efficiently exploit new parameter search techniques.
Our neural network model constitutes an important component of this research, and we have utilized machines, including Jazz, to upgrade and test various strategies for matching templates of neuronal network behavior gathered from experimental slices. The results so far have been mixed, and we have therefore delayed plans to scale up simulation runs. We continue to test approaches that would allow model-based determination of underlying, hard-to-measure experimental variables, including a promising new approach by H. Abarbanel. This strategy should be implemented in the fall, to be tested shortly thereafter. Depending upon its

effectiveness, the model would be scaled up to ~1/10 the scale of an experimental slice, and would require the resources estimated in the previous allocation request.

P**ublications and Presentations:**
W. van Drongelen, A. Martell, and H. C. Lee, " Neocortical Epileptiform Activity in Neuronal Models with Biophysically Realistic Ion Channels," in Computational Neuroscience in Epilepsy, Ivan Soltesz and Kevin Staley (ed). Elsevier, 2008.

Integrated 3-D Simulation of Neutronic, Thermal-Hydraulic, and Thermo-Mechanical Phenomena

PI: Tanju Sofu (Nuclear Engineering)

A new software system, known as the Numerical Nuclear Reactor (NNR), is being developed for high-fidelity reactor core simulations including neutronic and thermal-hydraulic feedback. The NNR offers a comprehensive core modeling capability with pin-by-pin representation of fuel assemblies and coolant channels. It is based on 3D neutron transport solutions to generate sub-pin level power distributions, and computational fluid dynamics for thermal feedback due to fluid flow and heat transfer.

Through the support of Electric Power Research Institute Fuel Reliability Program, NNR was modified for boiling water reactor (BWR) applications. Specifically, a new neutronic depletion analysis capability was completed. For crud deposition applications, the irradiated fuel assemblies in the reactor core get depleted or consumed, resulting in composition changes that affect the distribution of the neutron flux. In order to determine the new isotopic compositions in burned-out fuel, a depletion model is needed because only the fresh, as-manufactured fuel composition is known. The intrapin depletion capability implemented in NNR is based on exponential matrix method of the ORIGEN-S code for simulating once- or twice-burned fuel assemblies. NNR now provides a predictive capability to identify the operational conditions that lead to excessive crud buildup and establishes a modeling framework for assessment of mitigation options (Fig. 19).

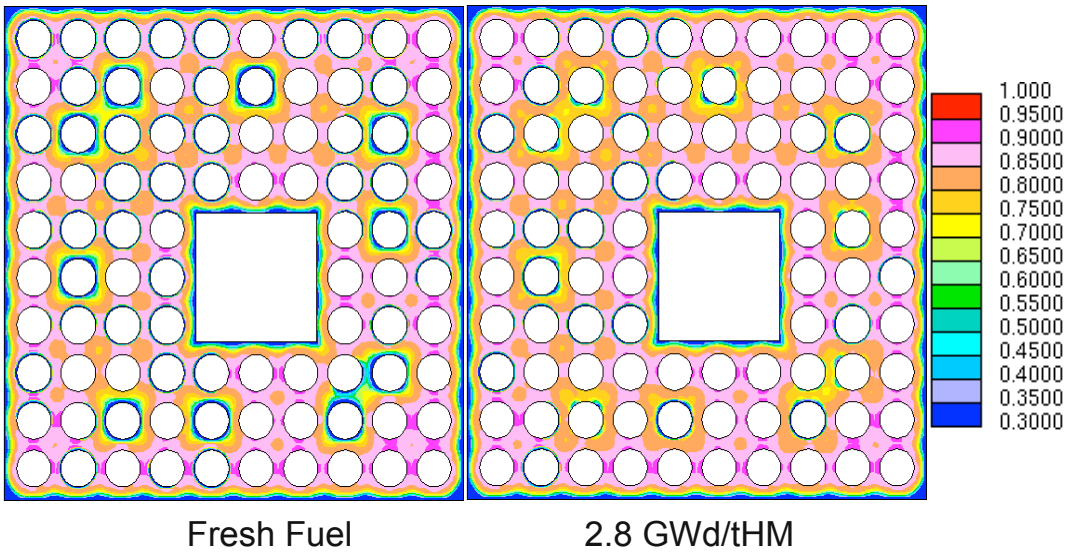


Figure 19. *Void fraction in core mid-plane for a typical fresh BWR fuel bundle (left) and after only three months of operation (right) as predicted using the NNR depletion analysis capabilities. The coupled NNR calculations for BWR depletion analyses typically require 20-30 processors and a week-long computations for fuel assembly-size problems.*

Grant:
This program is funded by the Electric Power Research Institute (EPRI) Fuel Reliability Program.

Parallel Tools Performance Testing

PIs: Robert Latham and Robert Ross (Mathematics and Computer Science)

The parallel-tools project continues to develop and study highly scalable software tools and libraries for parallel applications. Our efforts include a parallel file system (PVFS); an MPI-2 implementation (MPICH2); an MPI-IO implementation (ROMIO); work on higher-level libraries (Parallel-NetCDF); and tools and utilities to help capture, understand, and optimize the parallel I/O behavior.

As we do every year, we made extensive use of Jazz to evaluate novel approaches for high-performance I/O. All three fronts – PVFS, MPICH2, and pnetcdf – saw extensive testing and benchmarking. Thanks to the nightly tests we run on a portion of Jazz, we caught several regressions in both PVFS2 and ROMIO's PVFS2 driver. Jazz's node count and Myrinet interconnect made for a useful testbed for our experiments.

We also used Jazz resources as part of the ParaMEDIC distributed-computing project. This effort won the Bandwidth Challenge at SC2007 and a Best Paper award at ISC 2008.

Publications and Presentations:
Work done on Jazz has made its way into several product releases: PVFS2-2.6.1, MPICH2-1.0.7, and Parallel-NetCDF-1.0.2.

P. Balaji, W. Feng, J. Archuleta, and H. Lin, "ParaMEDIC: Parallel Metadata Environment for Distributed I/O and Computing," IEEE/ACM International Conference for High Performance Computing, Networking, Storage and Analysis (SC). Storage Challenge Award Winner, Reno, Nevada, Nov. 10-16, 2007.

P. Balaji, W. Feng, H. Lin, J. Archuleta, S. Matsuoka, A. Warren, J. Setubal, E. Lusk, R. Thakur, I. Foster, D. S. Katz, S. Jha, K. Shinpaugh, S. Coghlan, and D. Reed, "Distributed I/O with ParaMEDIC: Experiences with a Worldwide Supercomputer," in International Supercomputing Conference (ISC), Outstanding Paper Award, Dresden, Germany, June 17-20, 2008.

Quantum Monte Carlo Calculations of Light Nuclei

PIs: Stefano Gandolfi, Kenneth M. Nollett, Muslema Pervin, Steven C. Pieper, and Robert B. Wiringa (Physics)

This project uses quantum Monte Carlo [Green's function (GFMC) and variational (VMC)] methods to compute ground-state and low-lying excited-state expectation values of energies, densities, structure functions, transitions, astrophysical reaction rates, and so forth, for light nuclei. Realistic two- and three-nucleon potentials are used as input. Our goal is a description of all of these systems and processes using a Hamiltonian that also provides an excellent description of nucleon-nucleon scattering and nucleonic matter. Such a "standard nuclear model" can then be used, for example, to compute low-energy astrophysical reaction rates that cannot be experimentally measured.

During 2008 Jazz was used for many aspects of this project. The fast turnaround of Jazz makes it the machine of choice for all but our biggest calculations, which are done on Blue Gene or (decreasingly) at NERSC. The specific projects this year fell into four categories:

Transition Matrix Elements. One of our goals is to reliably compute the matrix elements that determine the rates of nuclear decays in light nuclei. These include the magnetic dipole (M1) and electric quadrupole (E2) matrix elements for photon emission and the Fermi (F) and Gamow-Teller (GT) matrix elements for weak decay. In the past two years we have learned how to evaluate these matrix elements using stored GFMC wave functions that were originally generated in binding energy calculations. Results for E2, F, and GT matrix elements were in good agreement with experimental data, where available. Results for M1 transitions were ~20% smaller than experiment, as expected, because of the omission of two-body meson-exchange current (MEC) contributions. After we added these MEC corrections, which are fixed in magnetic moment calculations, we found that the M1 transitions are now in excellent agreement with

experiment. Additional calculations of various transitions in A=8 nuclei were made during 2008, and this work will continue in 2009.

Two-Nucleon Momentum Distributions. In 2007 we began a study of two-nucleon momentum distributions in light nuclei using the VMC method. We computed two-nucleon momentum distributions rho(q,Q) in A=3,4,6,8 nuclei for the special case where the total momentum of the pair Q=0, i.e., the knocked-out pair come out back-to-back in the center of mass. We found the dramatic effect that, for our realistic nuclear forces with their strong tensor component, the number of np pairs can be 20-50 times larger than the number of pp pairs in the relative momentum range q = 300-500 MeV/c. This effect has now been seen in experiments at Jefferson Lab. The experiment and the theoretical explanation (including our work) were prominently featured in the Search & Discovery section of the July issue of *Physics Today*. We extended our calculations to finite Q in parallel kinematics and found that the large ratio of np to pp pairs quickly reduces to a factor of 2-3 as Q approaches 200 MeV/c. We published our prediction this past summer, and preliminary experimental results we have been shown are in excellent agreement with our calculation.

Dependence of Nuclear Binding on Hadronic Mass Variation. Some grand unified theories predict that fundamental "constants" such as the electromagnetic fine structure constant or bare quark masses could vary temporally or spatially during the course of the universe's evolution. There are some hints of such variation in quasar absorption spectra, the Oklo natural nuclear reactor, and big bang nucleosynthesis (BBN). In 2007 we began a study of how nuclear binding energies would vary if the input hadron (nucleon, nucleon resonance, pion, and vector meson) masses varied with changes in the underlying bare quark mass. This year we extended our study to some low-lying excited states to examine how spin-orbit splittings of nuclear levels in A=5-9 nuclei would be affected by quark mass variations. This gives rough estimates for much larger nuclei (e.g., 150Sm and 229Th, which could provide sensitive tests of time variation of some fundamental constants (Fig. 20).

Neutron Drops. Neutron drops are a collection of neutrons interacting via a standard NN and NNN Hamiltonian with an added artificial external well. The well can be adjusted to change the density or surface thickness, and it could be nonspherical. If the NN and NNN part of the Hamiltonian is realistic, the energies and density profiles from such calculations can provide useful input to energy-density functionals. Our GFMC method is limited to only 16 neutrons in the well due to its exponential growth with the number of neutrons. A related method, auxiliary field diffusion Monte Carlo (AFDMC) has only a power law growth and can do up to 100 neutrons but is potentially less accurate. We have used Jazz to compute 8- to 14-neutron drops by AFDMC for comparison with GFMC calculations for the same systems. The results show that AFDMC is accurate enough for our purposes. Jazz is also being used to compute bigger drops.

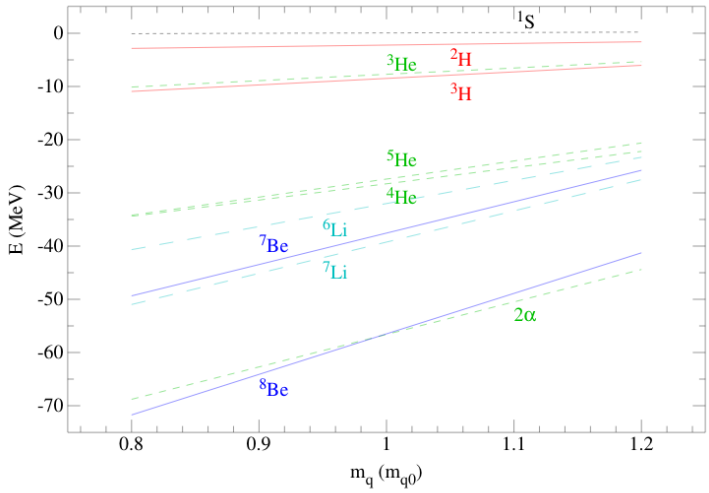


Figure 20. *Calculated variation of nuclear binding energies with current-quark mass.*

Publications and Presentations:

V. V. Flambaum and R. B. Wiringa, "Dependence of Nuclear Binding on Hadronic Mass Variation," Phys. Rev. C 76, 054002-1:11 (2007).

M. Pervin, S. C. Pieper, and R. B. Wiringa, "Quantum Monte Carlo Calculations of Electroweak Transition Matrix Elements in A=6,7 Nuclei," Phys. Rev. C 76, 064319-1:9 (2007).

R. B. Wiringa, R. Schiavilla, S. C. Pieper, and J. Carlson, "Dependence of Two-Nucleon Momentum Distributions on Total Pair Momentum," Phys. Rev. C 78, 021001(R)-1:3 (2008)

V. V. Flambaum and R. B. Wiringa, "Enhanced Effect of Quark Mass Variation in 229Th and Limits from Oklo Data," arXiv:0807.4943 [nucl-th], preprint, 2008.

M. Pervin, S. C. Pieper, and R. B. Wiringa, "Ab Initio Calculations of Electroweak Transitions in A=8 Nuclei," 2007 Annual Fall Meeting of the Division of Nuclear Physics of the American Physical Society, Newport News, Virginia, October 10-13, 2007; abstract in Bulletin American Physical Society 52, no.9, 28 (2007)

R. B. Wiringa, S. C. Pieper, M. Pervin, "GFMC Calculations of Isospin-Mixing in 8Be," 2007 Annual Fall Meeting of the Division of Nuclear Physics of the American Physical Society, Newport News, Virginia, October 10-13, 2007; abstract in Bulletin American Physical Society 52, no.9, 30 (2007)

S. C. Pieper, "Quantum Monte Carlo Calculations of Light Nuclei," in Proc. International School of Physics "Enrico Fermi," Course CLXIX, edited by A. Covello, F. Iachello and R. A. Ricci (SocietÃ Italiana di Fisica, Bologna, 2008) arXiv:0711.1500v1 [nucl-th]

S. C. Pieper, "The Illinois Extension to the Fujita-Miyazawa Three-Nucleon Force," in AIP Conf. Proc. 1011, 143-152 (2008)

Chemotaxis

PIs: T. Emonet (Molecular, Cellular and Developmental Biology Department, Yale University), P. Cluzel (Institute for Biophysical Dynamics, University of Chicago), C. Macal and M. North (Center for Complex Adaptive Agent Systems Simulation).

The aim of our project is to unveil design principles of biological networks by using agent-based numerical modeling and mathematical methods borrowed from statistical physics. Cells process information and make decisions using biochemical networks. Some biological functions are carried out at the single-cell level, while other behaviors emerge at the population level mediated by cell-to-cell communication.

We have developed the Network Free Stochastic Simulator (NFsim) to efficiently handle the problem of combinatorial complexity present in many signaling systems. NFsim is a generalized biochemical reaction simulator for rule-base models that utilizes an agent-based stochastic simulation algorithm. We demonstrate the capabilities of NFsim by constructing an integrated model of the full bacterial chemotaxis system, which we simulated on Jazz. The eventual goal is to use NFsim to extend the capabilities of our agent-based platform AgentCell to simulate a wide range of highly multiscale stochastic systems. NFsim implements agent-based methods to attain performance that scales with the number of events rather than the size of the reaction network.

These computations have paved the way for closer collaborations between analytical treatments, computational modeling and wet lab experimentation of *E. coli* behavior, which potentially has broad implications for many biological systems.

Publications and Presentations:
M. W. Sneddon W. Pontius, J. Faeder, and T. Emonet, "NFsim: Managing Complexity in Stochastic Simulations of Reaction Networks," Poster at the 2nd q-bio Conference on Cellular Information Processing, Santa Fe, NM, 2008.

Large-Scale Parallel Simulation of Subduction Zone Geodynamics

PIs: Matthew Knepley (Mathematics and Computer Science) and Richard Katz (St Anne's College, Oxford)

We are interested in the physical and chemical consequences of melting and freezing on Earth. Melting of mantle rocks at plate tectonic boundaries leads to chemical segregation and differentiation of the Earth's crust from its mantle. Over time, this process leads to the formation of distinct continental plates. The details of the process are poorly understood. Freezing of sea-ice is another example of chemical segregation. Ice formed by freezing of seawater is free of salt. A dense, salty brine accumulates between ice crystals, and this brine flows through the ice-crystal mush and into the open ocean below. This process has important implications for ocean circulation and hence for climate change.

To study these phenomena, we incorporated the enthalpy method into PETSc-based simulations of fluid flow with solidification and melting. The enthalpy method allows for a consistent description of equilibrium, multicomponent thermodynamics. It is a simple but powerful framework to state many different problems in a way that lends itself to easy solution.We also implemented a modular, parallel, PETSc-based particle tracking scheme for passive tracer advection in 2D fluid flows. This scheme can be easily added to a time-dependent PETSc code.

In 2008, we used Jazz extensively for simulations of both magmatic transport beneath mid-ocean ridges and reactive convection in mushy layers of salt crystals, an analogue for sea-ice formation. The magma dynamics work showed that the efficiency of magmatic focusing beneath mid-ocean ridges can be very high. The simulations are now being used to probe the consequences of mantle heterogeneity for magmatic flow and geochemical transport (Fig. 21).

These simulations will provide a means to test leading theories of melt transport in the mantle. Observational constraints derived from seismology and geochemistry can be compared with our results to support or reject the physical model we are working with. Such comparisons will advance our understanding of the dynamics of the inaccessible Earth below the crust.

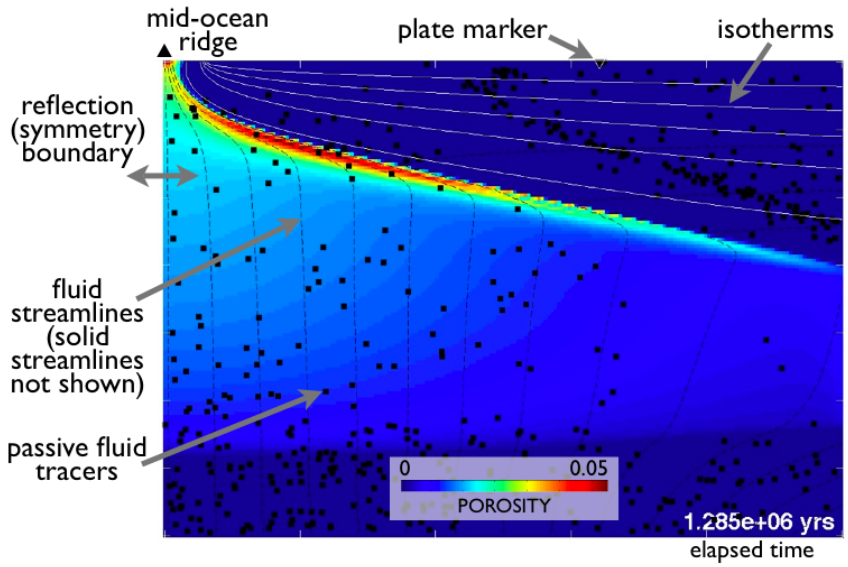


Figure 21. *Time-slice of porosity (volume fraction of fluid) in a 2D magma dynamics simulation. There is a reflection (symmetry) boundary condition at the left edge of the domain. The ridge axis, where magma erupts, is at the top left.*

Publications and Presentations:

R. F. Katz, "Magma Dynamics with the Enthalpy Method: Benchmark Solutions and Magmatic Focusing at Mid-Ocean Ridges," J. Petrology, doi:10.1093/petrology/egn058 (published on-line), 2008.

R. F. Katz and M. G. Worster, "Simulation of Directional Solidification, Thermochemical Convection, and Chimney Formation in a Hele-Shaw Cell," J. Computational Physics, 227, no. 23 (2008) 9823-9840.

R. F. Katz, "Mantle Heterogeneity and Crustal Production in Magma-Dynamics Simulations of Midocean Ridges," Goldschmidt conference, Vancouver, 2008.

Accelerator and Target Simulations for the Rare Isotope Accelerator Facility

PI: Brahim Mustapha (Physics)

A new lattice design is being proposed for the Fermilab proton driver (FNAL-PD) linac. It is based partly on the lattice of the future International Linear Collider (ILC). Such a design will take advantage of the well-advanced ILC R&D and would require minimal new R&D. The purpose of the project was to study the performance of the new design and compare it to the original design.

The new major development in the beam dynamics code TRACK was the inclusion of beam loss due to H- stripping by black body radiation, residual gas interaction, and Lorentz stripping. Beam dynamics end-to-end simulations were performed on Jazz to study the robustness of the new design to machine errors and eventual beam loss. The results show that the ILC-based design is viable option for the FNAL-PD. The design of the FNAL-PD is not yet final and the results of these simulations should help the decision on the final design option (Fig. 22).

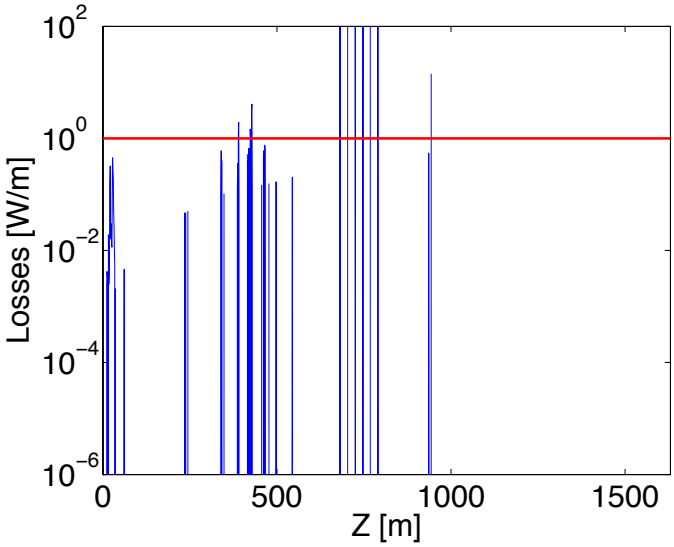


Figure 22. *Beam loss in watts/m in the FNAL-PD linac and transfer line. The lattice design is partly based on the ILC design.*

Publications and Presentations:

J.-P. Carneiro. D. Johnson, and R. C. Webber, "Start-to-End Simulations for the Proposed Fermilab High-Intensity Proton Source," in Proc. PAC-07 Conference, Albuquerque, NM, pp. 1676-1678, 2007.

Toolkit for Advanced Optimization

PIs: Todd Munson and Jason Sarich (Mathematics and Computer Science)

The goal of the TAO project is to provide a portable numerical optimization library for large-scale scientific applications. To achieve this goal, we must be able to install, debug, test, and run applications on a variety of parallel architectures, including Jazz.

In addition to this software development and support, several current TAO applications are run at least partly on Jazz, include predicting the flow of subsurface contaminants in groundwater and improving the accuracy of the energy density functional for modeling nuclear behavior.

During 2008, several new capabilities were added to TAO, including Nelder-Mead implementation for derivative free optimization; finite-difference derivative check to test the validity of user application gradients and Hessians; a new limited-memory Broyden-Fletcher-Goldfarb-Shanno method; new Newton trust-region, line-search, and trust-region line-search methods; and new conjugate gradient methods in PETSc.

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