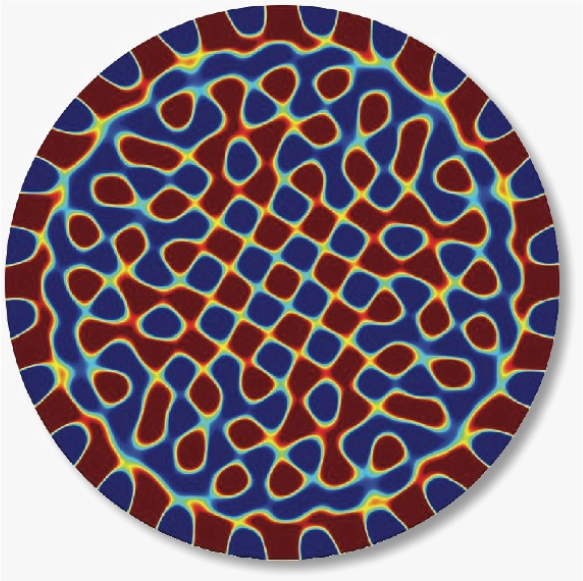
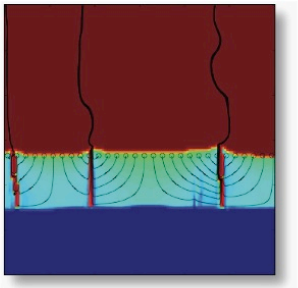
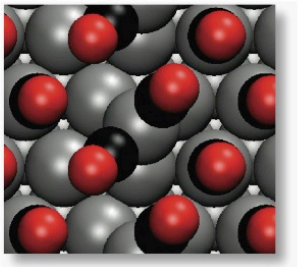
Argonne NATIONAL LABORATORY

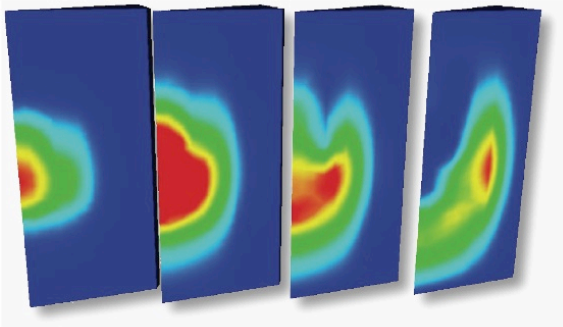
Argonne's Laboratory Computing Resource Center

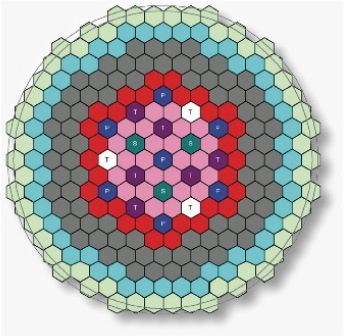
2007 Annual Report











About Argonne National Laboratory

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Argonne Laboratory Computing Resource Center

FY2007 Report

In the spring of 2002, Argonne National Laboratory founded the Laboratory Computing Resource Center, and in April 2003 LCRC began full operations with Argonne's first teraflops computing cluster. The LCRC's driving mission is to enable and promote computational science and engineering across the Laboratory, primarily by operating computing facilities and supporting application use and development. This report describes the scientific activities, computing facilities, and usage of LCRC operation in 2007 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.

Steering for LCRC comes from the Computational Science Advisory Committee, composed of computing experts from many Laboratory divisions. The CSAC Allocations Committee makes decisions on individual project allocations for Jazz.

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 consult@lcrc.anl.gov.

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Contents

Executive Summary v
The Laboratory Computing Resource Center 1
Objectives 1
Cluster Configuration 1
Cluster Usage 2
Users and Projects 3
Usage by Discipline 3
Job Size Characteristics 4
Scientific and Engineering Applications 5
Atmospheric Chemistry 6
Nuclear Engineering 7
Bridge Hydraulics 8
Collider Physics 10
Organic Semiconductors 12
Nanotechnology 13
DNA Repair 14
Nuclear and Particle Physics 17
Computational Electromagnetics 19
Climate Modeling 21
Computed Tomography 23
Global Climate Modeling 24
Multimethod Linear Solvers in Terascale PDE-Based Simulations 25
Aerodynamic Drag for Heavy Vehicles 27
Advanced Plasma Applications 28
Advanced Methods for Calculating Fundamental Atomic Properties 29
Validation of Neutronics Tools for Advanced Burner Reactor Design 31
CO Hydrogenation with Co Carbonyl Catalysts 32
3D Simulation of Neutronic, Thermal-Hydraulic, and Thermo-Mechanical Phenomena 35
Chemotaxis 37
Accelerator and Targets Simulations 38
Computational Nanophotonics 39
Voltage-Gated Potassium Ion Channels 40
Lattice Quantum Chromodynamics in Extreme Environments 41
Neocortical Seizure Simulation 43
Spin Wave Excitations in Magnetic Nanoparticles 44
Large-Scale Parallel Simulation of Subduction Zone Geodynamics 44
High-Fidelity Numerical Simulation of Nuclear Reactor Cores 46
Monte Carlo Analyses of Accelerator-Driven Subcritical Facilities 48

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.

In September 2002 the LCRC deployed a 350-node computing cluster from Linux NetworX to address Laboratory needs for mid-range supercomputing. This cluster, named "Jazz," achieved over a teraflop of computing power (10^{12} floating-point calculations per second) on standard tests, making it the Laboratory's first terascale computing system and one of the 50 fastest computers in the world at the time. Jazz was made available to early users in November 2002 while the system was undergoing development and configuration. In April 2003, Jazz was officially made available for production operation.

Since then, the Jazz user community has grown steadily. By the end of fiscal year 2007, there were over 60 active projects representing a wide cross-section of Laboratory expertise, including work in biosciences, chemistry, climate, computer science, engineering applications, environmental science, geoscience, information science, materials science, mathematics, nanoscience, nuclear engineering, and physics. Most important, many projects have achieved results that would have been unobtainable without such a computing resource.

The LCRC continues to foster growth in the computational science and engineering capability and quality at the Laboratory. Specific goals include expansion of the use of Jazz to new disciplines and Laboratory initiatives, teaming with Laboratory infrastructure providers to offer more scientific data management capabilities, expanding Argonne staff use of national computing facilities, and improving the scientific reach and performance of Argonne's computational applications. Furthermore, recognizing that Jazz is fully subscribed, with considerable unmet demand, the LCRC has framed a "path forward" for additional computing resources.

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 Mathematics and Computer Science Division operates the LCRC on behalf of the Laboratory. The LCRC's first computer cluster, called "Jazz," was installed in September 2002. 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.

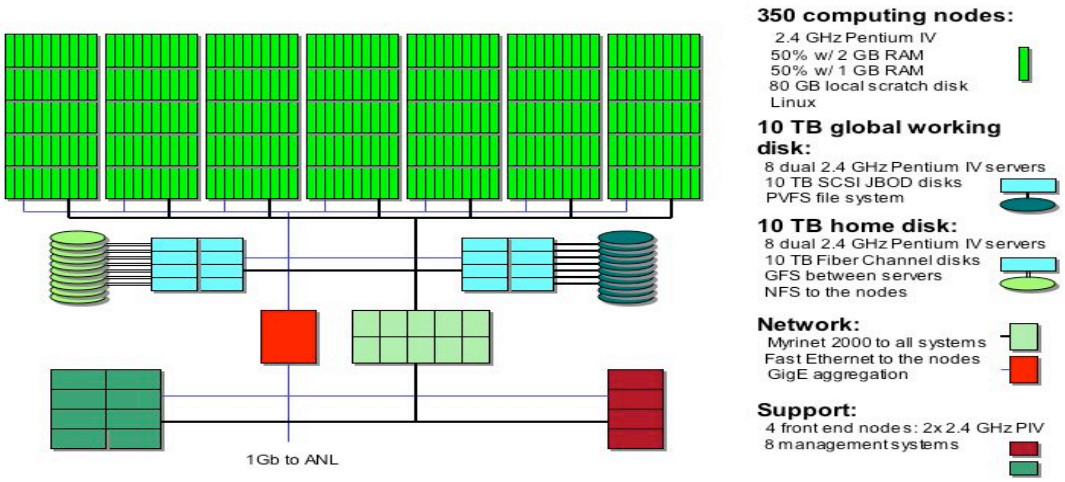
Objectives

During 2007, the LCRC emphasized the following objectives:

- Continue to operate Jazz as a highly effective production supercomputing resource.
- Encourage the use of Jazz for new projects and disciplines, with an emphasis on the Laboratory's initiatives.
- Help Argonne personnel improve the scientific reach and performance of their computational applications.
- Help large-scale users of Jazz identify opportunities to obtain allocations at national computing resources such as ALCF, NERSC, NLCF, MHPCC, PACI, and TeraGrid.

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 configuration is shown below.

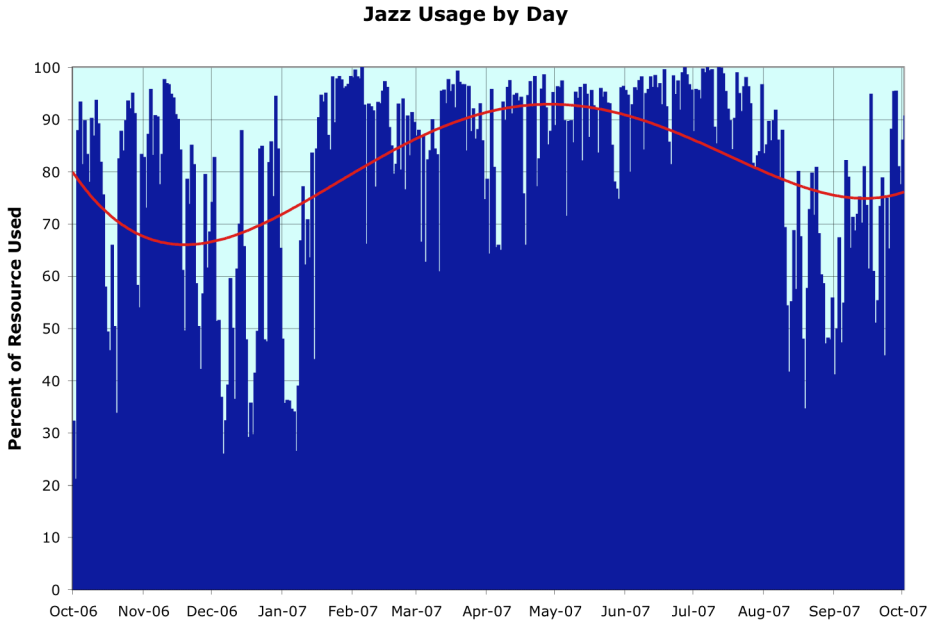


Cluster Usage

The usage of Jazz was high throughout most of fiscal year 2007, with usage over 80% and frequently exceeding 90%. 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. As can be seen, usage was very high for most of the year with two notable exceptions. For most of December and the start of January, few users were running jobs on Jazz for unknown reasons. It is possible that users were occupied by the holidays or other research. The lull in activity was communicated to the user community in mid-January, and usage quickly increased to over 90%. Then in mid-August, the LCRC implemented a new scheduling policy on Jazz to limit to one the number of background jobs an overdrawn project can run. It took about a month for the projects with positive balances to fill up the gap. Overall, this change was favorably received.

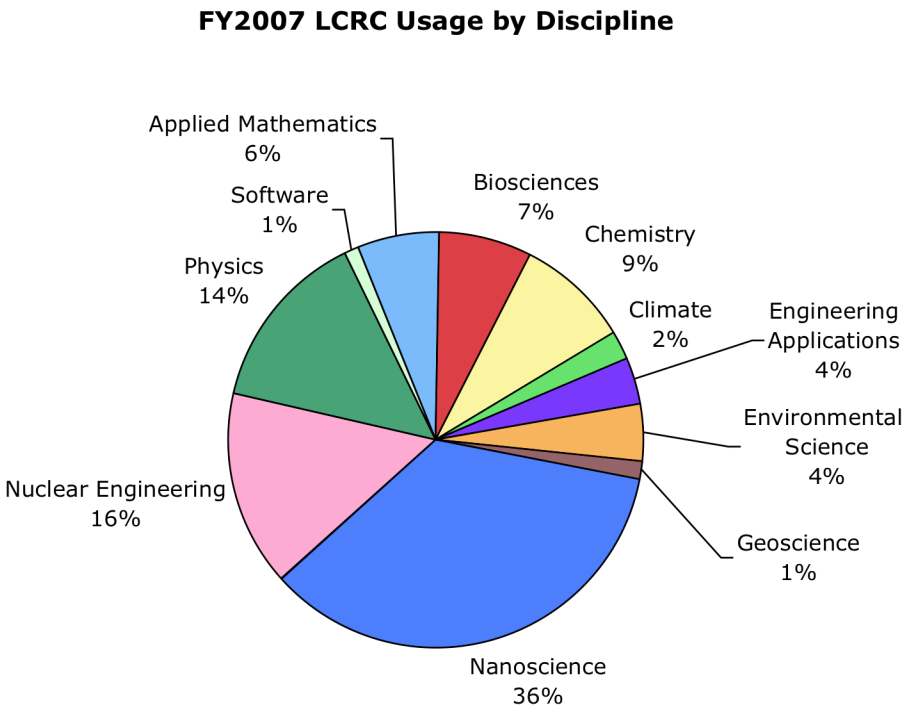


Users and Projects

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. 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. An investigator wishing to use Jazz for a longer period of time may apply for additional computing allocation via the Web site. Aside from these 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 Allocation Committee, composed of scientists from across the Laboratory.

Usage by Discipline

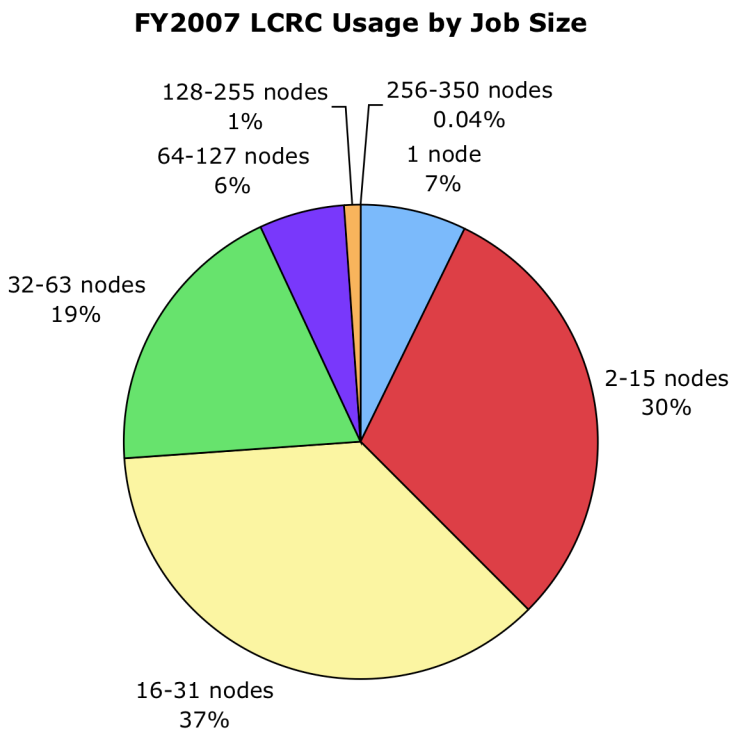
Jazz supports research in a wide range of disciplines, including biosciences, chemistry, climate, computer science, engineering, environmental science, geoscience, information science, mathematics, nanoscience, nuclear engineering, and physics. The chart below shows what fraction of the Jazz resource (number of node hours) was used by projects in each discipline during fiscal year 2007. Projects related to nanoscience, nuclear engineering, and physics made heaviest use of Jazz during the past year.



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 FY2007. Over 50% of the machine was used for jobs that employed 16–63 processors. About 8% of the jobs used 64–350 processors. The jobs that needed only one node accounted for about 7% (down from 12% in FY2006) of the total computing time used on Jazz. We encourage users to submit large parallel jobs so that the interconnect on the machine gets properly utilized.



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. Currently, over 60 projects from more than two dozen divisions 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 our 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 the Argonne Leadership Computing Facility (ALCF) and other national centers.

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

Strategic. Jazz is critical to 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 ALCF, NERSC, NCCS, 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 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 them 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 in FY2007. The examples span both the basic and applied missions of the Laboratory and include 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

PIs: Veerabhadran Kotamarthi and Beth Drewniak (Environmental Science)

The aim of our modeling activity is to further scientific understanding of the chemistry and distribution of oxidants in urban and rural air masses. Much of the output of our work is used for the air quality portion of environmental impact statements for federal agencies. Our work this year focused on the use of MOZART, a chemical transport model for ozone and related chemical tracers. Two mercury species are included in the model: elemental mercury (HGE) and oxidized or reactive mercury (HGO). All mercury is emitted as elemental in the model and later oxidized to reactive mercury. HGE dry deposition is set to zero in the model, as in many other models, since the soil re-emission of mercury is balanced by the dry deposition. Wet deposition of HGE is also set to zero because elemental mercury is generally not soluble in water. MOZART is driven with monthly climate data from the National Center for Environmental Prediction. The grid is roughly 2.8 degrees latitude x 2.8 degrees longitude, with 28 vertical levels extending from the surface to 2.7 mb. Surface emissions of various chemicals are derived from the Max-Planck-Institute for Meteorology. Mercury emissions are based on anthropogenic emissions reported in the journal *Atomospheric Environment* in 2006. Only anthropogenic emissions are included; natural emissions from the land and ocean are not represented.

Two model runs have completed to date. The first run was to initialize the background concentration of HGE in the atmosphere (HGO is initialized at zero since it has a short lifetime). Next, a base case was simulated with anthropogenic mercury emissions only. Mercury concentrations of HGE (Figure 1) were compared to other studies. The results are reasonable, although they are slightly lower because of the negation of natural emissions. Evaluating HGO from concentrations was difficult because most studies divide total mercury emissions into HGE and HGO emissions, whereas we modeled all emissions as HGE. Therefore, wet and dry deposition was used to determine the performance of the model for HGO. Mercury deposition of HGO from wet and dry sources were less than other studies, again a result of the neglect of natural emissions, but are still an acceptable estimate.

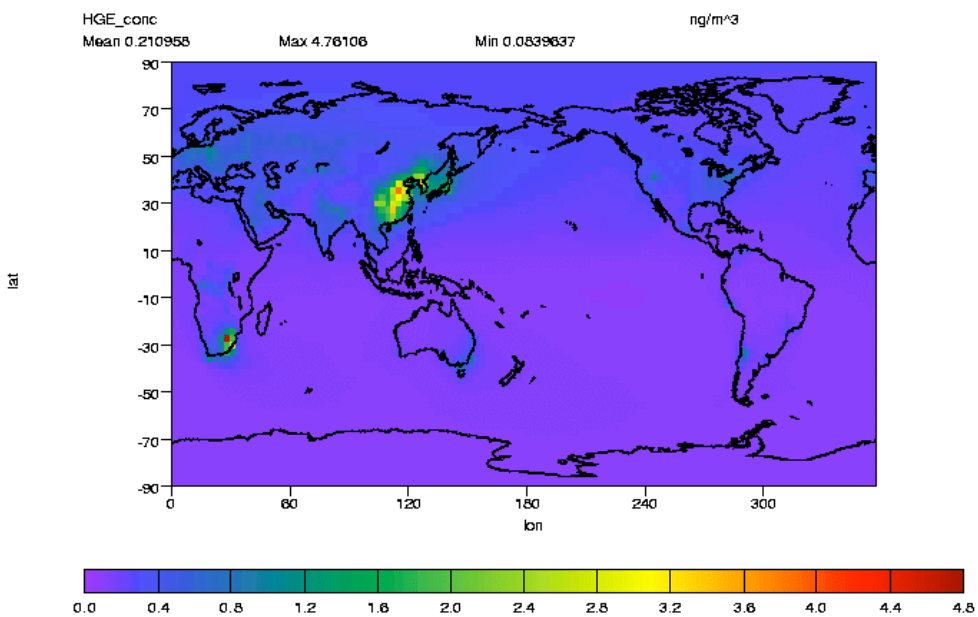


Figure 1. Annual mean mercury surface concentrations of HGE (ng m^{-3})

Nuclear Engineering

PI: William Pointer (Environmental Science)

We are developing a high-fidelity, full-core, pin-by-pin, fully coupled neutronic and thermal hydraulic simulation package for reactor core analysis. Our approach involves extending the capabilities for Eulerian-Eulerian two-phase simulation with the commercial computational fluid dynamics code Star-CD and validating the code for application to boiling water reactor (BWR) cores. Specific tasks include development of wall heat partitioning and bubble growth models, implementation of a topology map-based approach that provides the necessary capability to switch between the liquid and vapor as the continuous phase on a cell-by-cell basis, and development of appropriate models for the interphase forces that influence the movement of bubbles and droplets.

During 2007, our efforts focused primarily on development of the models to describe the forces acting on the bubble/droplet phase and testing of the extended framework implemented by external collaborators. In addition, as a validation of the predictive capability, we applied the model to an international benchmark problem for validation of BWR assembly analysis methods. Initial benchmark comparisons indicate that the extended framework not only provides comparable accuracy in prediction of macroscopic subchannel-averaged flow quantities to more traditional subchannel tools but also predicts general trends of the microscopic void distribution very well in comparison to the other computational fluid dynamics participants in the benchmark (Figure 2).

These computations have resulted in recognition of the potential of computational multiphase fluid dynamics (CMFD) for immediate to near-term application to problems of this type by the benchmark committee and expanded plans for involvement of CMFD tools in remaining phases of the benchmark. CMFD is currently a rapidly developing field, and these results have established Argonne as a leader in this effort.

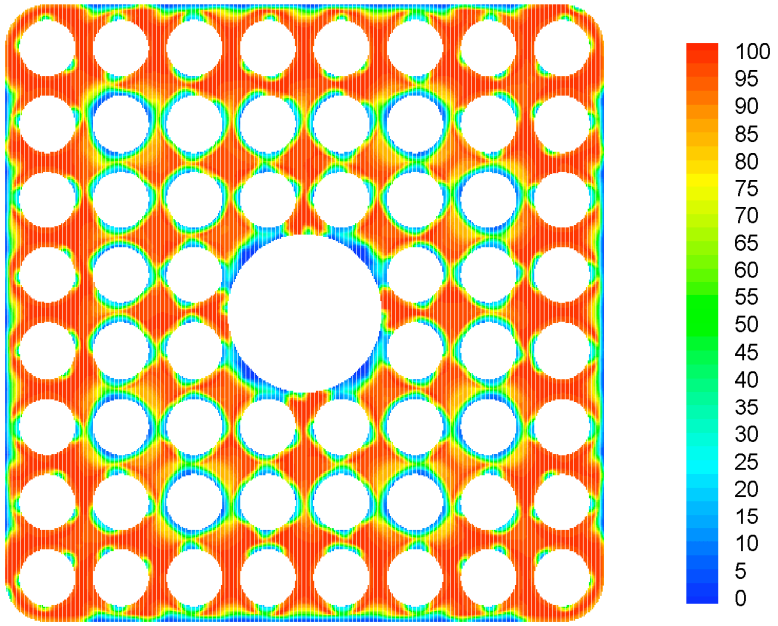


Figure 2. Predicted void fraction at the measurement plane in the BWR test assembly

Publications and Presentations:

W. David Pointer, "Eulerian Two-Phase Computational Fluid Dynamics for Boiling Water Reactor Analysis," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007), Monterey, CA, April 15-19, 2007.

T. Sofu, J. W. Thomas, D. P. Weber, W.D. Pointer and T. Downar, "Coupled BWR Calculations with the Numerical Nuclear Reactor Software System," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications, Monterey, CA, April 15-19, 2007.

A. Tentner, W. D. Pointer, T. Sofu, and D. Weber, "Development and Validation of an Extended Two-Phase Computational Fluid Dynamics Model for the Analysis of Boiling Flow in Reactor Fuel Assemblies," in *Proceedings of ICAPP 2007,* Nice, France, May 13-18, 2007.

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 rely 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 computational fluid dynamics (CFD) domain.

Our CFD simulations have addressed a range of hydraulics research, including the assessment of lift and drag forces on bridge decks when flooded (Figure 3), optimization of bridge deck shapes to minimize pressure flow scour, analysis of sediment transport and its influence on scouring, evaluation of active or passive scour countermeasures to mitigate the damage, and study of environmental issues such as fish passage through culverts. During 2007, we investigated the applicability of the commercial CFD codes Fluent and Star-CD for predicting these phenomena. Using Jazz, we were able to address the scalability of these simulations to large numbers of processors, particularly for the simulation of full-scale bridge deck interactions.

These results shed new insight on the fundamental nature of spatiotemporal chaos in an experimentally accessible fluid system that can be used to improve our understanding of more complex real-world systems such as the dynamics of the weather and climate. Numerical simulations of experimentally realistic Rayleigh-Benard convection systems using the full three-dimensional, nonlinear Navier-Stokes equations also provide a quantitative link between theory and experiment (Figure 4).

The next step will be to determine the agreement between the code predictions and experimental data for various modeling options. When validated using the broad experimental database, the simulations based on commercial CFD software will allow expanded parametric analysis and provide a means of evaluating directly the effects of scaling.

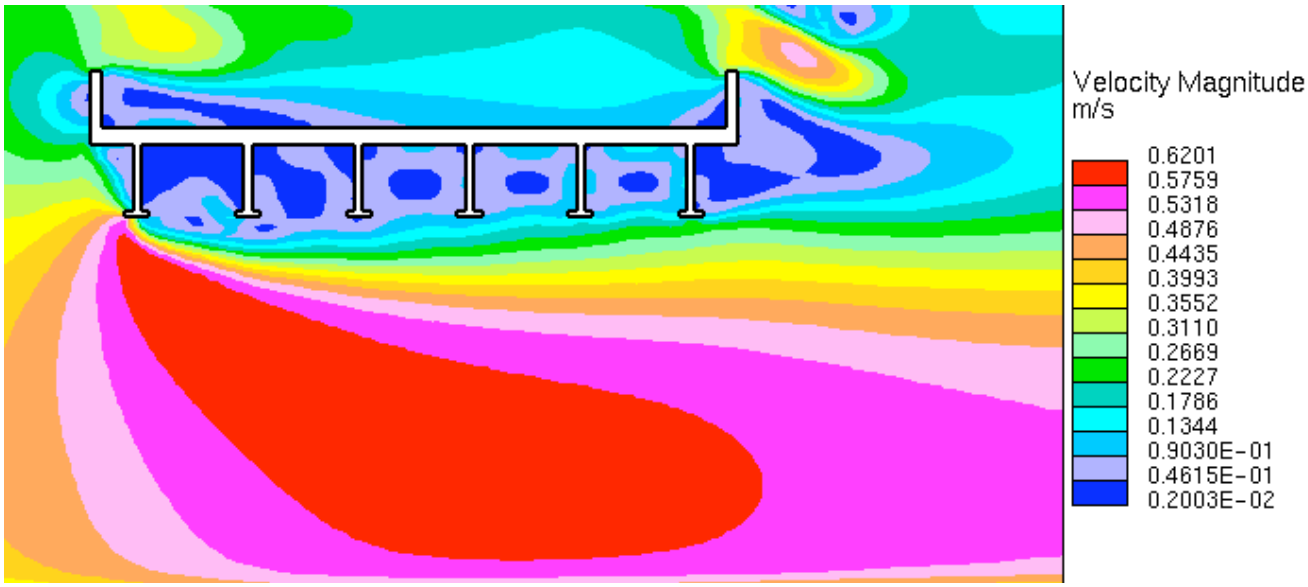


Figure 3. Flow field around an inundated bridge deck

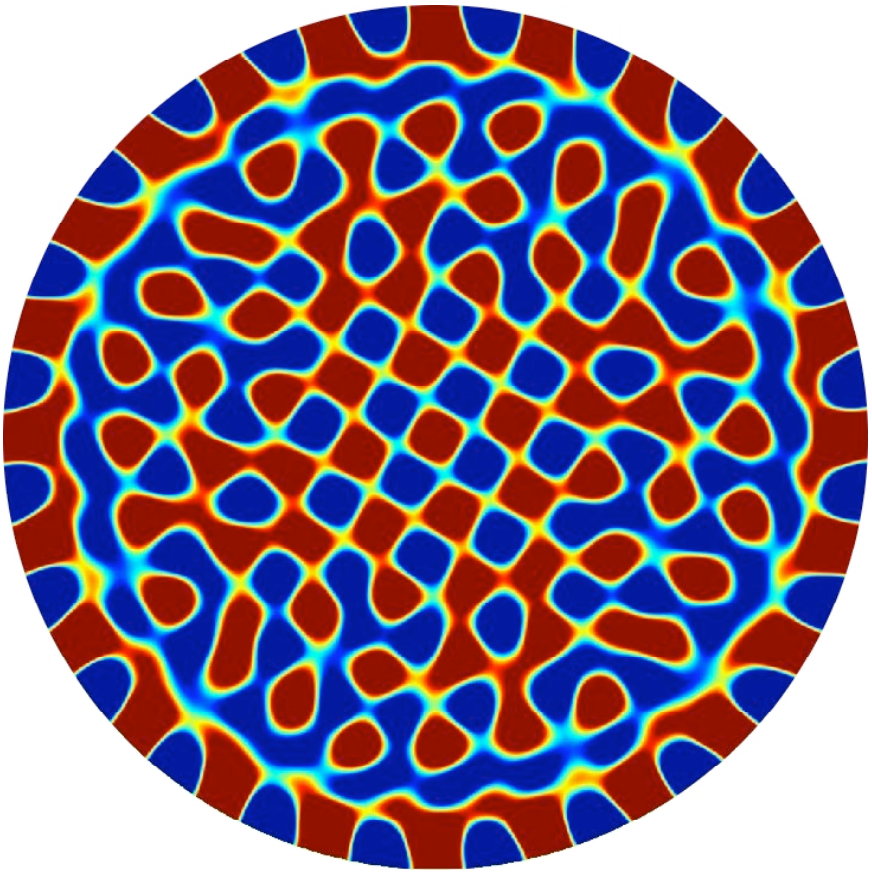


Figure 4. Square patterns in Rayleigh-Benard convection

Publications and Presentations:

P. L. Mutyaba, T. Kimmel, and J. D. Scheel, "Patterns in Rayleigh-Benard convection for high rotation rates," Division of Fluid Dynamics Meeting, Salt Lake City, UT 2007.

M. R. Paul, "Quantifying Spatiotemporal Chaos in Rayleigh-Benard Convection: New Insights from Numerics," Georgia Tech, March 2007.

M. R. Paul, M. I. Einarsson, P. F. Fischer, and M. C. Cross, "Extensive Chaos in Rayleigh Benard Convection," *Physical Review E* (2007).

M. R. Paul, "Spatiotemporal Chaos in Fluid Convection: New Insights from Numerics," University of Kentucky, April 2007.

J. D. Scheel, "The Amplitude Equation for Rotating Rayleigh-Benard Convection," accepted by *Phys. of Fluids* (2007); also presented at the SIAM Conference on Dynamical Systems, Snowbird, UT, May 2007.

Collider Physics

PI: Edmond Berger (High Energy Physics)

Supersymmetry is the leading candidate for new high energy physics that goes beyond the Standard Model description of particle physics. This compelling theory predicts the existence of a significant number of new particles that should be observed at the CERN Large Hadron Collider (LHC) scheduled to begin operation in 2008. 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. We are collaborating with Southern Methodist University in providing these improved predictions.

A "golden signature" for supersymmetry is the observation of three leptons plus missing energy coming from the decay of a chargino produced with a neutralino. Experimental analyses and data triggers are designed assuming that the Standard Model backgrounds to this channel are modest. It is essential both for ongoing analyses of Fermilab Tevatron data and for the development of strategies for LHC experiments to estimate as quantitatively as possible the overall magnitude and the expected population in phase space of both the supersymmetry signal and the dominant Standard Model backgrounds.

During the past year, we made detailed numerical simulations of the distributions in phase space expected from both the new physics signal and several standard model backgrounds, searching for kinematic variables and distributions that would best serve as discriminators (Figure 5). Some Standard Model backgrounds are huge, such as the background associated with a Z boson plus a bottom quark final state, (Z + b). However, after detailed analysis, 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, and more complex multivariable analysis strategies are being devised.

Several technical challenges arise when one is simulating processes that may occur one time in a trillion. Each iteration must pass a battery of computationally expensive tests that simulate how a physical detector would respond. Since a brute-force approach is not feasible, we first identified a method to factorize the problem into stages that could be iteratively optimized to remove most of the samples that

could not satisfy the final conditions. At this point we could run 100 million iterations for each simulated process and generate enough statistics to provide a reliable numerical estimate. The goal of this analysis was not simply to identify a new problem but to discover correlations in the results that would suggest a method for avoiding the problem. The ability to detect and write interesting data was required for us to perform the variety of postprocessing steps that could specialize to a given experimental analysis. However, the data store from the production of billions of iterations would have required multiple terabytes using standard data structures. Therefore, we developed optimized algorithms to extract a dense set of results that would later pass any relevant test. These results were written to a newly optimized data format. Postprocessing programs were then developed to read these data and allow for high-level analysis. Even with these significant algorithmic improvements, the overhead of maintaining systematic control for such small effects required the Jazz cluster's ability to compress each CPU-months-long calculation into a few days, so that an improved iteration could be performed.

Coupled with previous work on two-lepton final states, the results of this new project 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 in situ measures can be developed to quantitatively control the uncertainties.

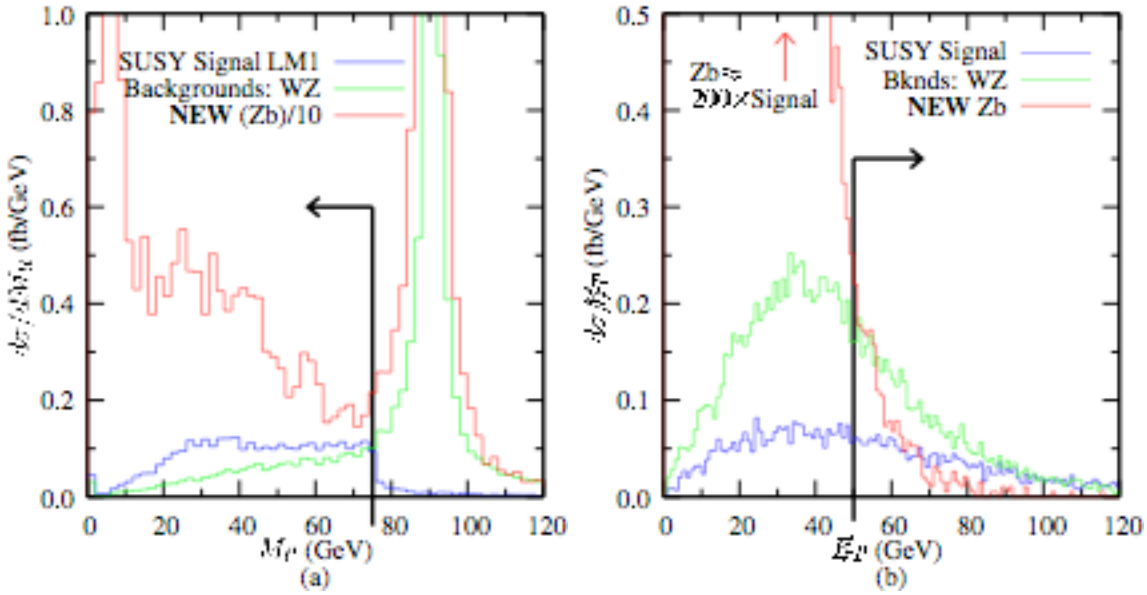


Figure 5. The (a) invariant mass of opposite-sign same-flavor leptons, and (b) missing energy, for events with a supersymmetric signal and two representative backgrounds. The newly calculated Zb background is more than 40 times larger than the WZ background (previously believed to be dominant). Arrows indicate acceptance cuts on the data that would significantly reduce the effect of this new background.

Organic Semiconductors

PI: Chaminda Kodituwakku (XFD)

Organic semiconductors are expected to become widely used in future applications such as efficient, low-cost solar cells is an area of great interest. Currently, copper phthalocyanine (CuPc) is one of the main materials being tested for solar cell applications, and initial work shows great promise. If the cost of solar power can be reduced sufficiently to make it comparable to fossil fuel costs, there would be enormous economic, environmental, and political advantages. However, relevant fundamental properties of CuPc for device applications, such as the excited state energies and properties, are not well understood.

To gain increased understanding, we are studying CuPC by using the electronic structure code Gaussian03. During the past year we measured electronic excitations and excitons on CuPc using inelastic x-ray scattering at the Advanced Photon Source. Gaussian03, which is more powerful than Gaussian98, enabled us to calculate occupied and unoccupied molecular orbitals as well as the possible electronic excitations. From these calculated results, we were able to explain most of our measured excitations (Figure 6). To date, we have calculated low-energy excitation states using up to 18 nodes; this number was chosen to involve the least amount of memory. We have measured data up to 12 eV. Our next step is to carry out accurate first-principles calculations for CuPc.

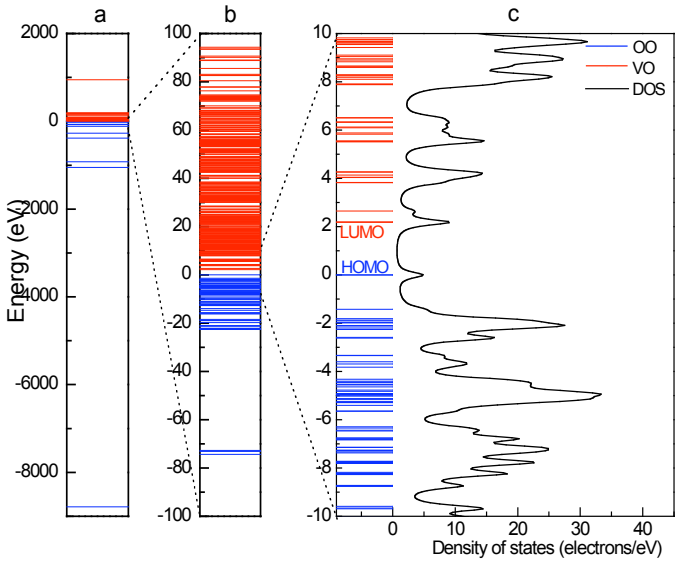


Figure 6. Calculated density of states of CuPc using the B3LYP hybrid density functional method. – shows the virtual orbitals (VO) and –shows the occupied orbitals (OO). (a) is the full set of VOs and OOs. and (b) is orbitals in between ±100 eV. Left side of (c) is OOs and VOs in between ±10 eV and right side is showing the calculated density of states with 300 meV resolution.

Publications and Presentations:

C. N. Kodituwakku, C.A. Burns, H. Sinn, A. Said, X. Wang, and T. Gog, "Inelastic X-ray Scattering Studies of the Charge Excitations in CuPc," preprint, 2007.

C. N.Kodituwakku, "Electronic Excitations in the Organic Semiconductor Copper Phthalocyanine," poster presentation, CuPc APS users meeting, Argonne, IL, May 2, 2007.

Nanotechnology

PI: Jeffrey Greeley (Center for Nanomaterials)

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. Because of the immense complexity of electrochemical liquid/solid interfaces, this field has been largely resistant to first-principles treatment. In the past few years, however, techniques have been developed that have begun to permit the theoretical analysis of electrocatalytic processes ranging from the electro-oxidation of carbon monoxide to the reduction of oxygen. Such 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. We are using these techniques, combined with simple thermodynamic formalisms to examine several electrochemical systems of interest to the fuel cell and catalysis communities.

We considered three major topics of catalytic significance during 2007. The first focused on the electro-oxidation of carbon monoxide at defect sites on platinum catalysts. For proper functioning of the hydrogen oxidation reaction in low-temperature fuel cells, it is essential that the anode catalyst (generally composed of platinum or platinum-containing alloys) be capable of efficiently oxidizing (and thereby disposing of) CO, a common contaminant in H_2 feed streams. To better understand how this reaction proceeds on different types of platinum surfaces and to identify surface structural features that might better catalyze CO oxidation, we performed extensive calculations to understand the energetics associated with the interaction of CO and water (the other key reactant associated with CO electrooxidation) with perfect Pt(111) terraces with clusters of one and two adsorbed Pt *adatoms* present, and Pt(211) steps (Figure 7). The latter surfaces represent models of defects that may, in some cases, be found on fuel cell anode catalysts. The calculations indicated that the highly undercoordinated adatoms are more active than are both perfect terraces and steps, suggesting that CO electrooxidation is a highly structure sensitive reaction that could be accelerated if highly undercoordinated surface features could be stabilized in environments relevant to technical fuel cells. Our results complement and enhance elegant experimental results obtained by coworkers in Argonne's Materials Science Division, and a combined theoretical/experimental paper detailing the preliminary results has been submitted for publication.

The second major effort involved studies of *dealloying* and corrosion processes in alloys of platinum and copper. In electrochemical cells, experiments have shown that, by operating at elevated electrode potentials, Cu may be selectively dissolved from a Pt-Cu alloy, leaving behind a compressed Pt lattice that is found to be highly active for electrochemical reduction of oxygen (a key reaction occurring on the cathodes of low-temperature fuel cells). We performed extensive calculations to determine the energetics of a variety of Pt and Cu mixtures at Pt-Cu-water interfaces; the indicated energetics were then used to calculate the electrode potentials at which Cu dissolves from the Pt. We found that Cu is stabilized when it is incorporated into Pt-Cu alloys on the dissolved Cu; the alloyed Cu dissolves at a higher potential than does pure, unalloyed Cu. These results agree well with experiments performed at the University of Houston, and a joint publication is now being prepared.

The third area of inquiry focused on nonaqueous heterogeneous catalysis. We analyzed the reaction of propane on subnanometer Pt clusters. Careful analysis of the energetics associated with the computed reaction pathways demonstrated that it is much easier to activate propane on subnanometer clusters than it is on bulk platinum samples. This result is in perfect agreement with recent experiments performed in Argonne's Chemistry division, and the experimental results associated with this work have demonstrated that subnanometer platinum can convert propane to propylene with unprecedented activity and selectivity.

The first two components of the project (CO electro-oxidation and Pt-Cu corrosion/dealloying) have contributed significantly to the understanding of experimental electrochemical results, and we hope that the work on CO electro-oxidation will ultimately lead to improved catalytic materials for low-temperature fuel cells. The third component (reaction of propane on subnanometer clusters) has focused attention on the critical role of defects and undercoordinated sites in this chemistry, and such insights may help to design the next generation of subnanometer clusters.

Publications and Presentations:

J. Greeley, "Nanoscale investigations of electrocatalysis," invited talk, ACS Fall Meeting, Boston, August 2007.

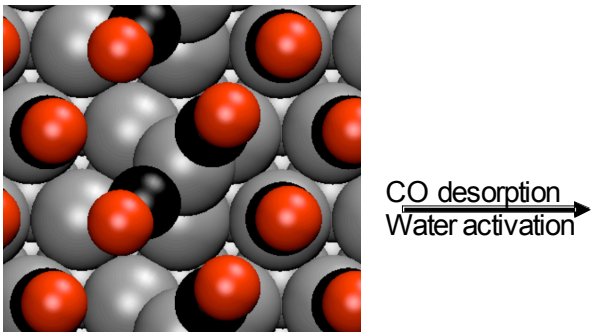


Figure 7: Schematic of CO electro-oxidation on adatoms on platinum surfaces

DNA Repair

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

Many proteins flip nucleotides from the DNA base stack into their active sites to remove or chemically modify bases for gene regulation and repair. We have been studying O6-alkylguanine-DNA alkyltransferase (AGT), which repairs alkylated guanine and thymine DNA bases by transferring the alkyl lesions irreversibly to an active site cysteine (Cys145). This unusual damage-reversal mechanism makes AGT of fundamental interest. Equally important, understanding its behavior is of medical significance because inhibitors are in clinical trials as anticancer therapeutics.

Simulations in 2006 revealed that the protein AGT flips damaged nucleotides for repair by a two-step process. This process is in contrast to the "push-pull" mechanism once speculated for nucleotide-flipping, in which the nucleotide that flips is "pushed" by a finger residue and "pulled" by specific interactins in the active site. The two-step process promotes a kinetic, rather than a thermodynamic, "gate-keeping" strategy for lesion discrimination. Such a mechanism allows the protein to scan the sequence rapidly in comparison to one involving full flipping.

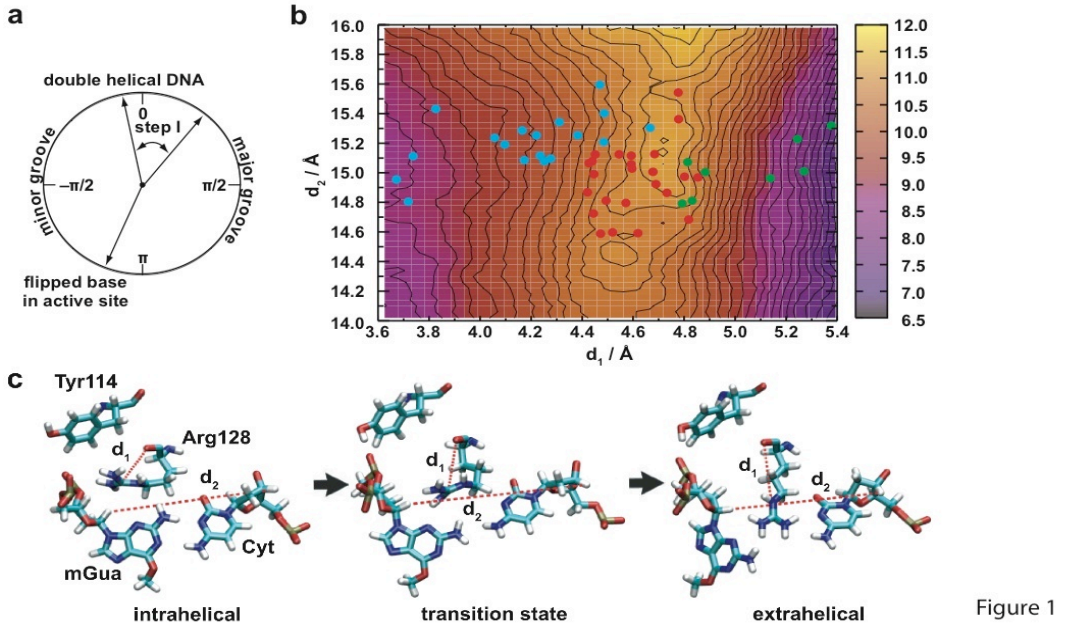
During 2006, we obtained explicit pathways for the first step in the two-step process. In 2007, we obtained pathways for the second step. Objective description of the paths requires identification of physically meaningful coordinates that are capable of distinguishing (meta)stable states from transition states defined dynamically by their probabilities to commit to a basin, *p*. Because of the large number of degrees of freedom in complex systems, relating p to structural and energetic properties of the system by trial and error is costly in terms of both human and computational resources and thus has been achieved for only a handful of relatively simple systems. Using informatic methods, we efficiently searched an enormous number of candidate physical variables for those combinations that best predict *p,* and we applied these methods to the AGT simulations to achieve a level of description unprecedented for a large biomolecular system.

Our results indicate that the finger residue (Arg128) captures spontaneous base pair fluctuations to stabilize an intermediate in which the lesion is extrahelical; a loop (residues Gly153 to Gly160) gates the active site and these motions determine the kinetics of the second step. Comparison of free energies for flipping guanine (Gua) and O6-methylguanine (mGua) suggested that the extrahelical intermediate identified enables kinetic discrimination between damaged and undamaged bases (Figures 8 and 9).

To set the work in context, transition path sampling has revolutionized the computational study of rare events in molecular systems over the past decade, but its application to complex biological systems has been limited. Novel means for generating initial paths, together with informatic methods that we introduced, now enable us to both harvest a statistically significant number of trajectories of a biomedically important stochastic process in its entirety and translate them into a physically understandable mechanism for the first time.

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," preprint, 2007.



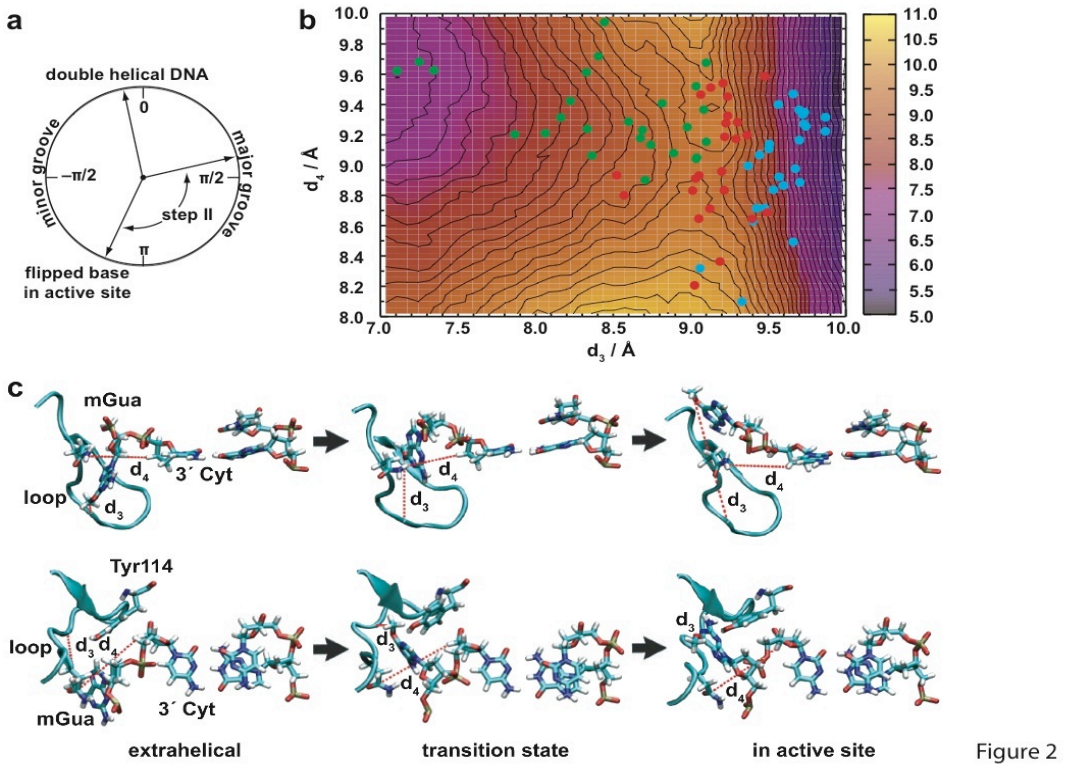


Figure 8. Flipping from the base stack to the extrahelical intermediate. (a) Range studied in terms of the pseudo-dihedral angle. (b) Free energy as a function of coordinates identified by informatic approach (contours spaced every 0.2 kcal/mol). Colored points indicate structures for which commitment probabilities (p) were calculated: mGua intrahelical (cyan), extrahelical (green) and at a transition state (red). (c) Representative structures for the transition.
Figure 9. Same as Fig. 8 for flipping from the extrahelical intermediate into the active site. In (b), colors indicate the extrahelical intermediate (green), transition states (red), and the base in the active-site (cyan). In (c), the upper and lower rows are two views of the same structures.

Nuclear and Particle Physics

PIs: Andreas Krassnigg, Craig Roberts, and Stewart Wright (Physics)

A central goal of contemporary nuclear and particle physics is to understand the properties of hadrons in terms of elementary excitations of quarks and gluons described by quantum chromodynamics (QCD). The formalism of Dyson-Schwinger equations (DSEs) provides a nonperturbative continuum approach to QCD. 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 information can be used both to illustrate exact results of the theory and to identify as yet unknown patterns. It is also an invaluable advantage of the approach compared to, for example, constituent-quark models. 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 of quarks means that no single quark has ever reached a detector. During 2007, we pursued two main directions: the structure of nucleons and their excitations in order to study the long-range part of the strong interaction, and the structure of mesons, focusing on their electroweak and strong form factors.

Nucleon Structure

In quantum field theory a nucleon appears as a pole in a six-point quark Green function, with the residue proportional to the nucleon's Faddeev amplitude. This is obtained from a Poincaré covariant Faddeev equation that adds all the possible quantum field theoretical exchanges and interactions that can take place between the three dressed-quarks constituting the nucleon. A merit of the Poincaré covariant Faddeev equation is that a modern understanding of the structure of dressed-quarks and dressed-gluons is straightforwardly incorporated; in other words, effects arising from the strong momentum dependence of these propagators are exhibited. During 2007, we rewrote the nucleon code to automate the construction of the Faddeev equation kernel; this has increased the speed by a factor of approximately 40. We used this framework to calculate and predict the *Q2*-dependence of the ratio of the neutron's electric and magnetic form factors. We expect to confirm our results with new data from Thomas Jefferson National Accelerator Facility (see Figure 10).

Meson Structure

In the Bethe-Salpeter amplitude of a pseudoscalar meson, one can identify structures representing nonzero quark orbital angular momentum (corresponding to L=1 in quantum mechanics). We investigated the orbital-angular-momentum content of ground and excited-state pseudoscalar mesons in the meson rest frame. For both states, angular momentum is most significant in the neighborhood of the chiral limit and decreases with increasing current-quark mass. Notably, at a given bound-state mass, the admixture of L = 1 components in the first radial excitation is roughly 15% greater than that in the ground state. Measured as a function of the current-quark mass, however, the situation is reversed.

We also started meson studies beyond the rainbow-ladder approximation. In particular we investigated an implementation of a quark-gluon vertex with a general structure in the Bethe-Salpeter equation and the corresponding Dyson-Schwinger equation for the quark propagator. The kernels of these two integral equations are linked by the axial-vector Ward-Takahashi identity, a relation whose satisfaction guarantees the correct implementation of the chiral symmetry of QCD and its dynamical and explicit breaking in the integral equations we solve and their solutions. Such a procedure based on a general vertex is complicated, which is reflected in the generation of the integral equation kernels. The corresponding code has reached the testing stage, but no concrete results have been obtained as yet.

The meson calculations have shown both the strengths and the weaknesses of the Bethe-Salpeter-equation approach. On the one hand, more complicated interaction terms will be needed to account for, e.g., the effects of quark orbital angular momentum in mesons and the structure and properties of radial meson excitations. On the other hand, we will need to take into account the character of a resonance for meson excitations; an adequate treatment of effects from strong decays of meson resonances is expected to play an important role in future studies in this project.

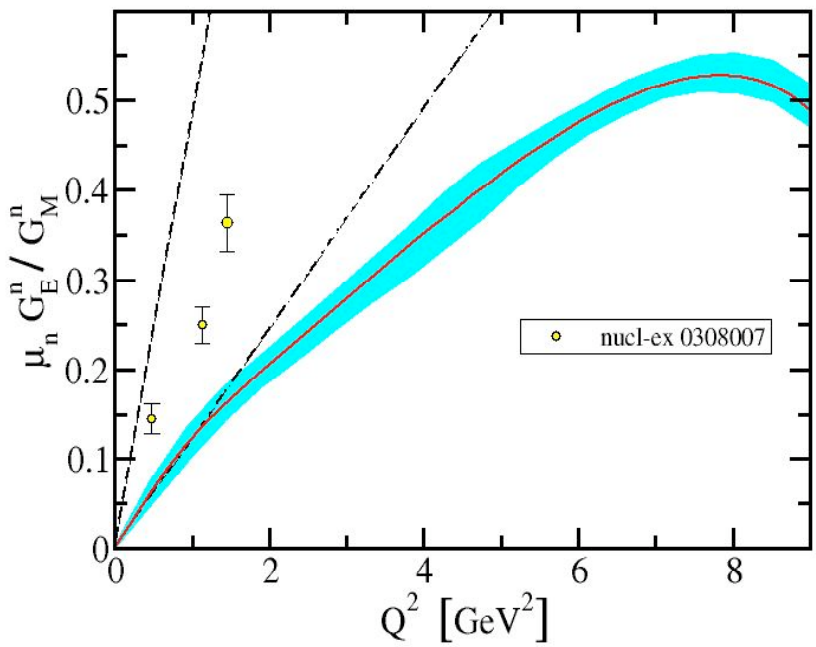


Figure 10. Predicted behavior of the ratio of the neutron's electric and magnetic form factors. The band shows an estimate of our error. The dashed lines show the expression –(rn2/6) Q2, with experimental and model values for the neutron charge radius. They are different because thus far the model describes only the quark-core contribution. Data are from R. Madey et al., *Phys. Rev. Lett.* 91 (2003) 122002. The figure is reprinted from *Nucl. Phys. A790*:10-16,2007.

Publications and Presentations:

M. S. Bhagwat, A. Höll, A. Krassnigg, and C. D. Roberts, "Theory and phenomenology of hadrons," *Nucl. Phys. A790*:10-16, 2007.

M. S. Bhagwat, A. Krassnigg, P. Maris, and C. D. Roberts, "Mind the gap," *Eur. Phys. J.* A31:630-637,2007.

M. S. Bhagwat, A. Höll, A. Krassnigg, C. D. Roberts, and S. V. Wright, "Schwinger functions and light-quark bound states," *Few Body Syst.* 40:209-235, 2007.

A. Krassnigg, "Bethe-Salpeter-equation studies of mesons," Workshop XXXV on Gross Properties of

Nuclei and Nuclear Excitations, "The structure and dynamics of hadrons," Hirschegg, Austria, January 15, 2007.

A. Krassnigg, "Integral-equation studies of meson physics," Universitätswochen für Theoretische Physik on "Conceptual and Numerical Challenges in Femto- and Peta-Scale Physics," Schladming, Austria, February 26, 2007.

A. Krassnigg, "The Bethe-Salpeter equation and mesons," invited talk, Workshop on "Confinement: Connecting the light- and heavy-quark domains," ECT*, Trento, Italy, March 13, 2007.

C. D. Roberts, "Baryons through the DSQCD looking glass," invited talk at the workshop Confinement: Connecting the Light- and Heavy-Quark Domains, ECT*, Trento, Italy, March 12, 2007.

C. D. Roberts, "Covariance, dynamics and symmetries, and hadron form factors," invited talk at the workshop "Exclusive Reactions at High Momentum Transfer," Jefferson Lab, Newport News, VA USA, May 23, 2007.

C. D. Roberts, "Dynamical chiral symmetry breaking and hadron structure," invited talk at the workshop on Strong Dynamics and Dynamical Chiral Symmetry Breaking, Argonne National Laboratory, Argonne, June 5, 2007.

C. D. Roberts, "Dynamics, symmetries, and hadron properties," invited talk, 11th International Symposium On Meson-Nucleon Physics and the Structure Of The Nucleon (MENU 2007), IKP, Forschungzentrum Jülich, Germany, September 10-14, 2007

C. D. Roberts, "Dyson-Schwinger equations – achievements and challenges," invited talk given at the Workshop on Dyson-Schwinger equations and their applications, Physics Department, Peking University, Beijing, China, August 14-18, 2007.

C. D. Roberts, "Hadron physics from Dyson-Schwinger equations," series of 4 lectures given at the Workshop on Dyson-Schwinger equations and their applications, Physics Department, Peking University, Beijing, China, August 14-18, 2007

C. D. Roberts, "Hadron properties and Dyson-Schwinger equations," invited talk given at the International School of Nuclear Physics, Erice-Sicily, 29th Course: Quarks in Hadrons and Nuclei, 16-24 September, 2007.

Computational Electromagnetics

PI: Misun Min (Mathematics and Computer Science)

Accurate and efficient numerical codes for solving electromagnetic problems have become critical. Current production codes use second-order finite-difference or finite-element time-domain methods that, because of their limited convergence rates, result in serious computational bottlenecks and high memory demands for the problems that require to resolve very high frequency electromagnetic fields. We have developed a high-order numerical code, called NEKCEM, that promises to overcome these bottlenecks.

NEKCEM is based on a spectral element, discontinuous Galerkin method that provides high-order accuracy than do traditional methods. Moreover, NEKCEM offers great geometric flexibility with body-fitted unstructured hexahedral meshes. Our experiments on Jazz show that CPU time increases linearly depending on the degree of freedom but is not dominated by increases in the degrees of the polynomials.

These results indicate that NEKCEM is likely to be valuable for high efficiency and accuracy.

Our work on Jazz has focused on implementing output format in parallel for NEKCEM. Nanopotonic simulations for the configuration such as forty nanospheres in funnel arrays require large of grids. Parallelization of the VTK output format for NEKCEM is necessary to visualize the electromagnetic field vectors on parallel machine. We designed output files in VTK format on each processor, and an XML file collecting the pieces of the VTK output data from each node to visualize a global solution on one processor using Paraview. Implementation has done to generate output in binary format, speeding up the loading time of the visual data 100 times faster than the previous format in ascii.

Wakefield simulations are critical for accelerator design. We have built meshes for various shapes of accelerating components: pillbox, collimator, and TESLA cavities that include linear, quadratic, circle, and elliptic variations in z-profile with circle or elliptic cross-sections. Studies for wake potentials are carried out for pillbox type and TESLA cavities. Parallelization of NEKCEM for wake field and wake potential calculations are implemented on Jazz (Figures 11 and 12). Further development should be carried out for picosecond bunch simulations on Jazz.

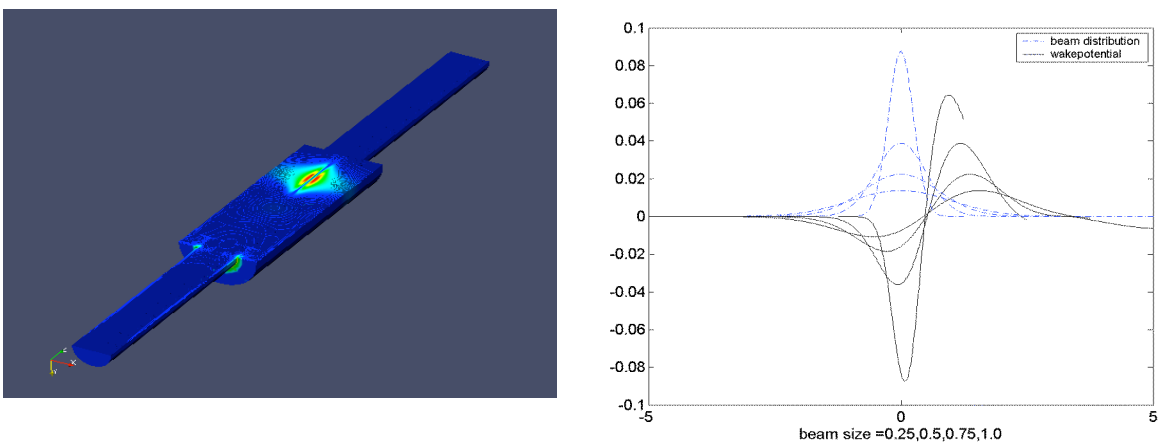


Figure 11. Gaussian beam moving on a pillbox cavity (left) and wake potentials for different bunch sizes (right).

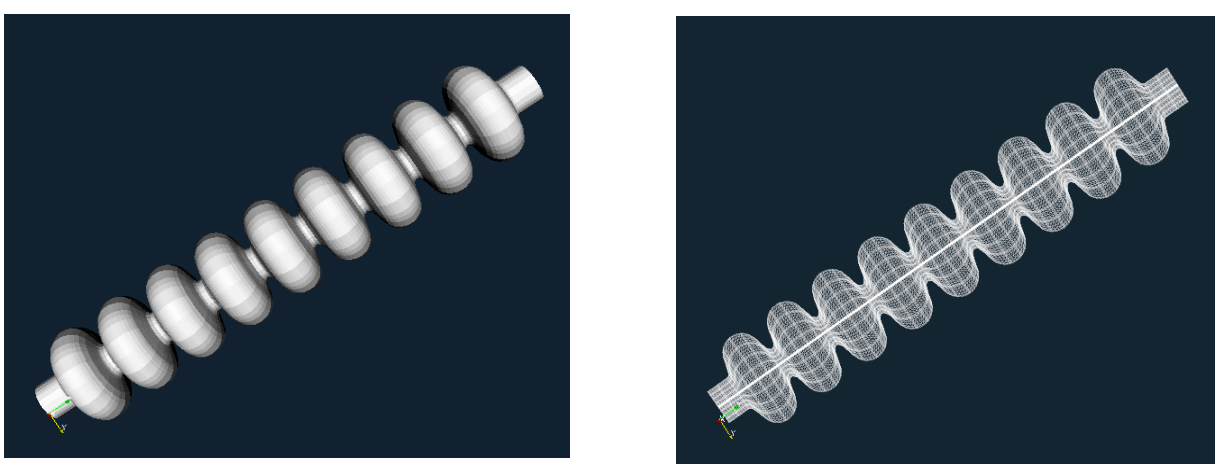


Figure 12. 9-cell TESLA cavity (left) and its spectral element hexahedral mesh (right)

Publications and Presentations:

M. S. Min, "Computational nanophotonics: NEKCEM," Office of Advanced Scientific Computing Research, Applied Mathematics Research Program Annual PI Meeting, poster session, May 2007.

M. S. Min, "Computational nanophotonics," Science Careers in Search of Women Conference, poster Session, Argonne National Laboratory, March 8, 2007.

M. S. Min, "Fourier spectral simulations for beam dynamics in accelerating structures," Minisymposium for the International Conference on Spectral and High Order Methods (ICOSAHOM), Beijing, China, June 18-22, 2007.

M. S. Min, "Spectral-element discontinuous Galerkin simulations with exponential time integrator for nanophotonics: NEKCEM software," International Conference On Spectral and High Order Methods (ICOSAHOM), Beijing, China, June 18-22, 2007.

M. S. Min, Y. H. Chin, P. F. Fischer, Y. C. Chae, and K. J. Kim, "Fourier spectral simulations for wake field in conducting cavities," in *Proc. of Particle Accelerator Conference (PAC),* THPAN090, 2007.

M. S. Min, Y. H. Chin, P. F. Fischer, Y. C. Chae, and K. J. Kim, "Fourier spectral simulations for wake field in conducting cavities," poster session in the 22nd Particle Accelerator Conference (PAC), Albuquerque, NM, June 25-29, 2007.

M. S. Min, P. F. Fischer, and Y. C. Chae, "Wake fields for TESLA accelerating structure: Spectral element discontinuous Galerkin simulations," in *Proc. of the 13th International Workshop on RF Superconductivity (SRF 2007),* TUP34.

M. S. Min, P. F. Fischer, and Y. C. Chae, "Spectral-element discontinuous Galerkin simulations for bunched beam in accelerating structures," in *Proc. of Particle Accelerator Conference (PAC),* THPAN091, 2007.

M. S. Min, P. F. Fischer, and Y. C. Chae, "Spectral-element discontinuous Galerkin simulations for bunched beam in accelerating structures," poster session in the 22nd Particle Accelerator Conference (PAC), Albuquerque, NM, June 25-29, 2007.

Climate Modeling

PI: Jay Larson (Mathematics and Computer Science)

The scientific challenge of developing advanced Earth system applications is daunting. Independently developed components may have incompatible interfaces or may be written in different computer languages. The high-performance computer platforms required by numerically intensive Earth system applications are complex, varied, rapidly evolving and multipart systems themselves. The Earth System Modeling Framework (ESMF) consists of software infrastructure for constructing and combining high-performance model components in the Earth science domain. It is in production use at the NASA Global Modeling and Assimilation Office, the U.S. Naval Research Laboratory, and the National Centers for Environmental Prrediction and is 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), Geophysical Fluid Dynamics Laboratory, MIT, and the Weather Research and Forecast model.

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 obtained several new results:
Performance. First-stage performance tests showed less than 5% overhead in time to solution for an ESMF-based model configuration compared to implementation based on the existing infrastructure (Model Coupling Toolkit). Moreover, performance tests conducted by JPL showed negligible run-time overhead for ESMF componentization.
Capability. The ESMF team completed prototypes of more flexible curvilinear, multipatch structured grids, unstructured grids, and a general regridding strategy. An initial implementation of new structured grids was released in July 2007. Initial regridding results were presented at the ESMF annual workshop on May 30-June 1, 2007, and the CCSM workshop on June 19-21, 2007.
Applications. Two applications transitioned to ESMF use this year were a HYCOM CICE coupled ocean-sea ice system and an ADCIRC-WASH123 coupled watershed system, for the U.S. Navy and Army, respectively. The number of ESMF science and computational components in the community at the working prototype level or beyond rose from 42 in July 2006 to 58 in July 2007.

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:

V. Balaji, "The Earth System Curator: Integration Technology for Models and Data," Princeton University, 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

Cecelia DeLuca, "Building Community and Capability through Common Infrastructure: ESMF and the Earth System Curator," NASA MAP meeting, College Park, MD, March 7-9, 2007.

Cecelia DeLuca, "ESMF/Curator Status," CCSM Software Engineering Working Group, Boulder, CO, March 16, 2007.

Chris Hill, "Coupling MITgcm and GEOS-5 using ESMF and MAPL," 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

Rich Hodur, "NRL Monterey Plans for Tropical Cyclone Modeling using the Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS)," 61st Interdepartmental Hurricane Conference, New Orleans, March 6, 2007.

John Michalakes, Tom Henderson, and Tom Black, "ESMF and the Weather Research and Forecast Model," 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

David Neckels, "A Parallel Rendezvous Regridding Algorithm," 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

David Neckels, "Wind Interpolation," CCSM Workshop, Breckenridge, CO, June 19-21, 2007.

David Neckels, "Derivative Preserving Interpolation with Application to Atmosphere-ocean Coupling," CCSM Workshop, Breckenridge, CO, June 19-21, 2007.

Don Stark, "An ocean nested regional climate model using POP and ROMS,", 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

Max Suarez, Arlindo da Silva, Chris Hill, Paul Schopf, V. Balaji, and Niki Zadeh, "Programming in ESMF with MAPL," 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

Alan Wallcraft, "Global Ocean Prediction Using HYCOM," presented at the First Annual Cray Technical Workshop, in Nashville, TN, February 28, 2007.

Shujia Zhou and Mark Iredell, "ESMF @ NCEP," 6th Annual ESMF Community Meeting, Boulder, CO, May 30-31, 2007.

Computed Tomography

PI: Eugene Koehl (Nuclear Engineering)

Scientists use 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, 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.

At Argonne, we are examining the issue of speed in the reconstruction of large volume, computed tomographic datasets obtained from x-ray sources, using Wintel/Pentium platforms. Our project comprises two parts. The first part seeks to reconstruct and display an 8-inch diameter volume of data from area detector arrays with 200-micron pixel resolution in less than 15 minutes. This work involves manipulating approximately a 2.5 GB dataset. The second part involves the reconstruction of a single, high-resolution computed tomography slice obtained from a linear, x-ray detector. The resulting image will accurately detail objects up to 30-inches in width, with a minimum 70-micron pixel resolution, with and without geometric magnification. Although only 10% of the large dataset size, the detector column count is an order of magnitude greater, pushing the number of computations for a single CT slice from 10^6 to 10^{12} (Figure 13).

During 2007, we addressed the problem of exceeding the 32-bit limit of typical compilers and operating systems when they are required to handle very large datasets: from 2 GB to 22 GB (when scanning objects ~14.5 inches in diameter). Some success has been achieved on single-processor Wintel systems; and we anticipate that the technology will allow highly detailed, near-real time imaging of small, stationary power system rotors and sections of larger mechanical systems comprising composite and emerging engineering materials.

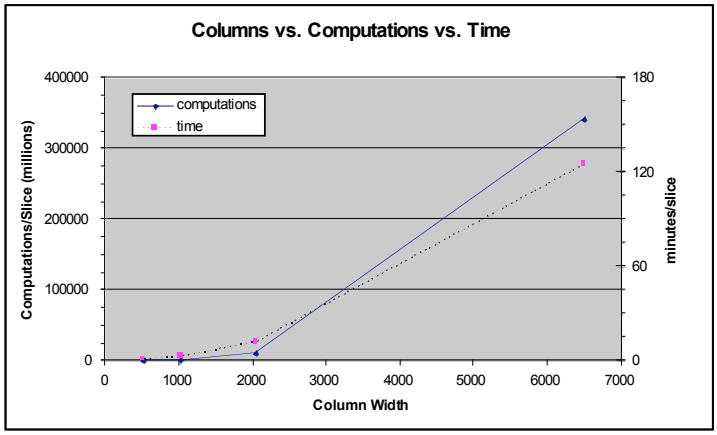


Figure 13. Number of computations and time required for various computed tomography slices

Global Climate Modeling

PI: Rob Jacob (Mathematics and Computer Science)

Climate model development is focused on increasing the fidelity of the simulation compared to the observations. At Argonne, we are seeking to understand how the interactions between the atmosphere, ocean, cryosphere, and land-mass distribution function to control climate on a geologic time scale. Based on the theory of Walker, at the million-year time scale the atmospheric CO_2 level is controlled mainly by a source, volcanism, and a sink, silicate weathering. We have built a program called GEOCLIM to study this theory. A main component in GEOCLIM is a coupled climate model called FOAM, or Fast Ocean Atmosphere Model. The main features of FOAM are a low-resolution model of the global atmosphere and an efficient model of the global ocean and a fully parallel implementation of the numerics. We combine FOAM output with dynamic vegetation and carbon cycle models to understand past concentrations of carbon dioxide in the atmosphere.

During 2007, we began work on the next major release of FOAM. We consolidated most of the physical constants used throughout the program into a set of text files that will make these values easier to identify and control by end users. It also removes duplication and inconsistencies within FOAM. Using Jazz, we ported FOAM to the NAG and Absoft compilers. We also coupled FOAM to the latest version of the ocean model Om3 and switched its compilation from single to double precision.

We have had some exciting results using our GEOCLIM model. Preliminary results in 2006 indicated that the breakup of Pangea (the supercontinent that existed during the Paleozoic and Mesozoic eras) led to a steady decrease in CO_2 concentration in the atmosphere during the Mesozoic era. In 2007, we studied the sensitivity of this result to a parametric law linking the rate of silicate weathering to the temperature and to the runoff. Using a set of relationships between runoff and silicate weathering as a function of the geoclimatic zone, we explored the impact of the "shield effect" (the vegetation in the tropics shields its bedrock from weathering) on the Mesozoic evolution of climate. Our results suggest that atmospheric CO_2 has been underestimated, evidencing a complex interplay between the paleogeographic setting and the shield effect (Figure 14). In particular, calculated atmospheric CO_2 during the early to middle Jurassic period rises up to 1600 ppmv, whereas it was limited to 700 ppmv when the shield effect was neglected, corresponding to a global warming of more than 4°C. This work emphasizes the need for numerical models that describe the growth of the weathering profiles that can be coupled to vegetation and climate model to investigate biogeochemical cycles and climate evolution, even at the geological timescale.

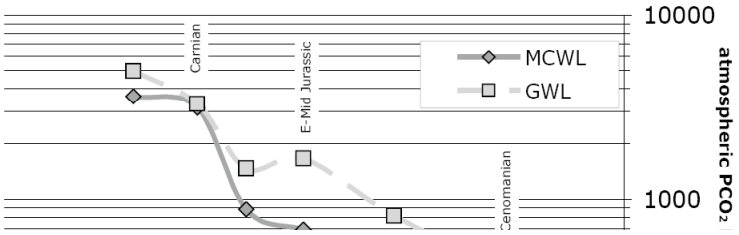


Figure 14. Mesozoic evolution of the CO_2 partial pressure calculated by the GEOCLIM model, using two different set of weathering laws: MCWL simulations used the previous parametric law, GWL are with the new law accounting for geoclimatic zones.

Publications and Presentations:

Y. Donnadieu, Y. Goddéris, R. Pierrehumbert, and G. Dromart, "Cold episodes inside Jurassic times: Is the carbonate deposition engine controlling atmospheric CO_2?" European Geosciences Union, Vienna, Austria, 2007.

Y. Donnadieu, Y. Goddéris, C. DeVargas, R. Pierrehumbert and G. Dromart, "The rise of nanoplankton calcification correlates with tectonically driven massive fall of atmospheric CO_2," International Conference on Paleoceanogaphy, Shangai, China, 2007.

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,* in press, 2007.

Y. Goddéris, Y. Donnadieu, C. De Vargas, R. Pierrehumbert, and G. Dromart, "The rise of nanoplankton calcification correlates with tectonically-driven massive fall of atmospheric CO_2," *EPSL*, in revision, 2007.

G. Le Hir, G. Ramstein, Y. Donnadieu, and R. T. Pierrehumbert, "Investigating plausible mechanisms to trigger a deglaciation from a hard snowball Earth," *C.R. Géosciences*, 339 (3-4): 274-287, 2007.

Multimethod Linear Solvers in Terascale PDE-Based Simulations

PIs: Boyana Norris, 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. Thus, we are exploring *polyalgorithmic multimethod linear solvers* in the context of several parallel applications, including flow in a driven cavity, compressible Euler flow, radiation transport, and fusion to potentially improve the execution time and reliability of linear system solution. We are developing composite solvers, which

provide linear solution by using a sequence of preconditioned iterative methods on a given system until convergence is achieved; this approach enhances reliability by overcoming the potential failure of a particular method. 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. This situation has motivated us also to develop 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.

During 2007 we used machine learning algorithms to generate functions that map particular linear systems to suitable algebraic solvers. A mapping function consists of a feature extractor to compute numerical quantities that are predictive of the performance of solvers and a classifier that maps each possible feature vector to a recommended solver. Our first set of experiments focused on driven cavity flow with pseudo-transient continuation (a standard PETSc example code), where we ran simulations on a dataset of about 15,000 entries. Our second problem set is composed of linear systems created during the execution of the M3D application from PPPL, a parallel three-dimensional plasma simulation code suitable for performing linear and nonlinear calculations of plasma in toroidal topologies. These preliminary results show the promise of machine learning technology in helping to select appropriate multimethod linear solver algorithms for large-scale applications

Our research on multimethod solvers for large-scale, PDE-based simulations using Jazz has motivated new research on computational quality-of-service (CQoS), a key component technology initiative within the SciDAC Center for Technology for Advanced Scientific Component Software (TASCS). We plan to apply these ideas in multimethod solvers within new multi-institutional SciDAC collaborations in fusion and accelerator modeling via the projects FACETS (Framework Application for Core-Edge Transport Simulations) and COMPASS (Community Petascale Project for Accelerator Science and Simulation). Transitioning these ideas into practice through these new collaborations is a significant step during which we will further motivate, validate, and extend this work as needed by the fusion and accelerator modeling communities.

As part of the CQoS initiative in the TASCS project, we are developing software that supports performance monitoring, analysis, and adaptation of important numerical kernels, such as nonlinear and linear solvers. We are in the process of developing capabilities for monitoring, checkpointing, and gathering of performance data, which 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:

S. Bhowmick, V. Eijkhout, Y. Freund, E. Fuentes, and D. Keyes, “Application of Machine Learning to the Selection of Sparse Linear Solvers,” preprint, 2007.

S. Bhowmick, D. Keyes, Y. Freund, V. Eijkhout, and E. Fuentes, “Application of Machine Learning for Solver Selection,” CScADS Workshop on Libraries and Algorithms for Petascale Applications July 30 - August 2, 2007, Snowbird, Utah.

S. Bhowmick, D. Keyes, Y. Freund, V. Eijkhout, and E. Fuentes, “Implementing Machine Learning for Solver Selection,” SIAM Conference on Computational Science and Engineering (CSE07), Poster, Costa Mesa, California, February, 2007.

D. Keyes and L. C. McInnes, "TOPS Solvers and Code Coupling: Opportunities in Core-Edge Fusion Simulations," FACETS Project Kickoff Meeting, November 2006, Boulder, CO.

L. C. McInnes, T. Dahlgren, J. Nieplocha, D. Bernholdt, B. Allan, R. Armstrong, D. Chavarria, W. Elwasif, I. Gorton, J. Kenny, M. Krishan, A. Malony, B. Norris, J. Ray, and S. Shende, "Research Initiatives for Plug-and-Play Scientific Computing," *Journal of Physics: Conference Series 78* (2007).

Aerodynamic Drag for Heavy Vehicles

PI: William Pointer (Nuclear Engineering)

Argonne is participating in a multilaboratory effort to enable and encourage the use of computational prediction capability by the heavy vehicle industry to aid in the improvement of fuel economy in class 3-8 trucks. The Argonne component is providing best practice guidelines for the use of current generation computational tools and a baseline for comparison with more advanced methodologies. Based on the guidelines developed to date, a series of applications studies have been completed to look at the effects of small changes in tractor geometry on fuel economy.

Work in 2007 focused on applying lessons learned from previous years to a series of parametric design studies that focused on the impact of small changes in the configuration of a tractor's radiator. The program as a whole has dramatically improved the efficiency of the process of building and running a model so that a very large machine is no longer needed for an individual case. Jazz has been critical to this year's efforts by allowing a large number of design study cases to be completed simultaneously as a demonstration of the potential for automated optimization of vehicle designs in the near future.

Results from prior years have had a significant impact, contributing to the adoption of CAE into the design cycle by all of the major manufacturers. This year's efforts have further emphasized the importance of designing an integrated system rather than focusing exclusively on the design of each part. The new 2007 EPA emissions standards and the looming 2010 emissions standards for tractor-trailer vehicles have greatly increased the burden on the engine cooling system so that much larger radiators may be needed to meet cooling needs. This knowledge is driving significant investment in electrification to enable the use of smaller radiators. This study has shown that signficant fuel economy savings cannot be realized by blindly reducing the radiator size with no consideration of the design of the full system. The study has also shown that small increases in radiator size can be absorbed with no significant fuel use penalty if the system is designed appropriately.

Publications and Presentations:

W. David Pointer, Tanju Sofu, and David Weber, "Applicability of Commercial CFD Tools for Assessment of Heavy Vehicle Aerodynamic Characteristics," in *Proc, of the Aerodynamics of Heavy Vehicles: Trucks, Buses and Trains*, Tahoe, CA, August 2007

Advanced Plasma Applications

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

Recent advances in laser and discharge systems with high repetition rate and high average power suggest the feasibility of modular, flexible, and relatively inexpensive microelectronic production facilities based on laser and discharge plasma sources. However, effective commercial utilization of given technology necessitates investigation and optimization not only of power sources but also plasma irradiation parameters, plasma energy deposition, target material, device design, and debris mitigation.
To this end, the HEIGHTS group at Argonne developed several versions of 2D and 3D computer models that include all the cited processes of laser-material interaction and discharge-produced plasma processes. The integrated models use the total variation diminishing (TVD) scheme in the Lax-Friedrich formulation to describe the laser produced plasma motion; an implicit scheme with sparse linear algebraic equations solver for heat transport in plasma and magnetic diffusion processes; an explicit scheme for heat transfer in neutral material; and a weighted Monte Carlo model for radiation transport and laser energy deposition.

During 2007, we enhanced these models in several ways. For the 2D case, heat transport and magnetic diffusion models were developed with splitting by directions and with a tridiagonal matrix solver. These modifications allow researchers to optimize sequential 2D code. For the 3D case, modeling of data distribution among different processors was changed. In the previous version the main processor controlled all the data in the domain. At each time step the main processor distributed data among other processors; the processors then calculated their part of domain, and the main processor gathered results. Now each processor owns data for its part of domain and exchanges information in neighboring cells. The processors save data in common files using MPI input/output subroutines. The new model decreases memory usage on main processor and enhances parallel code performance. Benchmarking results with the HEIGHTS-LPP packages are presented in Figure 15. HEIGHTS shows better agreement with experimental data than does the well-known LASNEX code.

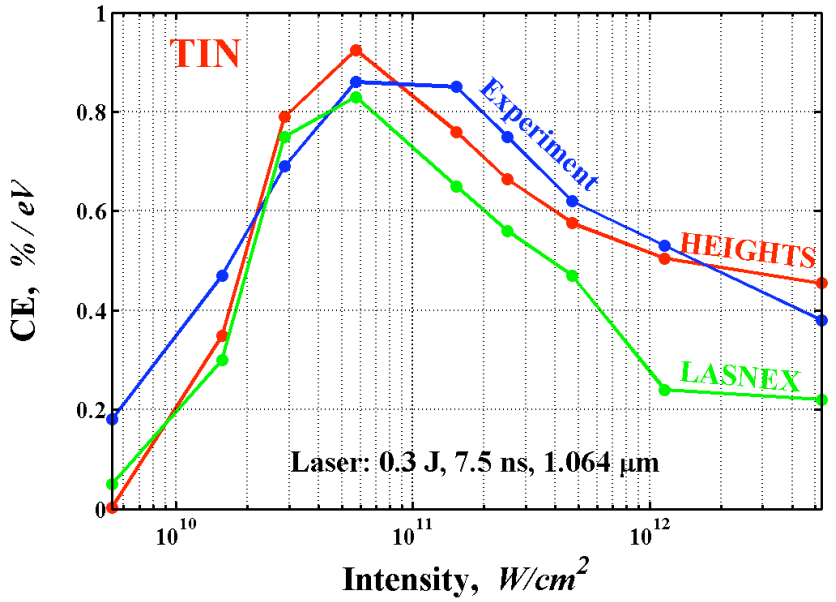


Figure 15. Efficiency of LPP device with tin planar target. Comparison of experimental and calculated results.

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*, vol. 25, no. 2, pp. 143-154, 2007.

A. Hassanein, V. Sizyuk, T. Sizyuk, and V. Morozov, "Optimization of EUV laser and discharge devices for high-volume manufacturing," in *Proceedings of SPIE. Emerging Lithographic Technologies XI*, San Jose, CA, vol. 6517, p. 65171X, SPIE, Bellingham, WA, 2007.

Advanced Methods for Calculating Fundamental Atomic Properties

PI: Vitali Morozov (Mathematics and Computer Science)

The HEIGHTS team at Argonne is developing a comprehensive integrated package for simulation laboratory and natural plasma sources. Typical examples of HEIGHTS applications are demonstrated by computer simulation of innovative plasma-facing fusion reactor surfaces for application both magnetic fusion and inertial fusion, target design and material lifetime under high-density irradiation for high-energy and nuclear physics applications, advanced fuel and nuclear reactor materials for fission, nanolithography devices for perspective chip manufacturing, discharge produced plasma and laser-target interaction simulation for high-energy density physics, and microlithography.

The core of HEIGHTS applications is a magnetohydrodynamics (MHD) model, which represents the conservation of mass, momentum, energy, and magnetic flux. The energy exchange is determined by a number of energy transport processes, such as magnetic diffusion, heat conduction, radiation energy loss and the others. Depending on the goal of the numerical simulation, the modeled device is subject to parametric study, optimization, and constraints. Results of the simulation are used to study the erosion and lifetime of device components, intensity and parameters of the generated plasma, operating conditions of the device, and so forth. The driving force of the device, such as the power supply, laser pulse, or ion beam, is implemented as a part of the total energy balance. The magnetohydrodynamic model, heat transport, and radiation transfer simulations depend on the accuracy and completeness of various plasma properties, such as equation of state, thermal conductivity, specific heat, ionicity, and opacities. Because these models depend on adequate calculation of energetic and probabilistic atomic properties, ionization and excitation rates, broadening of spectral lines, detailed description of line profiles, and shift of spectral lines in plasma, an adequate description of the atomic structures is essential.

Our efforts in 2007 focused on incorporating advanced atomic physics methods into the spectroscopically resolved generation of optical coefficients within the radiation transport calculation. The difficulty arises from the large number of spectral lines within the broad energy range. To stay practical, the radiation transport simulations can utilize preliminary tabulated opacities with no more than 3000-4000 spectral points, while the accuracy of atomic methods allows one to generate detailed coefficients with up to a million points to reflect very specific optical properties of plasma.

The very complicated structure of the optical coefficient and, therefore, the requirement to have a very fine energy mesh are generally unavoidable, because many-electron atoms and ions have an extremely large number of excited states. The resolution of the rate equations, which determine all possible transformations of the atom due to various collisional and radiative mechanisms in plasma, leads to inversion of practically intractable large matrices. Furthermore, validated atomic data is not always available for all quantum states and this leads to develop a variety of

simplified and yet adequate models. The models rely either on treating a reduced number of ions and extensive set of states or on examining a larger number of ions at the expense of averaged and less detail states for each ion. In HEIGHTS, we benefit from both approaches admitting several levels of atomic state refinement.

We have incorporated the resolution of full LSJ-split energy levels and correspondent dipole transitions into a collisional-radiation equilibrium approximation for generation bound-bound optical coefficients. As expected, the increased number of spectral lines has turned the coefficient indistinct to continuum in several energy ranges, with 10 to 100 times larger absorption in the picks of strong lines and approximately 10 to 100 times smaller at the picks of unresolved HFS lines. The influence of such a difference of the coefficients is not fully understood and requires additional study.

The second part of our project was to develop an efficient parallel algorithm for radiation transfer. During 2007, we successfully implemented several radiation transport methods with different ways of distributing the underlying MHD domain. If the domain is small, a current cell can be considered a center of collecting the photons over prescribed directions of the radiation movement. If the domain is distributed (more typical case), the radiation transport should account for transitory photon moves, which, because of the strong dependence of emission plasma properties from local thermodynamic parameters, lead to strong imbalance. We were successful in developing domain decomposition radiation transport with efficiency of approximately 0.5 for intermediate (up to 128 nodes) systems.

Results of tin opacity calculations for typical discharge-produced plasma parameters (Te=40 eV, d= 0.01 g/cm3) are shown in Figure 16. The left figure is the result of near 3000 HFS lines without electrostatic and spin-orbit interactions. The right figure is the result of detail transition accounting approximation (more that a million) with electrostatic and spin-orbit interactions included for LS scheme of addition angular moments.

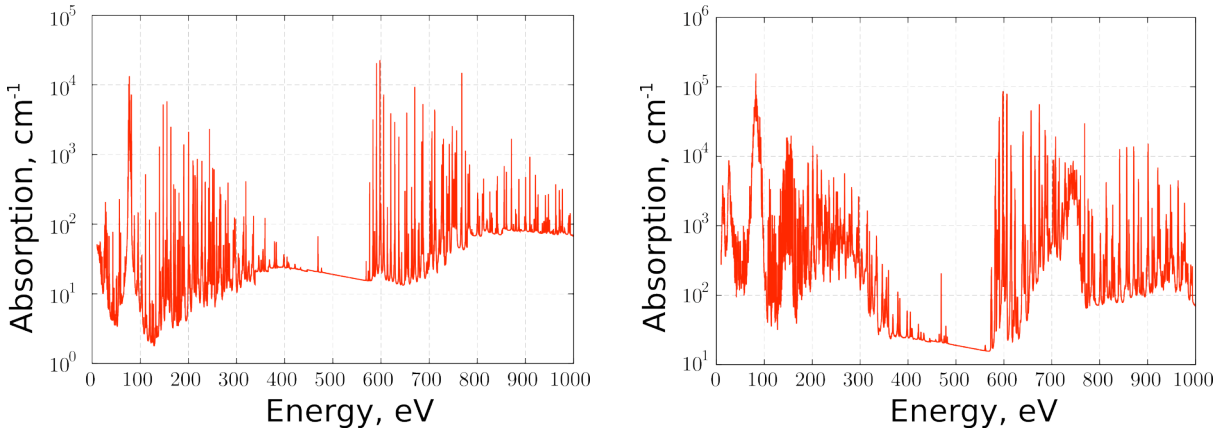


Figure 16. Sn opacity, calculated with configuration (left) and details transition accounting (right)

Publications and Presentations:

V. Morozov, " Computer Simulation and Numerical Methods of Detailed Atomic Physics Calculations for Various Applications," LANS seminar, Argonne National Laboratory, April 11, 2007.

V. Morozov, "Part I: HEIGHTS-ATOM—A Package for Calculation Atomic Characteristics," Argonne National Laboratory Report, 2007.

Validation of Neutronics Tools for Advanced Burner Reactor Design

PI: Taek K. Kim (Nuclear Engineering)

The Advanced Burner Reactor (ABR) is one of the three major technologies to be demonstrated in the Global Nuclear Energy Partnership program. The primary mission of the ABR is to demonstrate the transmutation of transuranics recovered from the light water reactor spent fuel, and hence the benefits of the fuel cycle closure to nuclear waste management. Design of the ABR and confirmation of its safety require a validated set of analysis tools for representing neutronics, irradiation behavior, and thermal-hydraulic, structural and mechanical, and chemical interaction and species transport phenomena in steady-state and transient conditions. Characterization of prediction uncertainties is central to the validation of the analysis tools.

Neutronics validation has been based mostly on the performance of a large number of critical experiments that allow a global validation of both data and calculation methods of global phenomena. The objective has been to define bias factors and associated uncertainties (to be used to define design/operation margins) for most design integral parameters. The Argonne suite of fast reactor neutronics analysis codes has been extensively validated against critical experiments and high-fidelity Monte Carlo solution. The neutronics methodologies including depletion calculations have also been validated by using a large experimental database derived from destruction measurements of EBR-II experimental test assemblies and processing irradiated EBR-II fuel assemblies in the Fuel Conditioning Facility.

Compared to conventional fast breeder reactors, however, the ABR would have additional neutronics issues: core and reflector interface effects due to the lack of fertile blanket transition zone, significant transport effects related to enhanced leakage due to a lower fuel density to achieve a lower conversion ratio, and degraded reactivity coefficients due to a higher minor actinide content and a high fissile to fertile ratio. More accurate prediction of fuel evolution is also desirable to characterize the spent fuel with fewer measurements in the reprocessing plant. In addition, The U.S. Cross Section Evaluation Working Group released in December 2006 the next-generation general -purpose Evaluated Nuclear Data File, ENDF/B-VII.0 as recommended nuclear data for advanced nuclear science and technology applications. Therefore, validation studies of Argonne neutronics analysis tools and nuclear data for ABR design applications have been initiated.

As an initial effort, a numerical benchmark problem (Figure 17) was developed based on the reference metal fuel core concept of 250 MWt Advanced Burner Test Reactor. Core multiplication factor, control assembly worth, sodium void worth, temperature defect, and power distributions were calculated and compared with MCNP5 Monte Carlo solutions. For MCNP5 Monte Carlo calculations at elevated temperatures, MCNP cross-section libraries were generated by using the NJOY code.

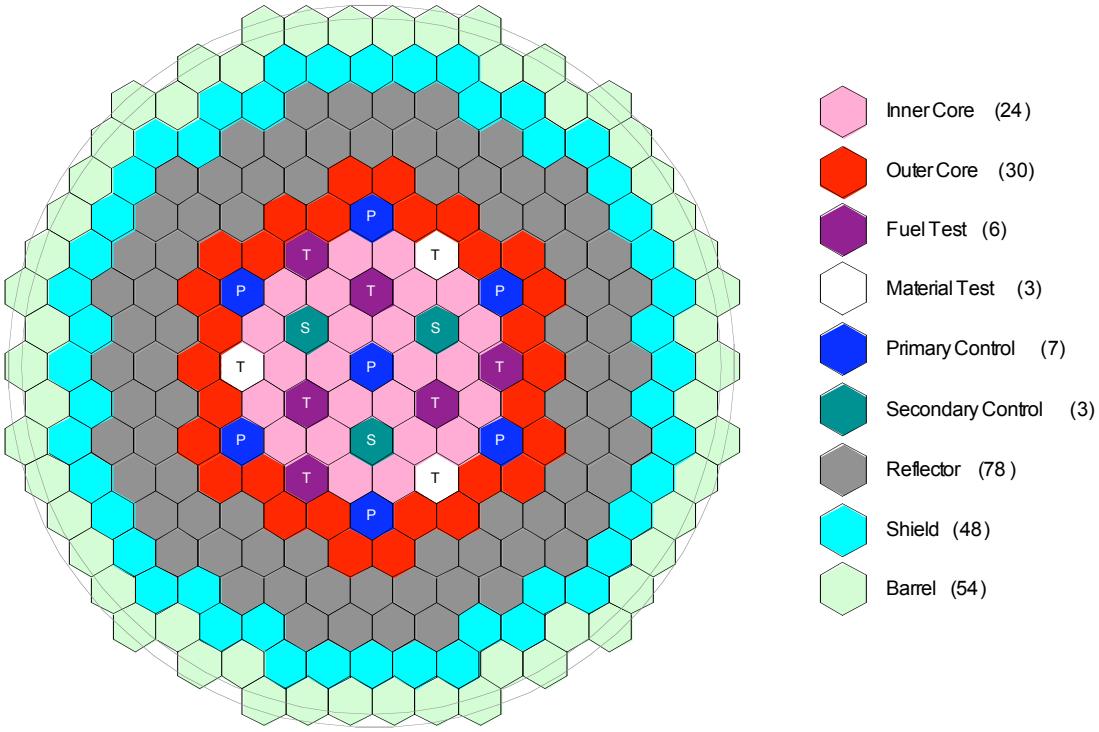


Figure 17. Core configuration of 250 MWt ABTR benchmark problem

CO Hydrogenation with Co Carbonyl Catalysts

PIs: Randall Meyer (Department of Chemical Engineering, University of Illinois at Chicago), Jerry Rathke and Robert Klingler (Chemical 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 this process 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 we can precisely identify the reaction pathways for the homogeneous catalyst and understand what factors influence the catalyst's selectivity, then we can use this knowledge to aid in the design of new heterogeneous catalysts.

In addition, Co-based catalysts are useful for two related reactions. First, the Co carbonyl catalyst has been used for hydroformylation of olefins to aldehydes in commercial processes dating back almost 70 years. However, despite such a long history of success, the underlying mechanism and rate limiting steps are not properly identified. Co carbonyl catalysts have also enjoyed success as homologation catalysts. Because of recent concerns regarding the price of petroleum-based fuels, there exists a renewed interest in ethanol. Currently, ethanol is primarily produced through fermentation of corn. However, this process requires a separation of water from the ethanol fuel product. As an alternative, a "dry" ethanol process has been developed at Argonne relying on the homologation of methanol with metal carbonyl catalysts.

We have used the VASP (Vienna *Ab Initio* Simulation Package) density functional theory code to investigate the hydrogenation of CO with Co-based homogeneous catalysts. The primary aim of our work is to understand how to improve selectivity of these catalysts. Recently we were able to identify intermediates for the production of methanol and methyl formate and ethylene glycol. The full potential energy surface is depicted in Figure 18. Two product pathways are possible based on the insertion of CO leading to either ethylene glycol and methanol (hydroxymethyl route) or methyl formate and methanol (methoxy route). Experiments have indicated that the methoxy route is preferred to the hydroxymethyl route when the hydrogenation reaction is performed supercritical CO. Furthermore, our calculation of the overall barrier to CO hydrogenation is in excellent agreement with experiments.

Additional calculations on $Mn(CO)_5$-based systems have begun. Barriers to hydrogenation products are found to be somewhat higher in Mn-based catalysts. We have also examined the ligand substitution on the catalysis. The use of phosphine ligands does not seem to greatly affect the overall reaction rate but according to calculations may shift the product distribution somewhat decreasing the amount of ethylene glycol and increasing methyl formate production.

Publications and Presentations:

"A Combined Theoretical and Experimental Study of CO Hydrogenation with Co Carbonyl Catalysts," presented at the 233rd Meeting of the American Chemical Society, Chicago, IL, March 25- 29, 2007

"Investigation of CO Hydrogenation Mechanisms using Co Carbonyl Catalysts," presented at the 20th North American Catalysis Society, Houston, TX, June 17-22, 2007

"Mechanistic Study of CO Hydrogenation with Co Carbonyl Catalysts," presented at the 13th International Symposium on the Relationships between Heterogeneous and Homogeneous Catalysis, Berkeley, CA, July 16-20, 2007

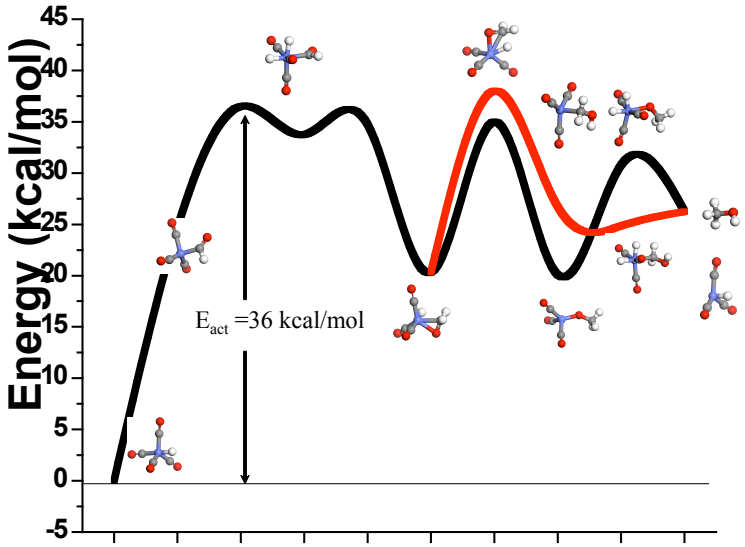


Figure 18. View of the potential energy surface for CO hydrogenation. The black line indicates the energy of intermediates leading to methanol production through the methoxy route. The red line indicates an alternative path leading to the formation of methanol through a hydroxymethyl intermediate.

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

PI: Tanju Sofu (Nuclear Engineering)

The Numerical Nuclear Reactor (NNR) software system is being developed to perform coupled neutronic and thermal-hydraulic calculations for light-water reactor core analysis with pin-by-pin representation of the fuel assemblies and intra-pin level thermal feedback. In 2007, we used NNR to address the operational and design issues related to fuel performance in boiling water reactor (BWR) fuel assemblies. Specifically, we used the code to analyze four fuel assemblies for an operating BWR plant to better understand the conditions that lead to formation of excessive crud and eventual fuel failure (Figure 19).

The results of these high-fidelity analyses of the selected fuel assemblies with explicit representation of individual fuel pins and surrounding coolant channels are being correlated with the observed crud formation patterns. The broad objective of this effort is to provide a comprehensive simulation capability to enhance quantification of margin to crud-induced fuel failure from fuel-duty perspective.

Our most recent accomplishment is to integrate in a single framework various software capabilities, including the extension of the neutronics module to treat heterogeneities in BWR core configurations, and a new Eulerian two-phase boiling model in the CFD-based thermal-hydraulic module. This integrated framework can now be used for coupled calculations including neutronic, hydraulic, and thermal effects.

Publications and Presentations:

D. P. Weber, Tanju Sofu, Won Sik Yang, Thomas J. Downar, Justin W. Thomas, Zhaopeng Zhong, Jin Young Cho, Kang Seog Kim, Tae Hyun Chun, Han Gyu Joo, and Chang Hyo Kim, "High Fidelity LWR Analysis with the Numerical Nuclear Reactor," *Nuclear Science and Engineering*, 155, 395-408 (2007).

T. Sofu, "Coupled BWR Calculations with the Numerical Nuclear Reactor Software System," Joint Intl. Topical Mtg. on Math. & Computation and Supercomputing in Nuclear Applications (M&C+SNA 2007), April 15-19, 2007, Monterey, California (2007).

A. Tentner et al., "Development and Validation of an Extended Two-Phase Computational Fluid Dynamics Model for the Analysis of Boiling Flow in Reactor Fuel Assemblies," in *Proceedings of 2007 International Congress on Advances in Nuclear Power Plants* (ICAPP 2007), May 13-18, 2007, Nice, France (2007).

Acknowledgment: This program is funded by the Electric Power Research Institute Fuel Reliability Program.

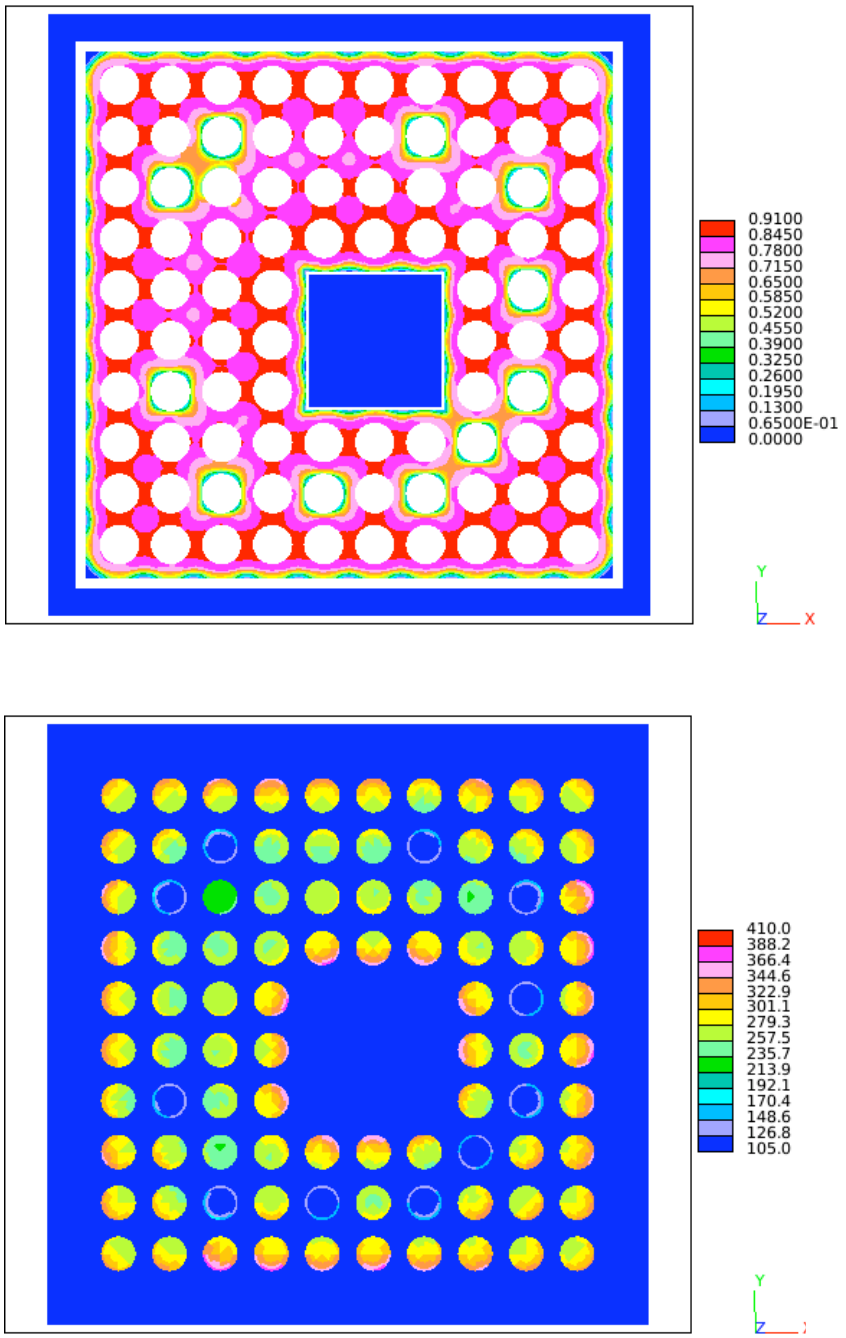


Figure 19. Pin power distribution in W/cc (top) and corresponding void fraction (bottom) in core mid-plane for a typical BWR fuel bundle using coupled NNR simulation capabilities

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, Argonne)

Bacterial chemotaxis in *Escherichia coli* is a canonical system for the study of signal transduction. A remarkable feature of this system is the coexistence of precise adaptation in population with large fluctuating cellular behavior in single cells. Using a stochastic model, we found that the large behavioral variability experimentally observed in nonstimulated cells is a direct consequence of the architecture of this adaptive system. Reversible covalent modification cycles, in which methylation and demethylation reactions antagonistically regulate the activity of receptor-kinase complexes, operate outside the region of first-order kinetics. Hence, the receptor-kinase that governs cellular behavior exhibits a sigmoidal activation curve that simultaneously amplifies the inherent stochastic fluctuations in the system and lengthens the relaxation time in response to stimulus. Because stochastic fluctuations cause large behavioral variability and the relaxation time governs the average duration of runs in response to small stimuli, cells with the greatest fluctuating behavior display the largest chemotactic response (Figure 20).

Previously, we had to remove all global variables from the legacy code stochastic simulator, StochSim, and modify AgentCell to allow for many cells per Java VM. Our current work opens the door for the modeling with AgentCell of biological problems involving cell-to-cell communications and more efficient and fully integrated multilevel simulations. 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.

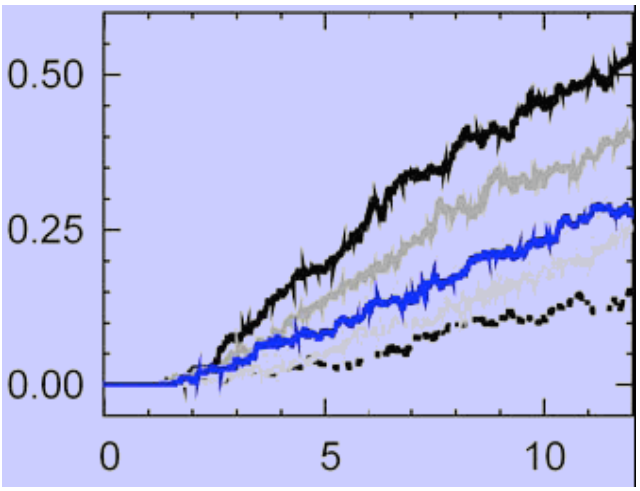


Figure 20. Effect of variations of [CheR] and [CheB] on the chemotactic response of a bacterial population of 400 cells. Digital swimming bacteria are exposed to a constant gradient of aspartate (M/µm, µM). Percentage of cells above 810/–=*dzdL*1)0(==*zL*1=*z* mm as a function of time: one (black), two (grey), four (light grey) wild-type [CheR] level. (Dashed line) response of wild type cells without gradient. (blue) Response of cells with wild-type level of [CheR] but four times the wild-type level of [CheB]. The CW bias is the same (CW=0.23) for mutant and wild-type cells. The initial position of the bacteria is mm. Chemotactic Response (y-axis) vs. Time [min] Chemotactic Response (x-axis)

Publications and Presentations:

T. Emonet and P. Cluzel, "Relationship between cellular response and behavioral variability in bacterial chemotaxis," preprint, 2007.

Accelerator and Targets Simulations

PI: Brahim Mustapha (Physics)

The Advanced Exotic Beam Laboratory (AEBL) has been proposed at Argonne as a reduced scale of the original Rare Isotope Accelerator (RIA) project, with about half the cost but the same beam power. AEBL will address 90% or more of RIA physics but with reduced multiusers capabilities. Our task was to study the proposed design through large-scale end-to-end beam dynamics simulations of the AEBL driver linac including all sources of machine error. To this end, we updated our beam dynamics code TRACK to support new types of accelerating structures, namely, the drift-tube linac (DTL) and the coupled-cavity linac (CCL). Considerable testing was performed to check their implementation.

A beam loss analysis showed that the actual design produce acceptable beam losses for the typical values of both misalignment and RF errors (Figure 21). The results of these computations indicate that the design proposed for the AEBL driver linac is acceptable overall. More design optimization may be needed to achieve more tolerance to misalignment and RF errors and to further limit beam loss for the typical values of errors.

These types of elements will allow future simulations of the SNS linac recently commissioned at the Spallation Neutron Source at Oak Ridge. With this we will be able to first benchmark the code against experimental data and to use the code to support machine operations.

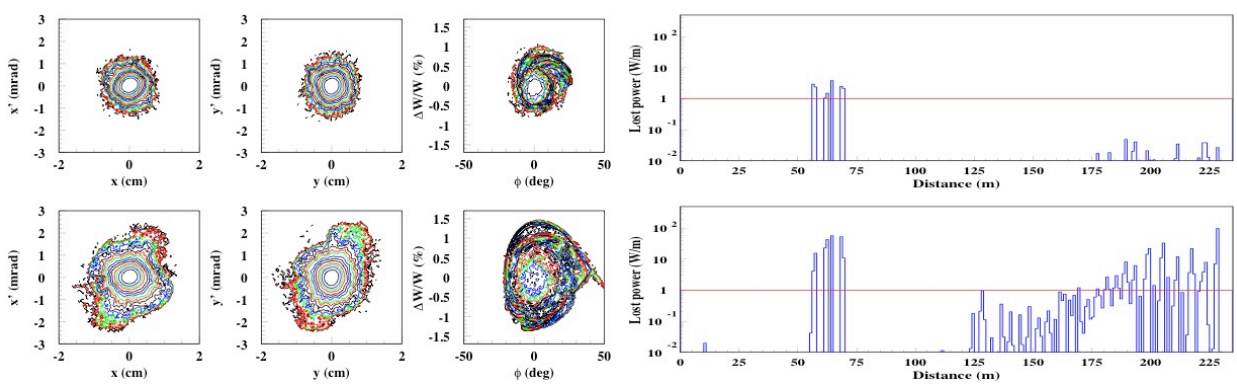


Figure 21. Left: Phase space plots for (1°,1%) RF errors (top) and (2°,2%) (bottom). Right: Beam loss in Watts/m along the linac for (1°,1%) RF errors (top) and (2°,2%) (bottom). For each configuration, 96 seeds were simulated with 2 x10^5 particles each that is a total of about 20 million particles.

Publications and Presentations:

B. Mustapha, P.N. Ostroumov and J.A. Nolen, "A Driver Linac for the Advanced Exotic Beam Laboratory: Physics Design and Beam Dynamics Simulations," in *Proceedings of PAC-07 Conference,* Albuquerque, New Mexico, June 25-29, 2007.

Computational Nanophotonics

PI: Stephen Gray (Chemistry)

How can energy be coupled into nanostructured environments and manipulated for specific purposes? These are basic questions in nanoscience and nanotechnology. In the subdiscipline of nanophotonics, the energy comes from photons that can be coupled into special excitations called surface plasmons (SPs). SPs are special because they localize energy in small spatial regions and can be propagated from one region to another. Applications of SPs range from killing cancer cells to chemical and biological sensing.

During 2007, we developed and applied a version of our 2D finite-difference time-domain (FDTD) code that allows for nonlinear material interactions. Building on our adaptive-mesh, parallel 2-D FDTD package, *Shapes*, we created a working version of an adaptive-mesh 3D code, *Forms*. These codes have been implemented for massively parallel environments and their scaling properties are being investigated. We also carried out extensive modeling of light interactions with periodic arrays of 100-nm diameter holes in thin metal films. The variation in the intensity of the transmitted light, as a function of incident wavelength, is a sensitive function of the nature of substrates placed on top of the hole arrays. We identified special peaks in the transmission spectra that were particularly sensitive to the substrate refractive index and analyzed their origins. Our calculations and analysis show how one can design hole array systems that are particularly sensitive to specified refractive index values. Such results are important to chemical and biological sensing applications where refractive index sensitivity is a key figure of merit.

Publications and Presentations:

Z. Meglicki, S. K. Gray, and B. Norris, "Multigrid FDTD with Chombo," *Comp. Phys. Comm.* 176, 109-120 (2007).

K. L. Shuford, M. A. Ratner, S. K. Gray, and G. C. Schatz, "Electric field enhancement and light transmission in cylindrical nanoholes *J. Comp. Theor. Nanosci.* 4, 239-246 (2007).

K. L. Shuford, S. K. Gray, M. A. Ratner, and G. C. Schatz, "Substrate effects on surface plasmons in single nanoholes," *Chem. Phys. Lett.* 435, 123-126 (2007).

X. Wang, G. C. Schatz, and S. K. Gray, "Ultrafast pulse excitation of a metallic nanosystem containing a Kerr nonlinear material," *Phys. Rev. B* 74, 195439 (2006) (5 pages).

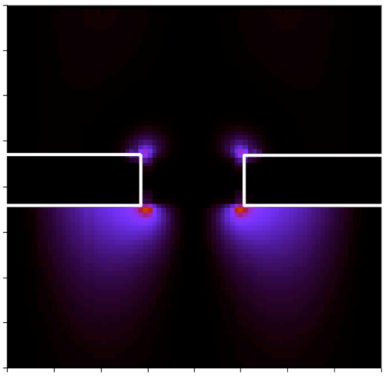


Figure 22. Electric field intensity of a plasmon resonance near a 100 nm diameter hole in a thin gold film. The film's borders are outlined in white. These resonances lead to transmission spectra highly sensitive to substrates.

Voltage-Gated Potassium Ion Channels

PIs: Benoit Roux and Yuqing Deng (Biology)

We are carrying out simulations of atomic models of the voltage-gated potassium channels. Our project addresses questions about the molecular mechanism that governs the function of voltage-activated ion channels that are selective to potassium ions (hence those ion channels are called Kv). These Kv channels open to conduct K+ ions under the influence of the transmembrane voltage. Their activity is fundamental to cellular excitability and the propagation of nerve impulses.

Last year, we used Jazz to carry out a 40 ns molecular dynamics simulation of a detailed model of the Kv1.2 channel with explicit solvent and membrane lipid—around 75,000 atoms. For this work, we used an MPI run of the CHARMM code in parallel. We also carried out some ab initio calculations using Gaussian on Jazz. The results from this simulation enabled us to evaluate the spatial variations of the voltage profile acting on the charged residues in the protein. The spatial variation of the potential is key for understanding the mechanism of activation of these kv channels. Our results were highlighted in the *Biological Journal* in the "News and Views" column, where it was stated that these simulations contribute greatly to clarifying the solvated environment of the atomic charges that play a key role in channel gating and in the transmembrane voltage.

We began extending these simulations to engineered mutants of the channels. Specifically, we replaced two amino acids by histidine, and we simulated the metal pairs with Zn^{2+}. These steps are useful because we have carried out the same mutations in the lab and detected that the channel become easier to activate in the presence of Zn^{2+} in those mutant channels. This observation helps us constrain the position of an important part of the protein, called the voltage sensor, with respect to ion conducting pore domain.

Publications and Presentations:

V. Jogini and B. Roux, "Dynamics of the Kv1.2 Voltage-Gated K1 Channel in a Membrane Environment," *Biophysical Journal* 93: 3070 (2007).

Benoit Roux, Vishwanath Jogini, Fatemeh Khalili, Klaus Schulten, Emad Tajkhorshid, Troy Whitfield, and Vladimir Yarov-Yarovoy, "Simulation provides key to the mystery of molecular machines," *SciDAC Review* (in press), 2008.

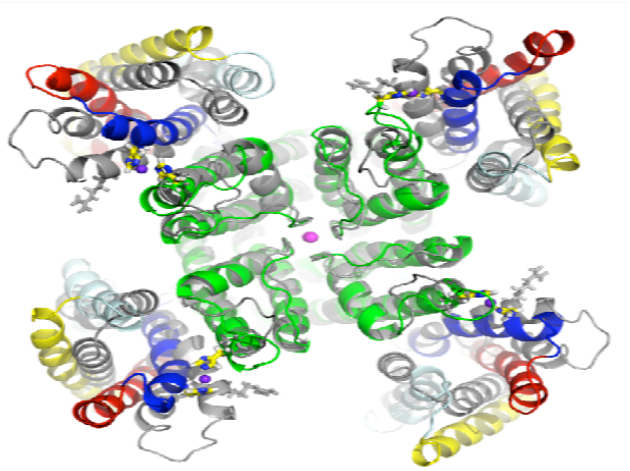


Figure 23. Kv1.2 channel with histidine-zinc-histidine metal bridges formed between the voltage sensor and the pore domain.

Lattice Quantum Chromodynamics in Extreme Environments

PI: Donald Sinclair (High Energy Physics)

Quantum chromodynamics (QCD) is the accepted theory of hadrons and their strong interactions. Lattice QCD defines QCD on a discrete space-time lattice to enable direct numerical simulations of the non-perturbative aspects of QCD such as hadronic masses and the strong interaction contribution to their matrix elements. In addition, lattice QCD enables us to study the thermodynamics of QCD. This is relevant to the theory of the early universe and neutron stars.

Our project involves the thermodynamics of lattice QCD at finite temperature or densities. We are studying hadronic/nuclear matter at finite temperature and density. In particular we are interested in the finite temperature transition to a quark-gluon plasma. We are using the rational hybrid Monte-Carlo method, a stochastic molecular dynamics approach. We also use the phase-quenched approximation, where the phase of the fermion determinant at finite quark-number chemical potential is ignored. With these methods, we search for a critical endpoint where the crossover from hadronic/nuclear matter to a quark-gluon plasma at high temperatures changes to a first-order phase transition. In addition, we are performing simulations aimed at calculating the equation-of-state of hot hadronic/nuclear matter.

These computations have excluded the existence of a critical endpoint for small chemical potentials. Such a critical endpoint is expected to be accessible to relativistic heavy-ion colliders. Moreover, the evolution of hot hadronic matter produced by relativistic heavy-ion colliders is determined by such thermodynamic quantities as pressure, entropyand energy densities (Figure 24). The equation of state describes the temperature dependence of these quantities. Hence these calculations should help in the understanding of experiments at facilities such as the Large Hadron Collider at CERN.

In addition, we began calculating the equation of state for hot nuclear matter in the low-density and high-temperature regimes. This work requires calculating the densities as functions of chemical potential for a number of fixed temperatures. This density describes the chemical potential dependence of the pressure.

Publications and Presentations:

J. B. Kogut and D. K. Sinclair, “Phase quenched lattice QCD at finite density and temperature,” ANL-HEP-CP-07-66, 2007.

J. B. Kogut and D. K. Sinclair, “The RHMC algorithm for theories with unknown spectral bounds,” *Phys. Rev. D* 74, 114505 (2006) [arXiv:hep-lat/0608017].

D. K. Sinclair, “Equilibrium thermodynamics of lattice QCD,” arXiv:hep-lat/0701010.

D. K. Sinclair, “Equilibrium thermodynamics of lattice QCD,” invited presentation, Expanding Horizons: The Scientific Legacy of Brosl Hasslacher, Los Alamos, NM, Nov. 3-4, 2006.

D. K. Sinclair, “Lattice QCD at finite T and small mu in the phase-quenched approximation,” invited presentation, 2006 International Workshop SCGT 06, Nagoya, Japan, November 21-24, 2006.

D. K. Sinclair, “Phase quenched lattice QCD at finite density and temperature,” presentation at YITP at 40, SUNY at Stony Brook, Stony Brook, NY, May 2-5, 2007.

D. K .Sinclair, “Phase quenched lattice QCD at finite density and temperature” (extended version), invited presentation, Lattice 2007, the XXV International Symposium on Lattice Field Theory, Regensburg, Germany, July 30 - August 4, 2007.

D. K. Sinclair, “QCD in extreme conditions,” presentation at Laboratori Nazionali di Frascati dell' INFN, Frascati, Italy, August 6-8, 2007.

D. K. Sinclair, “30+ years on the lattice,” invited presentation, Fermions and Extended Objects on the Lattice, Pedro Pascual Benasque Center For Science, Benasque, Spain, 2007, February 25 - March 2, 2007.

D. K. Sinclair and J. B. Kogut, “Searching for the elusive critical endpoint at finite temperature and isospin density,” *Proceedings of Science LAT2006*, 147 (2006) [arXiv:hep-lat/0609041].

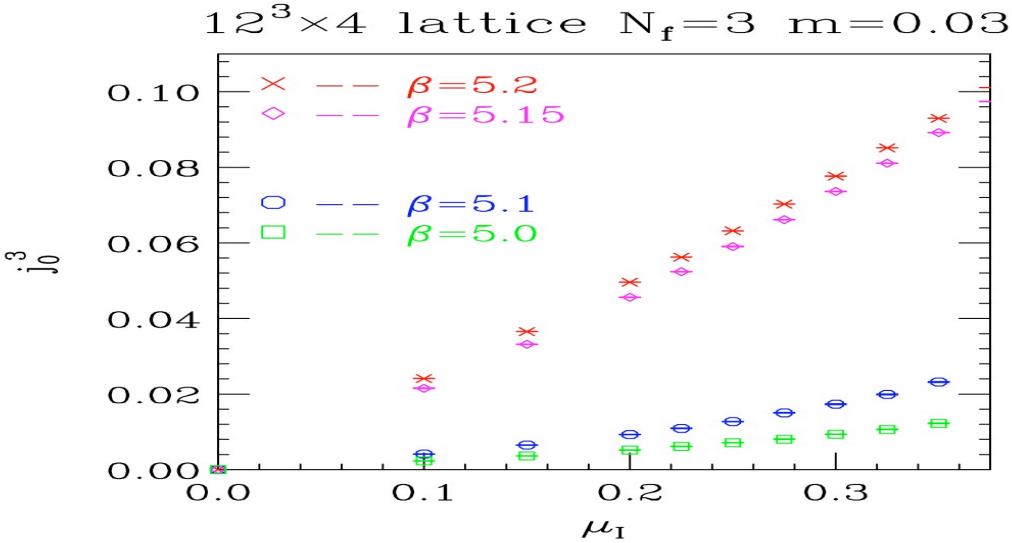


Figure 24. Density as functions of chemical potential for fixed betas (fixed temperatures). This density is the derivative of pressure with respect to chemical potential.

Neocortical Seizure Simulation

PIs: Mark Hereld (Mathematics and Computer Science)

Epilepsy is the third most commonly diagnosed neurological disease. Ideally, one would like to record from many cells simultaneously in vivo to create a picture of how seizures start and spread from a specific area of the brain (the focus). Unfortunately, in vitro experimental recording techniques are time-consuming and generally limited to a handful of simultaneous recording sites or cells, thereby providing an incomplete picture of the process at best. In vivo experiments are even more challenging. We seek to overcome some of these limitations by investigating seizure generation in a scalable computational model of neocortex. The cells and connectivity included in the model preserve the essential elements: multiple inhibitory and excitatory cell types, Hodgkin-Huxley based ion channels, and several types of interneuron connections that vary in topology and signaling speed. The model is being used to 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?

In 2007, we strengthened the model by adding additional biophysical features from these investigations (Figure 25). We investigated a novel mechanism for seizure initiation in which noise and small oscillations that exist in a network of neurons can be amplified by the behavior of the N-methyl-D-aspartate receptor. This receptor has an unusual current-voltage relationship in the presence of magnesium that reduces the threshold at which small oscillatory currents in the membrane can cause a cell to fire repetitively over a short period of time; present in high enough numbers, cells with an enhanced density of these receptors, bursting together, may synchronize network behavior enough to propagate a seizure. We found that some cells in mouse possess these properties and are susceptible to burst.

We also investigated the interesting rhythmic bursting between populations found last year in our simulations. Our efforts are focused on characterizing the dependence of these seizurelike oscillations on a variety of physical model parameters, so that we may compare them to similar recordings in the literature, and of ways to disrupt this behavior in the simulation. We performed a systematic study of automated parameter search techniques as a way to optimize model parameters with a minimum of handtuning. As models become more complex, handtuning becomes more of a handicap in aligning models with experimental setups. In the end, the results are mixed: the automated techniques are useful in getting the model close to optimal parameters but possess limited resolution once in the near-neighborhood of these values.

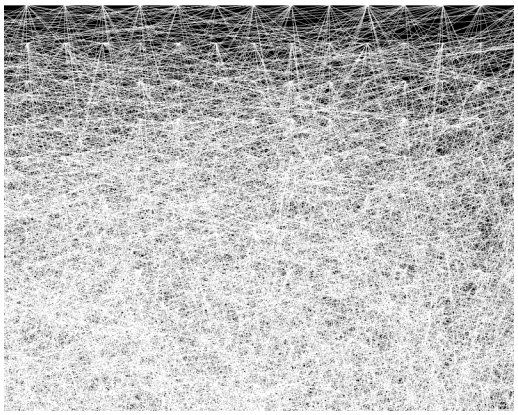


Figure 25. Visualizations of experimental model. automatically generated instance of the inhibitory connections (white lines) between deep pyramidal cells and basket1 cells corresponding to the line labeled '23' in the left diagram. The cells are on a regular special grid.

Spin Wave Excitations in Magnetic Nanoparticles

PIs: Ming Yan, Gary Leaf, and Barry Smith (Mathematics and Computer Science)

The mechanisms of spin-dependent electron scattering are important for controlling physical properties of nanoparticles. The nature of spin-wave spectra is one of the keys to understanding this mechanism. In particular, the lower-frequency eigenmodes determine the electronic behavior of these nanoparticles. We are investigating the dynamics of spin waves using the Landau-Lifschitz-Gilbert model for micromagnetic dynamics. Our experiments focus on determining the resonance frequency of a given particle in response to an applied rf power source. Since experimental measurements cannot determine whether the resonance is due to the excitation of the fundamental mode, simulations are required.

Our simulations mimic the experiments as much as possible. The particle size matches the fabricated size. The particle is saturated with a static field. For a given rf power, we vary the frequency of this source. For each frequency, the system is equilibrated, and the particle response is measured in a manner analogous to the Brilluoun measurements in the laboratory. The computations are three dimensional; and the algorithm, developed in house, has the feature that it can integrate long-time dynamics. This feature is critical for this study since equilibration is very slow near resonance frequencies when high power sources are involved.

Equilibration times can vary from 30 to more than 180 ns. A 15 ns simulation requires about 28 node-hours on Jazz. Using 90 ns as an average equilibration time leads to about 180 node-hours per frequency. The frequency grid varies from 0.1 to less than 0.025 GHz depending on nearness to resonance. This generates about 50 frequencies per power source setting, or about 9000 node-hours per power setting. At this time our experiments have generated four power settings, which yield about 36,000 node-hours.

Large-Scale Parallel Simulation of Subduction Zone Geodynamics

PIs: Matt Knepley (Mathematics and Computer Science), Richard Katz (Lamont Doherty Earth Observatory, Columbia University)

In the polar oceans, sea ice—a critical component of the climate system—freezes from the salty water below. Because salt is rejected from the growing ice crystals, a flux of salty dense water sinks into the open water, providing a driving force for global ocean circulation. Such sea-ice forms as a “mushy layer” of closely spaced ice-crystal dendrites bathed in an interstitial brine. This brine can move through the permeable mush, producing flow instability. As convection develops, reactions between the brine and the dendrites lead to “chimneys,” open tubes about 2 mm in diameter that drain dense brine from the mushy layer. The efficiency of brine drainage, and thus of the strength of salty downwelling beneath the sea-ice, is controlled by the formation of chimneys. Chimney formation is a complex, nonlinear process; to date, however, researchers have examined the dynamics mainly by linear stability theory. In the past year we have developed a simulation of mushy layer growth and chimney formation that accounts for all the inherent nonlinearity of the problem. This simulation shows that chimneys form through an interaction between vigorous convection in the compositional boundary layer at the mush—liquid interface, and by slower, porous convection within the mushy layer itself. The resulting porosity distribution is consistent with observations from experiments. Results of an example calculation are shown in Figure 26.

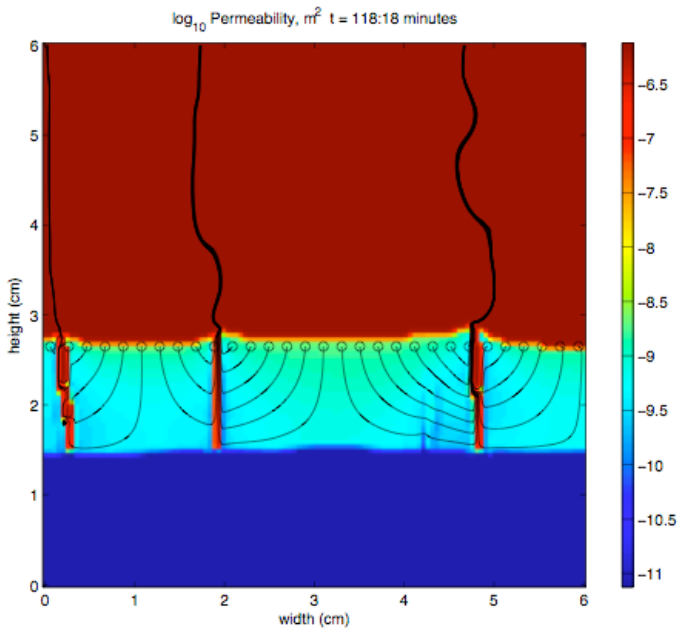


Figure 26. Brine convection through a mushy layer. The bottom boundary is held at a fixed cold temperature, the top boundary at a fixed, warm temperature. The colors represent the log of permeability. The top layer is open fluid; the middle is porous crystalline mush; and the bottom is pure solid at temperatures below the eutectic. Black lines originating at black circles are fluid streamlines. Note how fluid sinks through the mush but rises through the chimneys. Buoyancy comes from solidification of NH_4Cl into the mush, leaving a fresher, less dense fluid.

In addition, we studied magmatic processes in the mantle beneath volcanoes. Mid-ocean ridges on the ocean floor are formed when tectonic plates diverge; the volcanic ridges that form extend linearly for thousands of miles. Observations suggest that magma produced tens of kilometers deep in the mantle is quickly focused to these ridges. Magma dynamics theory is used to describe the mechanical interactions between magma and the mantle, but the complexity and nonlinearity of the theory have made it difficult to create models that consider both the full physics of the problem and the large time and length scales involved.

We are exploring a method that couples magma dynamics theory with an enthalpy method that treats freezing and melting as identical processes, avoiding the need to find parameterizations for melting rates and freezing rates. Our simulations show that freezing is critical to focusing magma toward the ridge axis: freezing of magma in the pores of the cold, sloping thermal boundary layer at the base of the divergent tectonic plates produces an impermeable barrier to flow and directs magma toward the ridge axis. Using simulations, we are exploring the parametric controls of this process to determine whether it can explain observations. In addition, we have developed a parallel Lagrangian particle-tracking method that helps to visualize the motion of fluid through the system. Particles are introduced by the application code and then tracked through the system, across processor boundaries, giving a picture of the time-integrated pattern of flow. The simulations strongly support the idea that magmatic focusing occurs along the base of the thermal boundary layer beneath the sea floor. The simulations also provide a context for testing other ideas about melt transport, for example, geochemical signals in lavas collected from the sea floor.

Publications and Presentations:

R. F. Katz, M. Knepley, B. Smith, M. Spiegelman, and E. Coon, "Numerical simulation of geodynamic processes with the Portable Extensible Toolkit for Scientific Computation," *Physics of the Earth and Planetary Interiors,* 163(1-4):52-68, 2007.

High-Fidelity Numerical Simulation of Nuclear Reactor Cores

PIs: Dinesh Kaushik and Andrew Siegel (Mathematics and Computer Science)

Recent work at Argonne has been focused on the development of a new high-fidelity system of software tools (SHARP) that model the overall nuclear plant behavior. At present, several methods are used in reactor analysis and other more general transport applications (shielding, deep well logging) to solve the neutron transport equation. The most common are diffusion-based nodal methods, discrete ordinates structured and unstructured methods, finite element-based spherical harmonics, combinatorial geometry-based collision probability, and characteristics. There exists substantial experience with all of these methods in the nuclear industry, and thus each individual method has well known advantages and disadvantages when compared with the other methods. As a consequence, these methods have been implemented such that they are best used for specific problems found in the nuclear industry (such as discrete ordinates for shielding and nodal methods for reactor physics analysis).

One of the most popular methods is the diffusion approximation. This approximation is typically employed at the whole-core level using assembly level homogenized cross sections in a nodal framework. To reproduce this capability (i.e., be able to rapidly solve problems based on homogenized assemblies), we have focused the initial development in UNIC (unstructured neutronics investigation code) on a second-order spherical harmonics method. The spherical harmonics method implements a continuous set of orthogonal functions to approximate the angular variable in the neutron transport equation and is generally well known in the nuclear industry. It is typically posed in either a finite-element or finite-difference spatial approximation, where both formulations lead to a large coupled system of equations for the angular approximation. Clearly for a large spatial domain and high-order angular approximation, the resulting matrix cannot be directly inverted because of the computational burden and storage expense. As a consequence, we have used the conjugate gradient solver available in the PETSc (Portable, Extensible Toolkit for Scientific Computing).

One example of the benchmarks we ran this year is the fourth Takeda benchmark. This benchmark is used to check the general solution capability of transport methods since it requires a relatively low angular approximation and contains virtually no heterogeneity. The geometrical 1/6 symmetry representation is given in Figure 27 along with the mesh that displayed full spatial convergence on the control rod withdrawn problem. The cross sections were provided and reference solutions obtained by using the VIM Monte Carlo code in multigroup mode. In this benchmark, three configurations were specified where the control rod is inserted fully, half, or removed. Figure 28 shows the four group flux solutions for the half-inserted control rod. The VIM Monte Carlo solution for the full-inserted control rod is 0.88001 ± 0.00038, for the half-inserted control rod is 0.9834 ± 0.00039, and for the withdrawn control rod is 1.09515 ± 0.00040.

This new coding initiative is focused on making immediate improvements to existing codes in addition to developing new methodologies that may not be immediately exploitable with current computing technology. The final tool will provide reactor analysts the ability to remove as many approximations as possible in their numerical modeling of nuclear reactors by performing a very high fidelity simulation of the system under study. The objective is to both reduce and resolve the bias in numerical simulation of nuclear reactor technology by combining the best available data, methods, and knowledge.

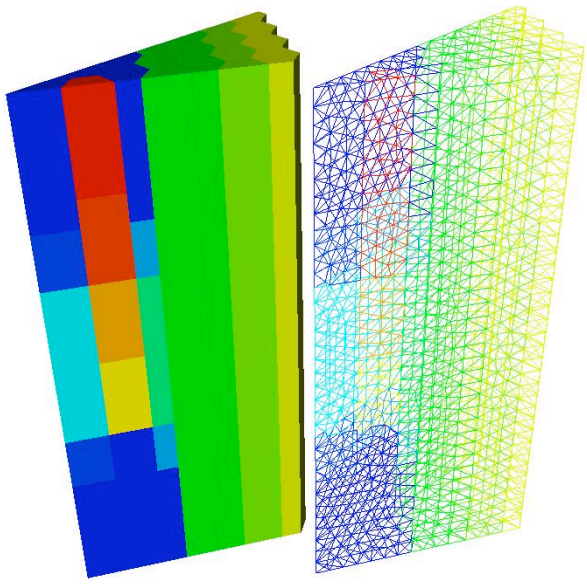


Figure 27. Fourth Takeda benchmark geometry and mesh

The relatively large inaccuracy in these results limits verification of the new code. Thus, additional, comparative solutions were obtained by using the nodal spherical harmonics code VARIANT. All of the calculations were completed on the Jazz cluster using 16 to 64 processors. From our space-angle convergence analysis, we believe the solutions obtained with the P_NFE component of UNIC and the VARIANT code are good, although additional spatial refinement may be necessary in both codes to get agreement. There is also some residual error in the Monte Carlo solutions likely due to insufficient fission source convergence.

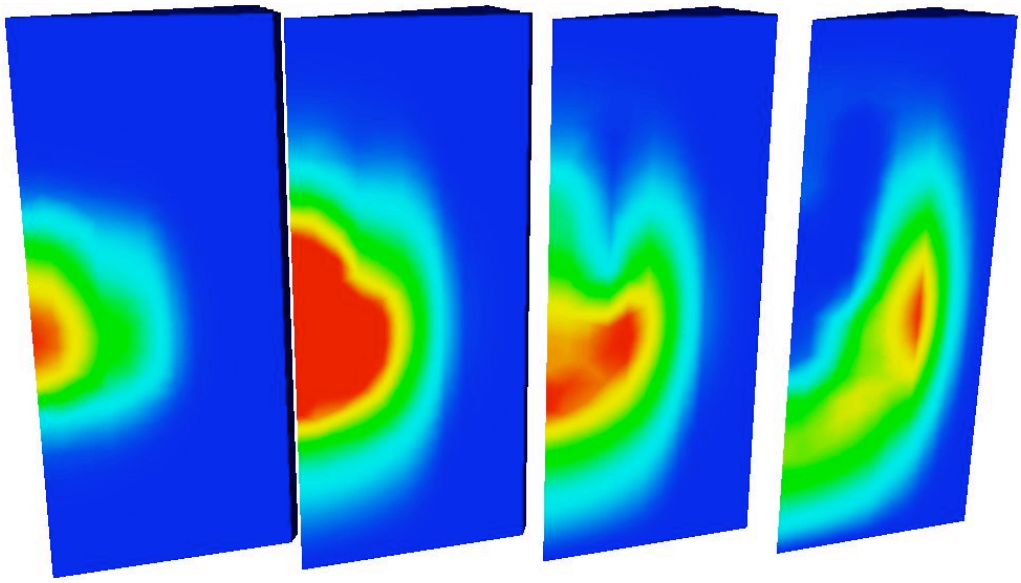


Figure 28. Fourth Takeda benchmark flux results for half-inserted control rod (first through fourth energy group fluxes are given left to right)

Publications and Presentations:

G. Palmiotti, M. A. Smith, C. Rabiti, M. Leclere, and D. Kaushik, A. Siegel, B. Smith, E. E. Lewis, "UNÌC: Ultimate Neutronic Investigation Code," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007), Monterey, California, April 15-19, 2007.

A. Siegel, T. Tautges, A. Caceres, D. Kaushik, G. Palmiotti, and M. Smith, "Software Design of SHARP," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007), Monterey, California, April 15-19, 2007.

M. A. Smith, G. Palmiotti, C. Rabiti, D. Kaushik, A. Siegel, B. Smith, and E. E. Lewis, "PNFE Component of the UNÌC Code," Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007), Monterey, California, April 15-19, 2007.

Monte Carlo Analyses of Accelerator-Driven Subcritical Facilities

PI: Yousry Gohar (Nuclear Engineering)

Accelerator-driven subcritical systems have been under development for different functions including medical isotope production, transmutation of transuranics and long-lived fission products, reactor physics experiments, and basic research with fast, thermal, and cold neutrons. We have been analyzing two different facilities. The first subcritical assembly has both fast and thermal neutron spectra in one configuration to achieve high neutron flux density as much as possible. This configuration, together with a high-neutron source, makes this facility interesting for performing kinetics research for accelerator-driven systems. The configuration has $k_{eff} < 0.98$ and it is driven by an external neutron source, a ^{252}Cf neutron source or a deuteron accelerator with deuterium or tritium target for producing neutrons. The subcritical assembly has a central fast neutron zone surrounded by a thermal neutron zone. The fast neutron zone multiplies the external neutrons through the fission reactions of highly enriched uranium and (n,xn) reactions of lead. The neutrons leak to the surrounding thermal zone. Between the two zones is an interface zone consisting of two layers. The inner layer has metallic natural uranium rods, and the outer layer has boron carbide rods that absorb thermal neutrons. Such a zone enables fast neutrons to penetrate into the thermal zone and prevents thermal neutrons from entering the fast zone from the thermal zone. The subcritical assembly is surrounded by a graphite reflector in the radial direction and borated polyethylene in the axial direction. The radial reflector and the backside of the thermal zone are covered by organic glass sheet. There are four axial experimental channels in the fast zone, three axial experimental channels in the thermal zone, and two axial experimental channels and one radial experimental channel in the reflector zone.

The MONTE CARLO geometrical model of the subcritical assembly is shown in Figure 29. The calculated performance parameters of the subcritical assembly were compared with the experimental measurements, and the comparison shows an excellent agreement.

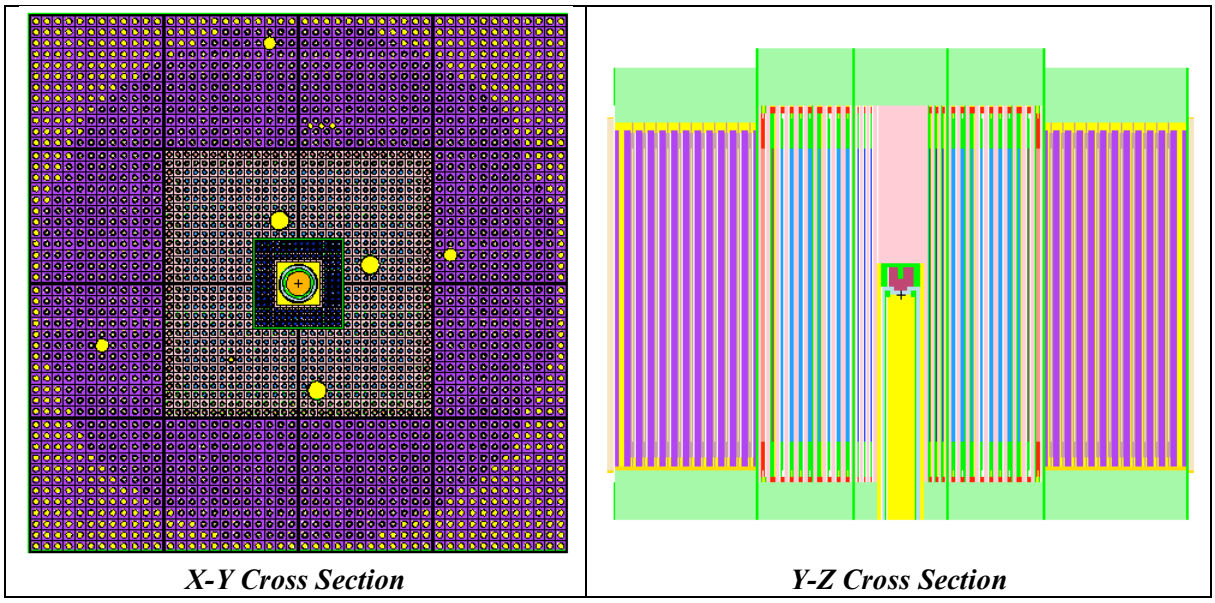
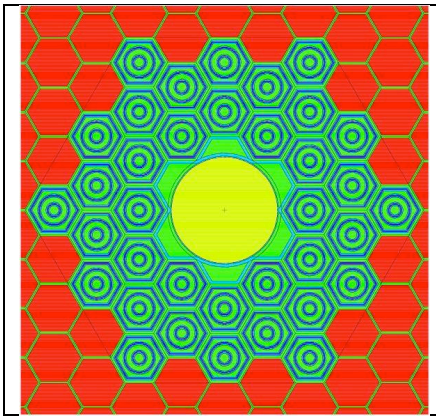


Figure 29. Monte Carlo geometrical model of the subcritical assembly with fast and thermal zones

The second subcritical assembly is driven by an electron accelerator and uses low enriched uranium fuel. The assembly's target uses tungsten or uranium for neutron production through photonuclear reactions from 100-KW electron beam. The neutron source intensity, spectrum, and spatial distribution have been studied as a function of the electron beam parameters to maximize the neutron yield and satisfy different engineering requirements. The subcritical assembly is designed to obtain the highest possible neutron flux intensity with a subcriticality of ~0.98. Different fuel materials, uranium enrichments, and reflector materials are considered for the subcritical assembly design. Analyses were performed to define the dose map around the facility during operation as a function of the heavy concrete shield thickness. The facility is configured to produce medical isotopes, perform basic research with neutrons, and train young nuclear professionals. Figure 30 shows the subcritical assembly configuration and its main parameters.



Natural uranium target, 36 fuel assemblies, Carbon Reflector, Water coolant, k_{eff}= 0.9840

Target Material	Electron energy, MeV	Averaged Flux over target length, n/s cm3	Total Energy deposition, kW
U	100	2.660E+13	330.027
	200	2.798E+13	339.63

Figure 30. Monte Carlo geometrical model and main parameters of the electron-driven subcritical assembly