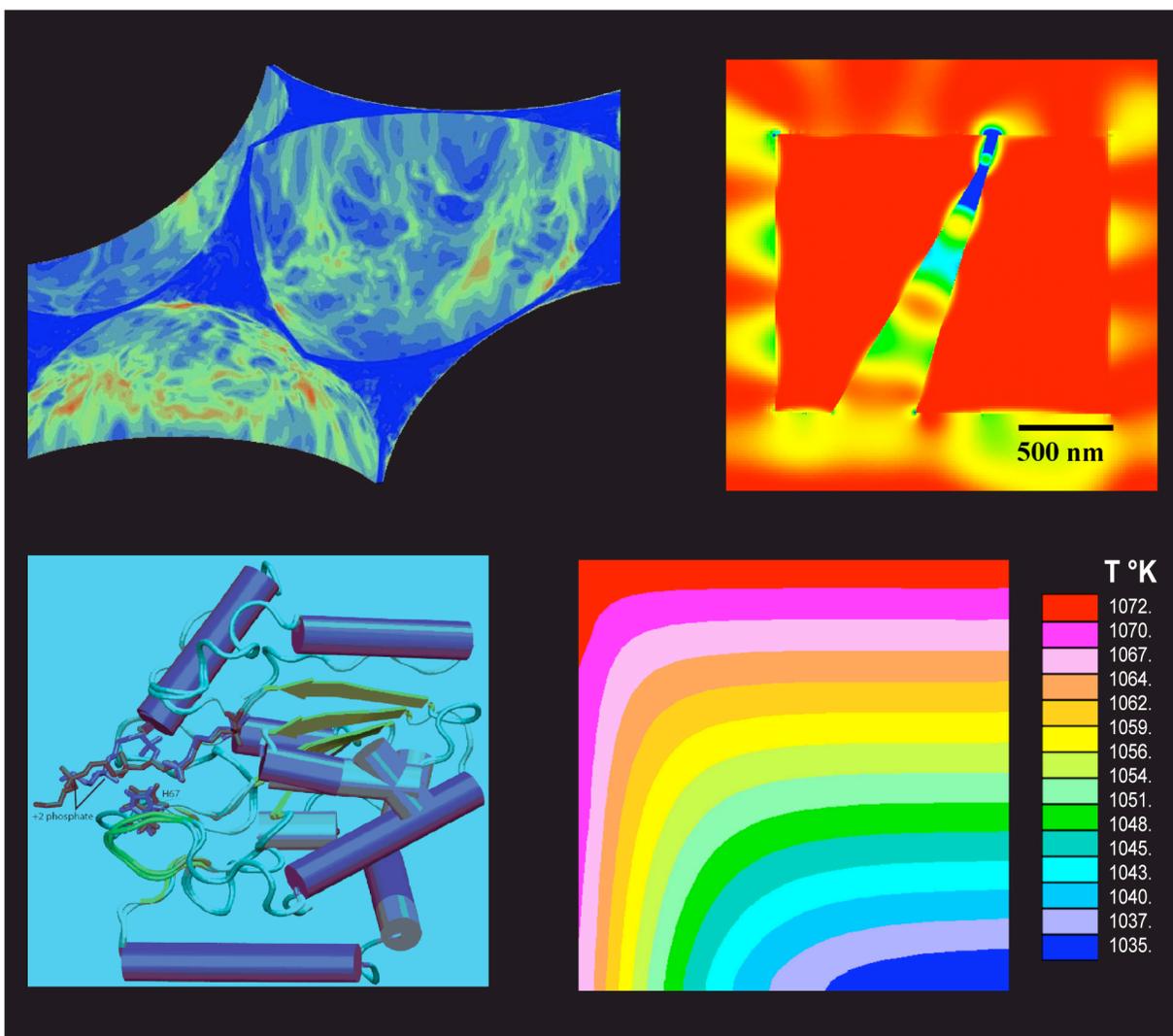


# Argonne's Laboratory Computing Resource Center

2005 Annual Report



**About Argonne National Laboratory**

Argonne is a U.S. Department of Energy laboratory managed by The University of Chicago under contract W-31-109-Eng-38. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne, see [www.anl.gov](http://www.anl.gov).

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# Argonne Laboratory Computing Resource Center

## FY2005 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 2005 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@lrcr.anl.gov](mailto:consult@lrcr.anl.gov).

*Ray Bair*  
Director, Laboratory Computing Resource Center  
[bair@lrcr.anl.gov](mailto:bair@lrcr.anl.gov)



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## Executive Summary

Argonne National Laboratory founded the Laboratory Computing Resource Center 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.

The first goal of the LCRC was to deploy a mid-range supercomputing facility to support the unmet computational needs of the Laboratory. To this end, in September 2002, the Laboratory purchased a 350-node computing cluster from Linux NetworX. 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 fifty 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 2005, there were 62 active projects on Jazz involving over 320 scientists and engineers. These projects represent 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 improve 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 develop comprehensive 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 begun developing a "path forward" plan 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 was installed in September 2002. The cluster was named "Jazz" because we expected that the mix of disciplines and applications operating on the system would be diverse, wide ranging, and continually changing. Moreover, the name is easy to remember.

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.

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 get started. An investigator wishing to use Jazz for a longer period of time may apply for additional computing allocation via the Web site. All project requests are judged on the basis of scientific merit by the LCRC Allocation Committee, composed of scientists from across the Laboratory.



During 2005, the LCRC put special emphasis on the following objectives:

- Continue to operate Jazz as a highly effective production supercomputing resource.
- Expand the use of Jazz to 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 NERSC, NLCF, MHPCC, PACI, and TeraGrid.
- Develop and submit a plan for expanding LCRC computing resources.

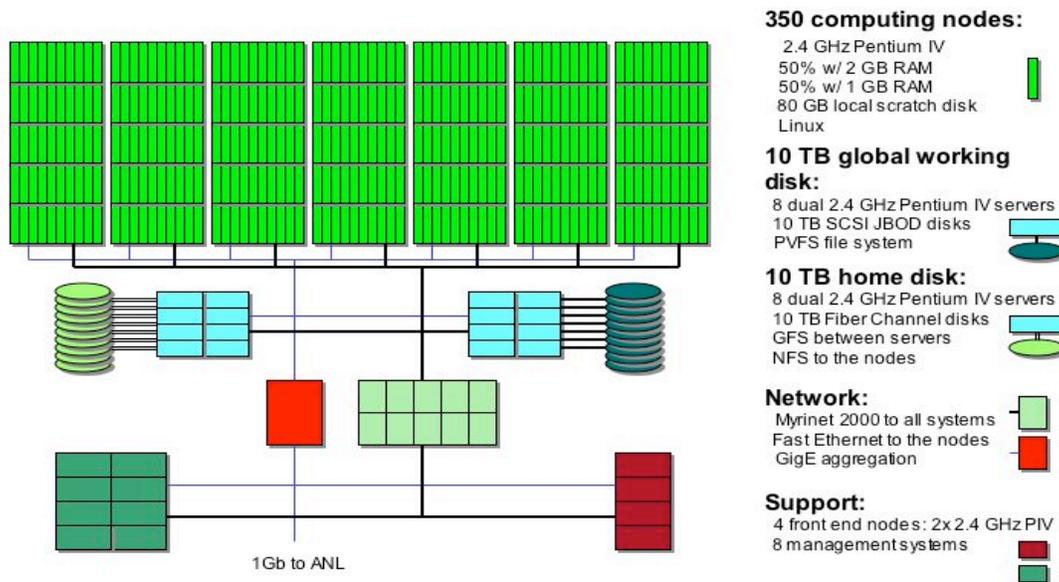
For further information about the LCRC and Jazz, please see the LCRC Web site at <http://www.lcrc.anl.gov/>, or send email to [consult@lcrc.anl.gov](mailto:consult@lcrc.anl.gov).

# The Jazz Computing Cluster

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.

## Cluster Configuration

Jazz comprises 350 computing nodes, each with a Pentium Xeon processor and a connection to both Myrinet and Ethernet communication networks. The system has 20 TB of disk storage, half in a global shared file system and half in a high-performance parallel file system.



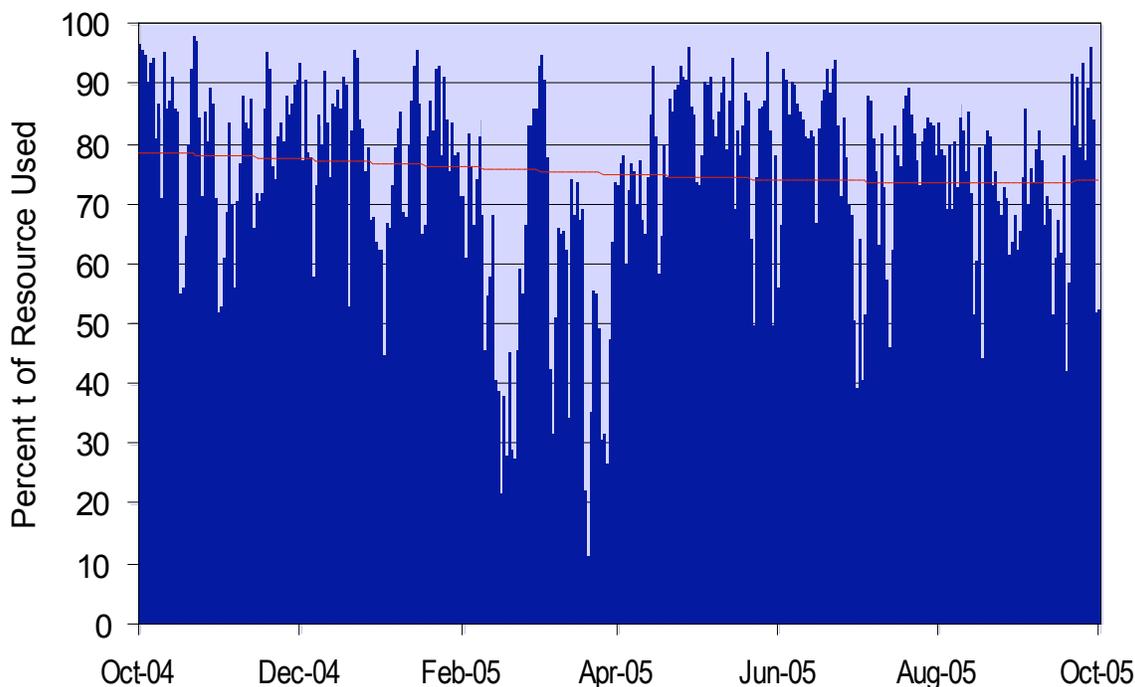
## Cluster Usage

As can be seen in the chart below, the usage of Jazz was steady, averaging 75% in fiscal year 2005. On this chart 100% would mean that all 350 nodes were used continuously for that day. 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.

Demand for compute resources on Jazz throughout the year was sufficient to maintain its maximum sustainable level, but utilization of Jazz was down during certain periods owing to a few events, decreasing the yearly average. In February, the operating system on the compute nodes was upgraded, resulting in lower usage while user applications and libraries were recompiled and tested against the new system. In March, Jazz experienced problems with the home file system and with the hardware for the parallel file system (PVFS) servers, which limited the number of jobs that could be run. Moreover, starting in late spring and continuing through the summer, a significant number of the compute nodes experienced intermittent failures on the high-speed interconnect network (Myrinet). The cause of the problem was difficult to determine, but the Jazz support staff did an outstanding job of identifying the

power supplies in the compute nodes as the source. As nodes failed, they were removed from the job queue; this action caused a steady decline in the availability of nodes, reducing the overall utilization of Jazz. Not until the bulk of the failing power supplies were replaced in September did utilization return to its maximum sustainable level. In anticipation of other power supply failures, we plan to proactively replace the power supplies in the remainder of the nodes in order assure full availability of the cluster.

### Jazz Usage by Day



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.

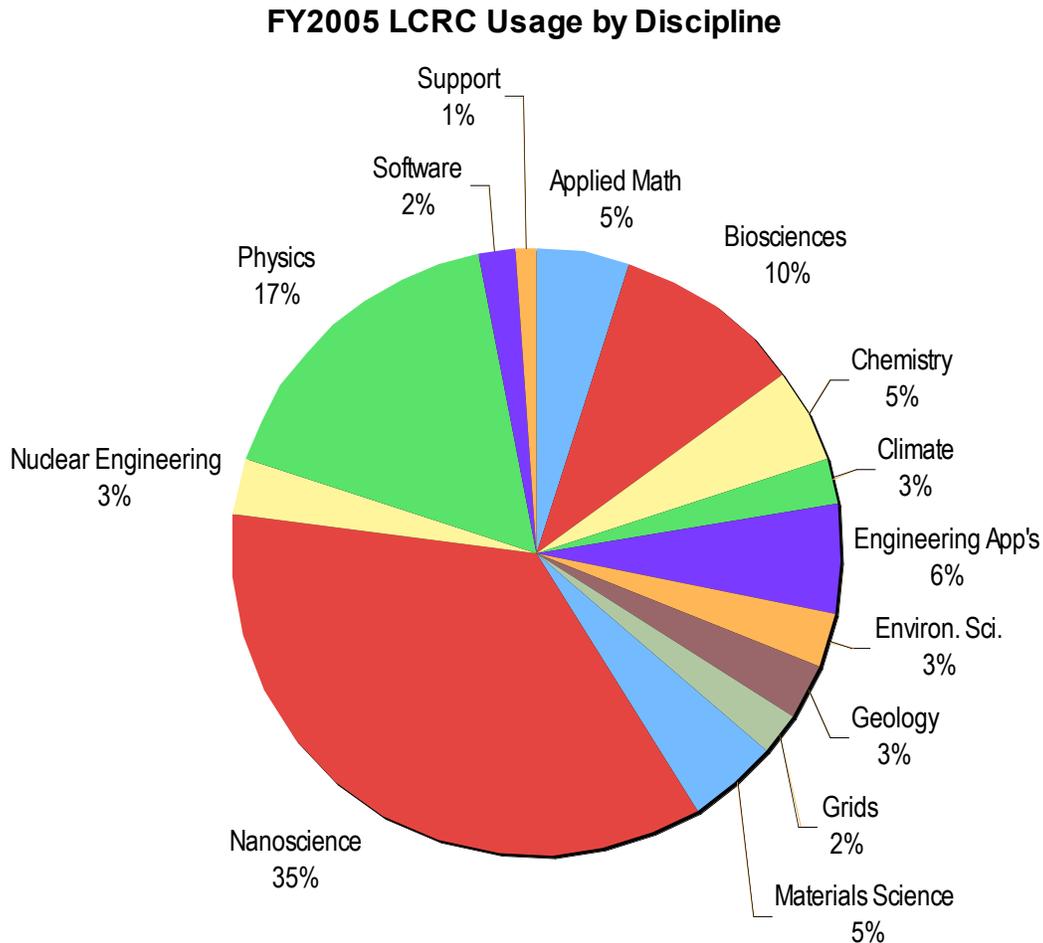
### **Users and Projects**

Argonne staff may obtain a startup account for 1,000 hours, to become familiar with the Jazz system and evaluate its applicability to their work. 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.

In FY 2005, 19 new LCRC projects were started, and 123 new user accounts were created. By the end of FY2005, there were over 350 active user accounts and 70 active LCRC projects.

## Usage by Discipline

Jazz supports research in a very wide range of disciplines, as indicated by the chart below. Here the size of the slice is proportional to the fraction of the Jazz resource (number of node hours) used by all projects in a particular area, during FY2005. These fractions change over time as new projects are added. In FY2005, nanoscience, physics, and biosciences dominated the Jazz usage.



## 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 FY2005. About 50%

of the machine was used for jobs that employed 16–64 processors. About 14% of the jobs used 64–128 processors. The jobs that needed only one node accounted for about 12% (up from 6% FY2004) 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 like 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 15 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 national centers.

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

- **Strategic.** Jazz is critical to essentially 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. For many of these strategic projects Jazz is the only large computing resource available.
- **Production.** An important component of LCRC's mission is to provide a fast and reliable resource for the Laboratory's production modeling and simulation activities. Some of these production codes are still under development; others are fully mature. Often Jazz is the largest resource available to a research group; for other production applications, Jazz fills the need for quick turnaround on mid-range runs, where larger runs are done on systems bigger than Jazz at NERSC 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.

## LCRC Research Highlights

In this section, we present examples of research performed with Jazz through 2005. 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 with Jazz, 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, specialized forms of computational fluid dynamics, Monte Carlo solvers, and “first principles” solutions.

## An Integrated Modeling System for Evaluating the Impact of Aerosols on Regional and Urban-Scale Climates (AERO-MODEL)

PI: V. R. Kotamarthi, Environmental Research

Reducing the uncertainty in evaluating the impacts of tropospheric aerosols on global- and regional-scale climate has been identified as a critical need in climate studies. Poor representation of processes and underresolution in space and time have limited the understanding of human impact. In the Aero-Model group in Argonne’s Environmental Research division, we are exploring how well-resolved simulations on the regional scale can solve some of these problems. To carry out such simulations, we are integrating various community applications including CMAQ and MM5. Currently, replacement of the I/O with parallel netCDF is near completion and should bring significant improvement in performance.

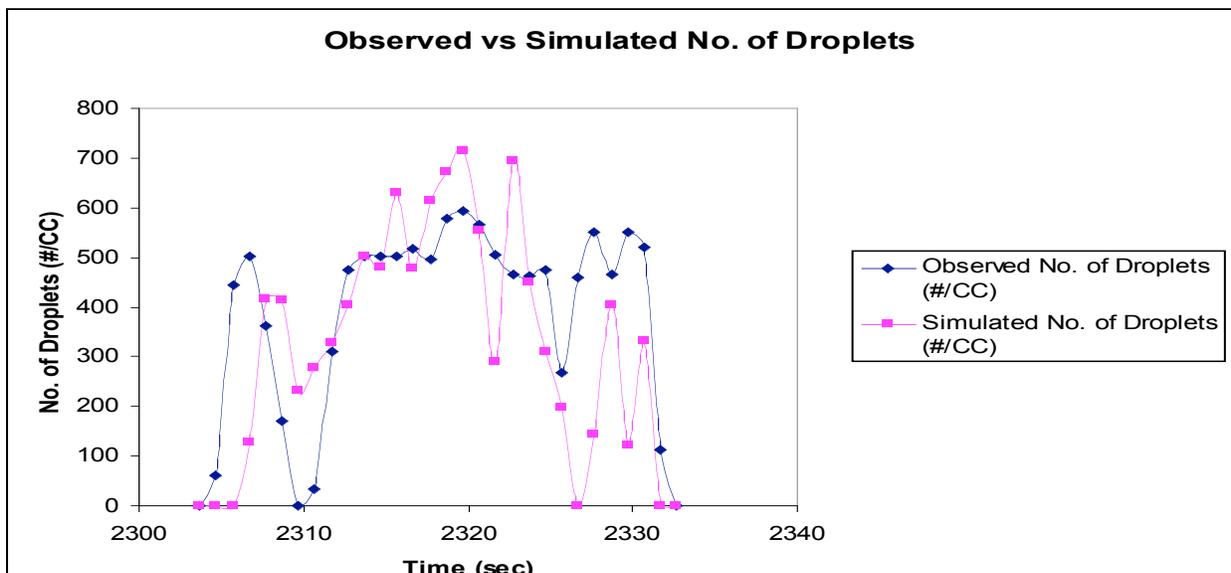


Figure 1: Offline simulation of the aerosol activation parameterization and the final observed and simulated number of droplets.

Additionally, we have started evaluating one of the key components of the indirect effect of aerosols on climate—specifically, the size and the number of cloud droplets formed under enhanced aerosol loading. The primary focus is on data from the ARM (Atmospheric Radiation Measurement) IOP (Intense Operational Period) May 2003 CIRPUS (Center for Interdisciplinary Remotely-Piloted Aircraft Studies) Twin-Otter flights, which were flown over the Southern Great Plains (SGP) site near north-central Oklahoma. Data was collected with instruments located within or attached to the aircraft. The aircraft was equipped with standard meteorological sensors to retrieve temperature, pressure, and humidity and with more sophisticated sensors to measure cloud droplet concentration. The acquired data was then used to constrain a computer code simulating aerosol activation to predict the number of droplets formed under the prescribed conditions. The parameterization is now implemented in the WRF model for calculating the aerosol activation (this work was performed by Prof. Hayder Abdul-Razzak, 2005 Summer FAST faculty with the MCS and ER divisions). The event shown in Figure 1 is being simulated with the complete WRF model. Such simulations are expected to provide a definitive description of the expected errors in calculating droplet size distribution in these models and the effect of grid size and its impact on resolving the updraft velocity. The updraft velocity is shown as a major parameter in our offline calculations.

## **Impact of Aerosols on Regional and Urban Scale Climates (ATMOS CHEM)**

PI: V. R. Kotamarthi, Environmental Research

To further our understanding of the chemistry and distribution of oxidants in the urban and rural air masses, we are focusing on such key unresolved processes as

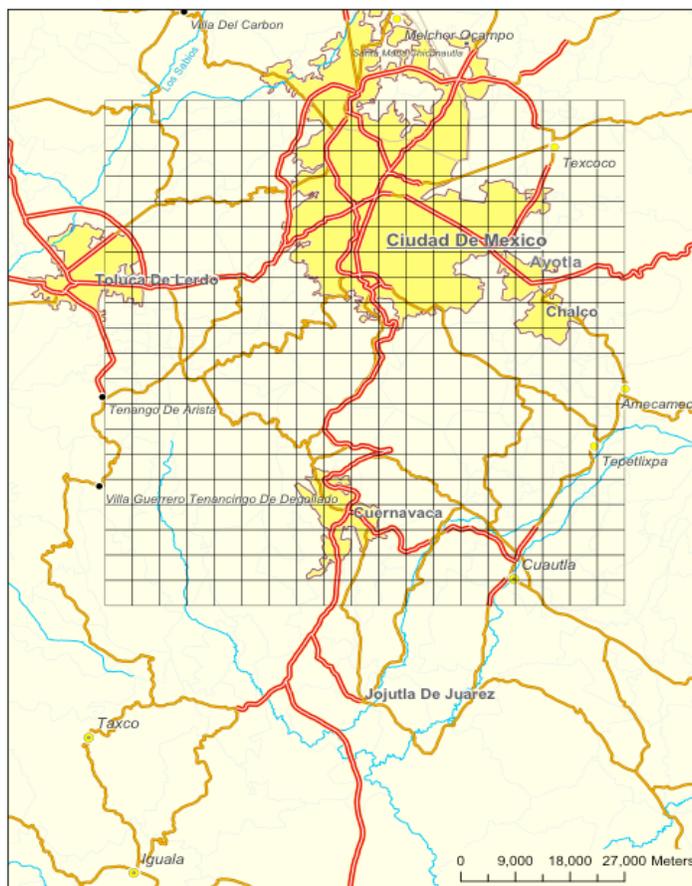
- The importance to oxidant chemistry of rapid surface reactions cycling NO<sub>x</sub> and HO<sub>x</sub> reservoir species to NO<sub>x</sub> and HO<sub>x</sub>,
- Different HC lumping schemes and their effect on the NO<sub>y</sub> and HO<sub>x</sub> partitioning as it relates to the formation of oxidants, and
- Oxygenated hydrocarbons and their impact on determining the urban and rural boundary layer oxidant levels.

Given the computational burden of running chemical transport models, it is highly desirable to have fast and accurate approximations to selected outputs of these models. We present two methods to approximate ammonia wet deposition output from the Community Multiscale Air Quality (CMAQ) model, a regional-scale 3-D chemical transport model. The first method involves a greatly simplified version of CMAQ, called Tracer, that requires 1/40 the processing time of CMAQ. The second method is an extension of Tracer, called Multitracer. Both methods make use of a CMAQ run under a reference emission scenario and provide good approximations to CMAQ outputs under different emission scenarios. The first approximation method requires a Tracer run under the new emission scenario; the second approximation requires only a matrix multiplication between a precomputed matrix that approximates the transport in the model, obtained from a single Multitracer run, and the new emission. Both methods were developed using the Jazz computing resources.

Based on the second predictor, we are now exploring an inverse modeling method for ammonia that makes it possible to adjust emissions by a different factor for each of 100 subregions of the spatial domain. Testing with pseudodata yields a good match between the inverse modeled emissions and the actual emissions. Estimates of emissions using actual observations in the eastern United States show a reasonable adjustment field.

### Mexico City Study

We are performing comprehensive 3-D model simulations to assess the various sources of black carbon measured by the Mexico Valley Metropolitan Area (MVMA) field experiment during April–May 2003. The contribution of a regional forest fire in the Yucatan Peninsula to the measured black carbon in the MVMA is estimated based on model simulations and measurement constraints. The 3-D modeling system uses MM5 to simulate the meteorology and provide the dynamics to the CMAQ chemistry-transport model (Figure 2), which simulates the sources, sinks, and distribution of aerosols during the MVMA. A tracer version of the CMAQ model will also be used to evaluate the sensitivity of the modeled black carbon to several source configurations. Initial calculations of the meteorological conditions using the MM5 mesoscale meteorological model for April 2003 have been completed and are being analyzed.



**Figure 2: Inner domain modeled by using MM5 and CMAQ for the Mexico City calculations. This domain will also be used for analyzing the data set collected during the DOE ASP 2006 MILAGRO field experiment.**

### Publications/Presentations

1. H.K. Im, M. L. Stein, and V. R. Kotamarthi, Predicting CMAQ’s ammonia wet deposition and a novel approach to inverse modeling, *J. Geophysical Research*, 2005 (accepted).
2. J. S. Gaffney, N. A. Marley, M. M. Cunningham, and V. R. Kotamarthi, Beryllium-7 measurements in the Houston and Phoenix urban areas: Estimation of upper atmospheric ozone contributions, *J. Air and Waste Manage. Assoc.*, 55, 1228–1235, 2005.

## Large-Scale Discrete Adjoint and Sensitivity Computations (AUTODIFF)

PI: Paul Hovland, Mathematics and Computer Science

A massive optimization problem has been carried out within the “Estimating the Climate and Circulation of the Oceans” (ECCO) project (<http://www.ecco-group.org>). The problem involves a state-of-the-art global general circulation model that was fit to a variety of satellite and in situ observations (order

$10^8$  observational elements) by using the method of Lagrange multipliers, often referred as the “adjoint method.” Automatic derivation of the adjoint operator from the nonlinear parent code has proved to be an essential ingredient. The tool used so far is Transformation of Algorithms in FORTRAN (TAF), a commercial tool developed by the company Fastopt. Use of TAF in practice is extremely labor intensive, yet it clearly demonstrates the enormous power of automatic differentiation (AD) tools, particularly when operated in the adjoint, or reverse, mode.

To assure the future availability of such tools independent of a single small commercial vendor, and to bring to bear the much wider expertise in the computer science community, we are developing a new open source tool, OpenAD. Novel features will address the issue of nonsmooth gradients due to switches, thresholds, and limiters in the model’s parameterization schemes. The objective is to enable the use of higher-order derivative information (beyond first-order tangent linear and adjoints) such as the Hessian of the cost function to posterior variances in control space.

Software advancements in 2005 included incorporation of static to the OpenAD tool via the OpenAnalysis toolkit. In addition, improved two-level checkpointing strategies were developed and implemented, and the ability to exploit the structure of simple iterative loops was added. The result of all of these improvements was an order of magnitude speedup.

Simulations on Jazz with the prototype OpenAD tool have been successfully applied to study adjoint-based sensitivities of a barotropic ocean model to changes in bottom topography. More precisely, we investigated the sensitivity of mass transport through the Drake Passage, a key oceanographic quantity, to changes in bottom topography everywhere in the domain. Sensitivities are mediated through the flow field represented by the model dynamics. This sensitivity map was achieved through a single adjoint model integration (Figure 3). The computations carried out in FY2005 have proven the feasibility of adjoint-based calculations for a scalable model using OpenAD derived code. The new calculations anticipated for FY2006 will extend to a fully fledged ocean general circulation, MITgcm (<http://mitgcm.org>).

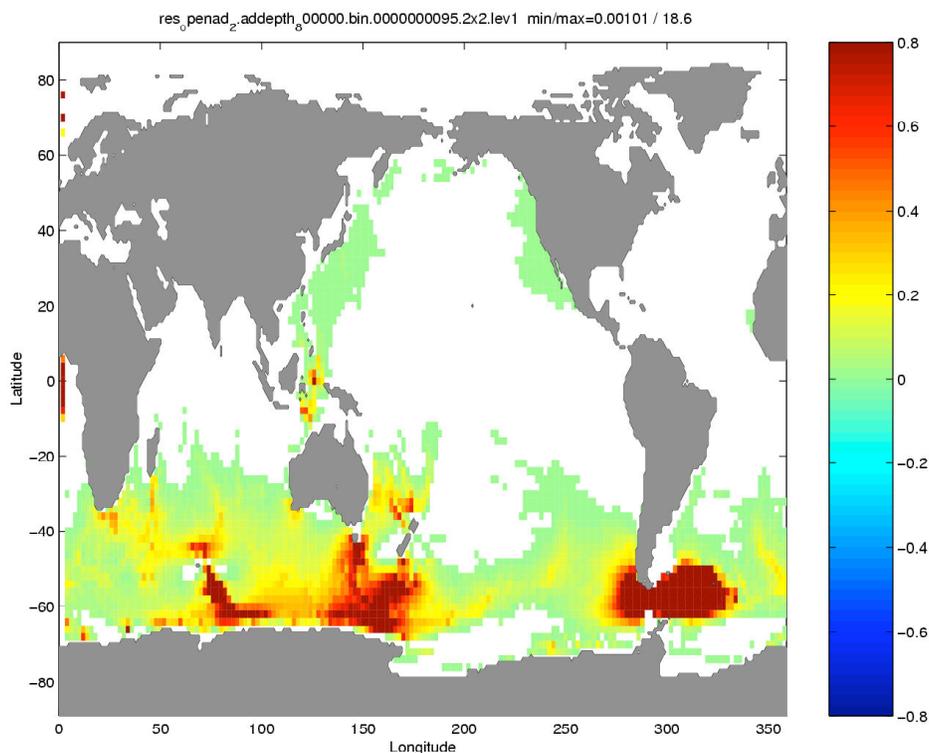


Figure 3: Sensitivity map of mass transport through the Drake Passage.

## Studies of the Water-Gas Shift Reaction over Mono- and Bimetallic Catalyst Surfaces (BIMETALLIC-WGS)

PI: John Krebs, Chemical Engineering

Our group is involved in the development of catalytic materials for the reforming, or conversion, of hydrocarbon fuels to a hydrogen-rich gas mixture that can be fed to hydrogen fuel cells. In addition to hydrogen, the breakdown of hydrocarbon fuels also produces carbon monoxide and carbon dioxide. Carbon monoxide has been shown to inhibit the activity of hydrogen fuel cells at levels of 10–100 ppm. Because levels of CO in the product stream are as high as 10%, methods of reducing these levels have been implemented. The water-gas shift (WGS) reaction,  $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2$ , is being used to remove the CO contaminant and produce additional hydrogen (Figure 4). Currently, the most active WGS catalysts suitable for use in fuel processors are Pt-based catalysts. Although very effective, these catalysts are expensive; hence, effort is being directed to develop a less expensive, nonprecious-metal-based WGS catalyst. However, these less expensive catalysts can also generate methane, thereby consuming the desired hydrogen.

To address this problem, we are exploring ways to modify the absorption properties of Co and Ru with the addition of a second metal. Theoretical calculations focus on the energetics of the WGS and methanation reactions over mono- and bimetallic surfaces. Studies of monometallic systems were conducted first to establish general trends over the areas of interest in the periodic table. Experimental results coupled with theoretical studies of the WGS reaction over monometallic surfaces are being employed to design bimetallic, WGS selective Ru or Co-based catalysts.

While modeling of the adsorption of molecules on the surfaces of metals is well established, its use in directing heterogeneous catalyst development is relatively new.

### Publications/Presentations

1. T. Krause, J. Krebs, M. Ferrandon, and C. Demecik, "Water gas shift catalysis," DOE 2005 Annual Review, May 23–26, 2005, Arlington, VA.

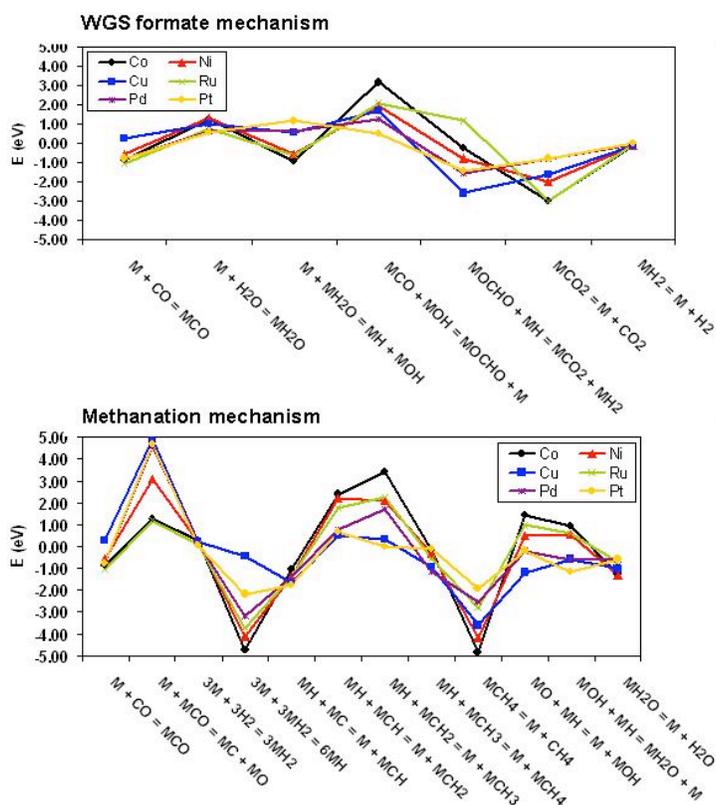
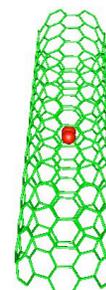


Figure 4: Water-gas shift (WGS) formate mechanism.

## Wave Packet Dynamics with Cartesian Coordinates (CARTESIAN)

PI: Stephen Gray, Chemistry

Quantum dynamics simulations of atoms and molecules are important for understanding a wide range of problems in chemical physics, atmospheric and combustion chemistry, and nanoscience. The aim of this project is to develop a Cartesian-coordinates-based code for such quantum studies. The code will solve the time-dependent Schrödinger equation governing the motion of atoms and molecules, generating wave packets that can be analyzed to infer dynamical information. Most quantum mechanical methods for molecular problems involve internal coordinates and complicated angular momentum considerations that are cost-effective for few-atom systems. A conceptually simpler approach is to represent the wave packet in Cartesian coordinates. While the wave packet is much less compact, the required operations to generate its time evolution are simpler and more readily implemented on parallel computers. As one begins to consider larger polyatomic systems, or even atoms or molecules moving in nanostructured environments (Figure 5), a purely Cartesian representation, implemented in a parallel computing environment, should prove to be one means of obtaining accurate quantum mechanical information.



**Figure 5: Diatomic molecule confined to a carbon nanotube.**

For a general  $N$ -atom problem, there are  $3N$  Cartesian coordinates. Allowing for the constant velocity of the center of mass of the system, one can reduce the necessary number of Cartesian coordinates to be included in a calculation to  $3N-3$ . The wave packet is then a function of these  $3N-3$  coordinates. Clearly, even for small  $N$ , the scale of the problem can be vast if, say, 10–20 grid points are required to describe each Cartesian dimension. Of course some problems can be simplified by assuming some atoms or bonds are fixed—a common approach in practice. However, the more general problem will be a good candidate for future petaflops computing architectures.

Keeping these points in mind, we are designing the Cartesian wave packet code to allow parallelization over any number of Cartesian coordinates. The parallelization scheme (i.e., 1-D, 2-D, and higher-domain decompositions) is also a variable. To date, we have written and assembled most of the software components, and we have validated the code for parallelization of a 4-D problem with explicit parallelization over two of the four dimensions. Our tests on Jazz involved up to 108 processors and showed about a 70-fold speedup, about 65% of the perfect, linear scaling limit. We also carried out a challenging 6-D application to the combustion-important methyl radical, which involved a mixed representation (three Cartesian and three internal coordinates) that employed some of the parallel techniques developed in this project.

### Publications/Presentations

1. D. M. Medvedev, L. B. Harding, and S. K. Gray, Methyl radical: Ab initio global potential energy surface, vibrational levels, and partition function, *Mol. Phys.*, in press 2005.

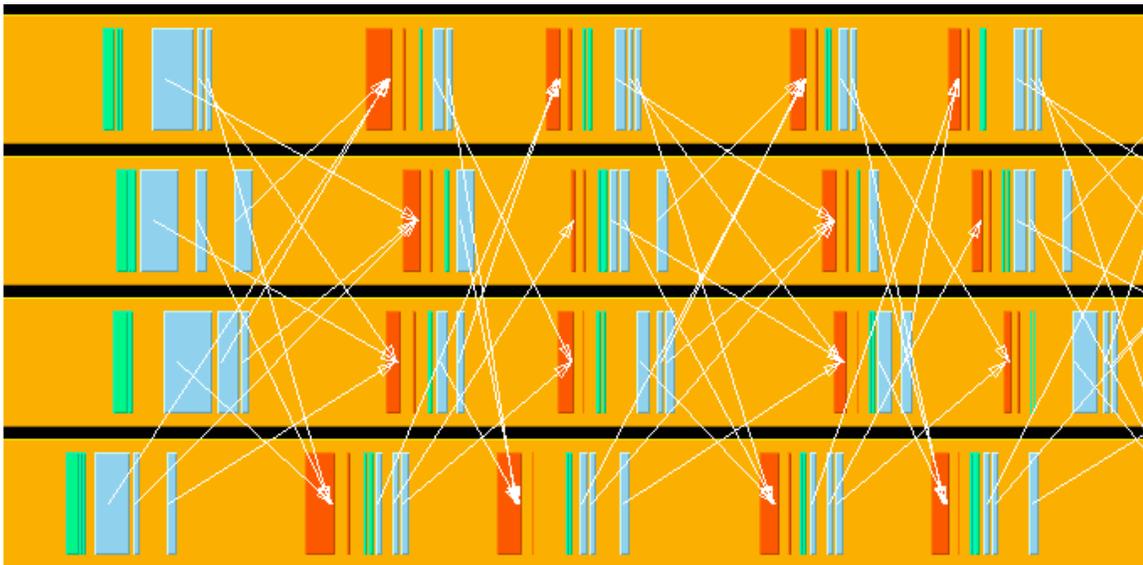
# Development and Performance of the Community Climate System Model on Linux Clusters (CCSM2)

PIs: Michael Jacobs, Michael Tobis, Mike Steder, and Ray Loy, Mathematics and Computer Science

The Community Climate System Model (CCSM) is a fully coupled global climate model that provides state-of-the-art computer simulations of the Earth’s past, present, and future climate states. CCSM is the primary model for global climate research in the United States and is supported on a variety of computer systems. It is also being used for assessing impacts of climate change for the Intergovernmental Panel on Climate Changes (IPCC) Fourth Assessment. CCSM is the result of a community modeling effort sponsored by the National Science Foundation and the Department of Energy.

We are examining the possibility of whether a flexible scripting language such as Python can be useful as the high-level coupler description layer of a high-performance, distributed-memory parallel model. We believe we can improve the productivity of physical scientists running multiple physics models using Python. By building and using Babel interfaces to performance critical compiled coupler modules (MCT), we intend to test the hypothesis that the flexibility offered by a scripting language can outweigh the performance penalty. Jazz has been the primary development platform for the Python effort; the availability of the parallel machine was critical for progress.

We have also studied the Parallel Ocean Program (POP) code, a component of CCSM, with the goal of improving its parallel efficiency. POP 2.0 has been instrumented with MPE calls for visualization by using the Argonne-developed Jumpshot tool (see Figure 6). We studied the performance of this instrumented version of POP on Jazz, which is one of the officially supported platforms for CCSM—the only Linux cluster with that distinction, which makes it ideal for development work. The analysis of POP suggests that performance gains can be realized by aggregating messages in its communication routines.



**Figure 6: Jumpshot analysis of the instrumented POP 2.0 code running a test case on 4 processors. The image shows MPI communications at the end of the barotropic driver. Horizontal bars correspond to individual processors, the horizontal axis representing time.**

## Computational Nanophotonics with Chombo (CHOMBO)

PI: Zdzislaw Meglicki, Mathematics and Computer Science

Among the challenges of present-day scientific and engineering computations are multiscale models. These call for resolving details of various structures at various levels. Modeling of nanophotonic devices is a good example. Here we may have larger microscale optical conditioning structures combined with nanoscale active signal processing elements. The current focus of this project is the development of a code for numerical simulation of such devices by using multigrid and adaptive mesh refinement (AMR) methods. Later we plan to convert the code into a dynamically reconfigurable toolkit, similar to the well-known data visualization program AVS. To this effect we have based the code on the Chombo toolkit developed by at LBNL. The C++ toolkit provides basic primitives for multigrid and AMR operations, parallelization, and data movements while at the same time allowing for the physics of the modeled system to be coded in plain Fortran. This approach has obvious advantages as it hides the complexity of AMR and parallelization and enables the user to focus on the physics itself.

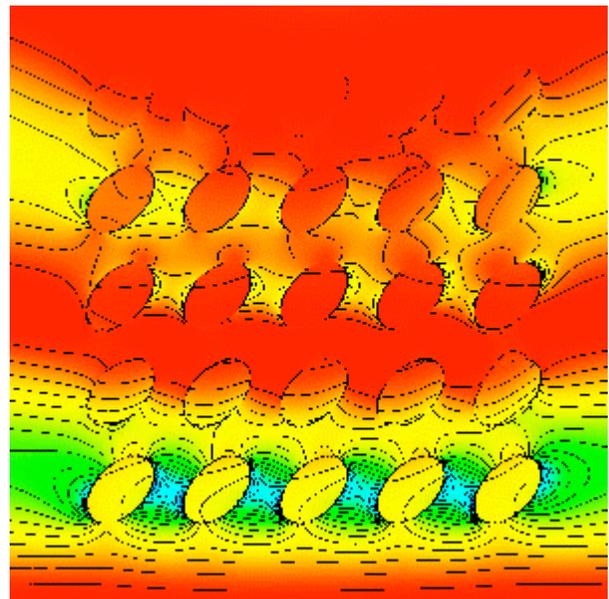
We have used the Jazz cluster to test our code, especially for parallel runs. Access to the system helped us identify and remedy semantic, coding, performance, correctness, and stability problems. Jazz was indispensable in providing a stable, highly functional platform for this work. So often, systems are provided for production work but not for development. Here we found an environment that was highly suitable and configured for both.

In the process we have obtained a number of new technical results that may be directly applicable to nanophotonic structures (Figure 7). These include cavity signal conditioning, various optical funnel configurations, superlattice configurations, and metallic nanograin systems.

As the application is developed further and the toolkit constructed, we expect the system to be used by engineers and scientists working on nanophotonic devices. We also expect that users themselves will provide additional modules that will broaden the scope of the application.

The code developed in FY2005 is two dimensional. We have developed and implemented rich, flexible, and easy-to-use semantics for device layout specification: The name of the code, “Shapes,” derives from this feature. We have also modified the code to express the staggered grid mapping of Maxwell electrodynamics explicitly within the Chombo layer itself. This feature is important as it affects the way data is moved between various levels of the multigrid.

Frequency domain output can be now generated for an arbitrary number of frequencies. I/O is provided both in parallel-HDF5 and in Gnuplot-readable text-file formats. The code and its associated facilities



**Figure 7: Scattering of an electromagnetic wave, 3000 Å long (near ultraviolet), on a grid of nano-dimensional elliptical silver cylinders. The cylinder's long axis is 37.5 nm, and the eccentricity is 0.79. The spacing between the cylinders is 45 nm.**

are fully documented in reports and in Unix-style man pages, all of which have been installed on the Jazz cluster.

## Computational Nanoscience (COMPANO)

PI: Peter Zapol, Chemistry/Materials Science/Center for Nanoscale Materials

Computational nanoscience projects involving density functional theory, molecular orbital theory, and tight-binding methods were performed at the LCRC facility this year.

Titanium dioxide nanoparticles are currently receiving a lot of attention because of their inherent suitability for advanced photochemical applications. Size, phase, and morphology of the nanoparticles are the critical parameters determining their performance in particular applications. A thermodynamic model [1] devised to describe the shape of nanoparticles as a function of size was used last year to predict the phase stability of titanium dioxide nanoparticles, with particular attention given to the cross-over of stability between the anatase and rutile phases [2, 3]. This work has now been extended to titanium dioxide nanoparticles in water, to examine the effects of various adsorption configurations on the equilibrium shape and the phase transition [4]. Moreover, the studies were extended to include hydrated surfaces of rutile and anatase. We also modeled the pH dependence of the anatase and rutile nanoparticle thermodynamics, using varying coverage of the surfaces by H, H<sub>2</sub>O, OH, and O adsorbates. Density functional calculations performed on Jazz were used to accurately determine surface energies and surface tensions. These calculations used generalized gradient approximation (GGA) and ultrasoft pseudopotentials, followed by projected augmented wave (PAW) single point calculations, as implemented in the Vienna Ab initio Simulation Package (VASP). The effects of nanocrystal morphology on the phase transition were addressed and comparisons drawn with previously reported studies.

Inconsistencies in experimental thermochemical analysis of the anatase to rutile phase transition have led to speculation as to the physical and chemical parameters affecting the stability of TiO<sub>2</sub> at the nanoscale. Using a thermodynamic model, we present predictions of the transition enthalpy of nanocrystalline anatase and rutile as a function of shape, size, and degree of surface adsorbate coverage, showing that thermochemical results can differ for various faceted or spherical nanoparticles. The results show that surface adsorbates induce changes in the shape of rutile nanocrystals and anatase nanoparticles and that the size at which the phase transition may be expected varies significantly with pH.

Explicit calculations of nanoparticles require a large number of atoms to be considered. Tight-binding methods offer an attractive alternative to first-principles calculations. The reliability of tight-binding methods requires a comparison to more rigorous density functional calculations for relatively small systems. To this end, we used DFT to optimize anatase nanoparticle of 105 atoms. Structural properties, such as radial distribution function, were compared to results of tight-binding calculations, showing good agreement. This work has been extended to tight-binding calculations of up to 1365-atom anatase nanoparticles [6].

### Publications/Presentations

1. A. Barnard and P. Zapol, A model for the phase stability of arbitrary nanoparticles as a function of size and shape, *J. Chem. Phys.* 121, 4276 (2004).

2. A. Barnard and P. Zapol, Effects of particle morphology on the phase stability of TiO<sub>2</sub> at the nanoscale, *Phys. Rev. B*, 70, 235403 (2004).
3. A. S. Barnard and P. Zapol, Predicting the energetics, phase stability and morphology evolution of faceted and spherical anatase nanocrystals, *J. Phys. Chem.*, 108, 18435 (2004).
4. A.S. Barnard, P. Zapol, and L.A. Curtiss, Modeling the morphology and phase stability of TiO<sub>2</sub> nanocrystals in water, *J. Chem. Theory. Comput.* 1, 107–116 (2005).
5. A. S. Barnard, P. Zapol, and L.A. Curtiss, Anatase and Surfaces with adsorbates representative of acidic and basic conditions, *Surf. Sci.*, 582 172 (2005).
6. Y. Lin, S. Erdin, A. Barnard, Peter Zapol, and J. W. Halley, *Modelling of TiO<sub>2</sub> nanoparticles*, preprint, 2005.

## Large-Scale Cumulative Reaction Probability Calculations (CRP)

PIs: Ron Shepard, Mike Minkoff, Mathematics and Computer Science

Partial differential equations (PDEs) arise in many scientific and engineering contexts and form the backbone of many computational science endeavors. Their accurate numerical solution by computer simulations has long been considered important by federal funding agencies. National initiatives such as DOE's SciDAC (Scientific Discovery through Advanced Computing) and NSF's cyberinfrastructure initiatives emphasize the essential role that scientific computing now occupies in virtually all research programs. These also identify a major remaining challenge: "to deliver on the promise of providing 'peak' computing power for scientific codes running on terascale computers," namely, massively parallel high-performance computing (HPC) platforms with thousands or tens of thousands of processors (CPUs).

Massive parallelization offers the promise of computing at a level that has never before been achieved. To realize the full potential requires the development of efficient parallel algorithms, however. Two of the most important techniques used in PDE simulations are iterative linear solvers and eigensolvers, whose optimization and efficient parallelization are addressed by this Jazz project. More specifically, this project seeks to implement certain optimized numerical methods on HPC platforms for general use by scientists from many disciplines.

The parallel codes are designed to be (1) *general*, in that they can in principle be applied to many different types of applications; (2) *usable*, that is, sufficiently modular as to serve as kernel routines for subsequent front-end development in specific disciplines; (3) *scalable*, over large numbers of CPUs; and (4) *optimal*, that is, very computationally efficient over a broad range of applications.

Jazz enabled us to perform parallel scalability tests of our iterative eigensolver and linear solver kernel routines, including both specialized routines and the fundamental matrix-vector product operation. These tests indicated that the latter does not scale efficiently for typical chemical physics application matrices, prompting the development of a new parallel implementation. Among the software enhancements during the past year were low-level solutions to the matrix-vector product problem; new, generalized versions of the kernel routines that can handle arbitrary grid sizes and number of CPUs were also developed (this generality is required by real applications, and also introduces the aspect of load balancing); dimensional combination features; and several new preconditioners. A new round of testing indicated that the revised matrix-vector product algorithm does indeed scale well over all of Jazz

(Figure 8). Parallel isoefficiency analyses indicate that both specialized and matrix-vector product routines may be effectively implemented over tens of thousands of CPUs.

In addition, Jazz was used in conjunction with the above routines to perform rovibrational spectroscopy calculations for triatomic rare gas clusters. Calculations for the  $\text{Ne}_3$  trimer system indicate anomalous rovibrational structure not seen previously in molecular systems. More broadly, the parallel iterative kernel routines developed on Jazz and, in the future perhaps implemented on much larger HPC clusters, will enable researchers in physical chemistry and other disciplines to perform PDE calculations for a much broader class of applications than heretofore possible.

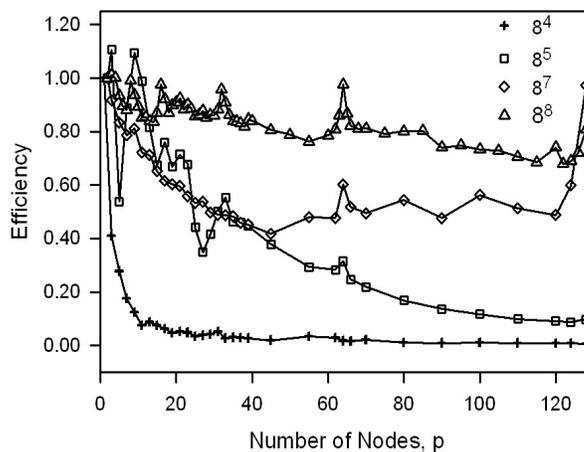
## Kinetics of Enzymatic DNA Repair (DNA\_REPAIR)

PIs: Aaron Dinner and Stuart Rice, Office of the Director

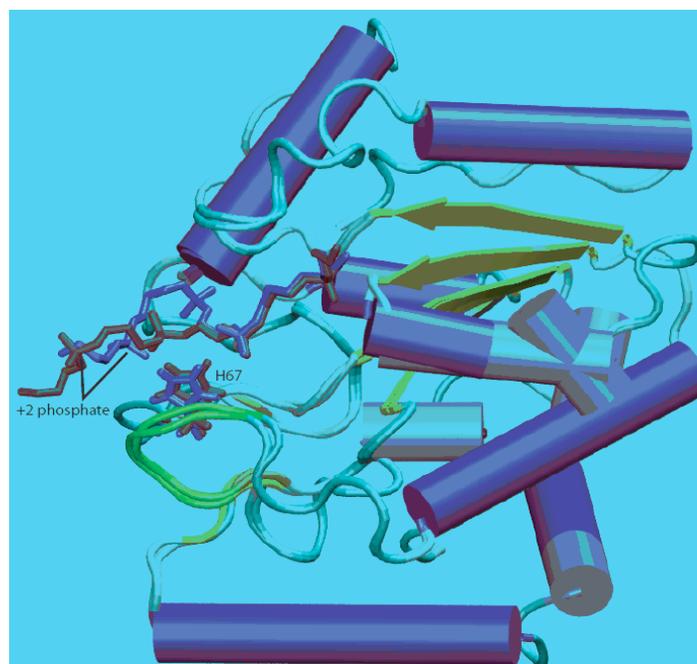
The DNA repair enzyme uracil DNA-glycosylase (UDG) removes bases that are normally restricted to RNA (uracil) from DNA. Misincorporation of deoxyuridine and deamination of cytosine cause several hundred uracil bases to arise in the DNA of a human cell every day. Except where it replaces a thymine, such uracil is premutagenic and must be eliminated to maintain genomic integrity. UDG initiates this process by cleaving the glycosylic bond of deoxyuridine in DNA to yield an apyridimic site.

In contrast to most enzymes, the activation energy is lowered primarily by substrate electrostatic interactions. Phosphate groups in the DNA backbone stabilize an oxocarbenium cation intermediate.

We performed dual topology free energy perturbation simulations to resolve apparent discrepancies between simulations and experiments concerning the role played by one of these groups. In addition to the structure of the bound substrate, we obtained protonation states for an associated histidine residue that was indicated to have a large anti-catalytic effect (Figure 9).



**Figure 8: Parallel efficiency vs. number of Jazz nodes for the new implementation of the matrix-vector product routine, as applied to a model system of varying dimensionality (4–8) with 8 grid points per dimension.**



**Figure 9: Structures corresponding to the protonated endpoint. Except for one exposed helix, the two structures are quite similar, suggesting that the protein is well behaved.**

The free energy simulations involve extensive postprocessing to correct the results for approximations made to treat solvent efficiently. This step, completed in FY2005, demonstrated that the histidine in question (H67) is indeed protonated over the range of pH values studied in experiments. The free energy differences were decomposed to determine the protein residues that most strongly contributed to the observed values. Subsequently, we also mapped the free energy for DNA to bind in different modes to the protein. These calculations are vital for showing rigorously that recent kinetic experiments fail to probe the contributions of the controversial +2 phosphate group. The calculations resolve issues concerning a protein widely regarded as a paradigm for understanding DNA repair.

In the process of performing the continuum electrostatic calculations, we realized that the standard protocol neglects to account for an effect that arises from inconsistent truncation of the pairwise interactions. We introduced means for accounting correctly for this feature; this represents a significant methodological advance of general interest in molecular simulations.

## **Meson and Baryon Observables in a Dyson-Schwinger Approach (DSE\_EXC\_PION)**

PIs: Andreas Krassnigg, Arne Hoell, Stewart Wright, and Craig Roberts, Physics

Our project deals with a nonperturbative continuum approach to QCD, the fundamental theory of the strong interaction between quarks and gluons. This approach uses coupled integral equations to calculate the basic building blocks, the Green functions, of the theory. By describing quarks (the constituents) and hadrons as quark-antiquark or three-quark bound states on the same footing, we can 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.

The project's main directions at the moment are twofold. On one hand we investigate mesons and their radial excitations in order to study the long-range part of the strong interaction; this part of the interaction is not accessible by perturbative methods and requires a nonperturbative framework. On the other hand we investigate the structure of the nucleon by calculating its electromagnetic form factors. A manifestly Poincare covariant approach such as ours is ideal to compute form factors, in particular for regions of high momentum transfer.

In 2005, we used Jazz as follows:

- We investigated the parameter dependence of radial meson excitations in detail for pseudoscalars and scalars. This work involves calculations for various quark masses in order to attempt an identification of the excitations in the calculated spectra with states seen in experimental data.
- We studied the first radial excitation of the kaon and its leptonic decay constant. This work extended our investigations to systems with constituents of unequal masses.
- We calculated the electromagnetic form factor of the pion's first radial excitation and studied its model-parameter dependence. The charge radius of the states can be extracted from the form factor at zero momentum transfer. Results for excited-states charge radius exhibit a similarly strong model-parameter dependence as the bound state masses.
- We investigated possible extensions of the present model without the immediate danger of not being able to actually do the calculations required.

We also modified the code to allow for different choices of the model interaction from the input file for easy comparison of runs for different models. In this way, parameter dependence as well as model dependence of meson properties can be investigated with the same code. Additionally, two more versions of the code were created, to describe scalar mesons and their radial excitations and to describe mesons consisting of quarks with unequal masses.

The meson excited-state calculations have shown us a possibility to study the strong interaction in a systematic and powerful way. We expect that these calculations will continue to have considerable impact on our understanding of meson states, including charmonia, hybrids, confinement, and the concept of diquark correlations. The studies of the nucleon and its electromagnetic form factors will continue to contribute to the current debate regarding both the structure of the nucleon and the electromagnetic form factors by identifying contributions from the quark core vs. those from the pion cloud dressing the quark core.

### **Publications/Presentations**

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2. A. Krassnigg and P. Maris, Pseudoscalar and vector mesons as Q anti-Q bound states, *J. Phys. Conf. Ser.* **9**:153–160, 2005.
3. A. Holl, A. Krassnigg, C. D. Roberts, and S. V. Wright, On the complexions of pseudoscalar mesons, *Int. J. Mod. Phys. A* **20**:1778–1784, 2005.
4. A. Holl, A. Krassnigg, and C. D. Roberts, Confinement, CDSB, bound states, and the quark-gluon vertex, *Nucl. Phys. Proc. Suppl.* **141**:47–52, 2005.

## **Earth System Modeling Framework (ESMF)**

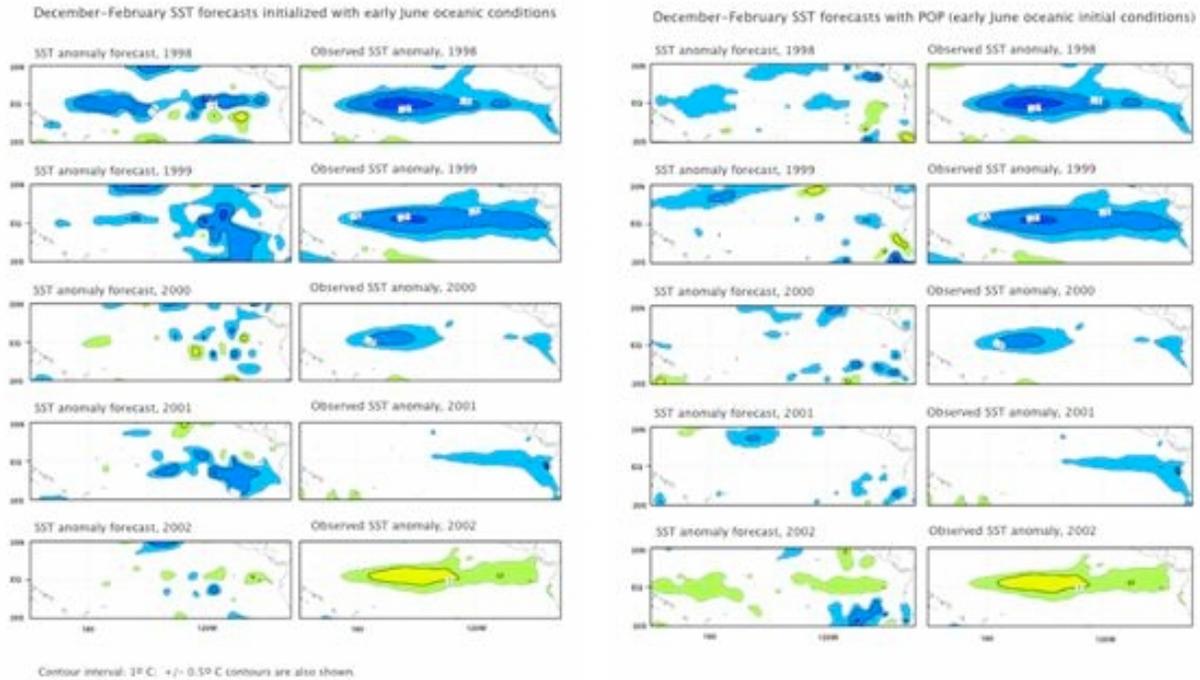
PIs: Jay Larson and Robert Jacob, Mathematics and Computer Science

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 being evaluated and adopted by leading models across the country, including the NOAA NCEP Global Forecasting System (GFS), the NASA GEOS-5 atmospheric GCM, Navy, Air Force and Army models, the Community Climate System Model (CCSM), MITgcm, UCLA models, and the Weather Research and Forecast (WRF) model (see Figure 10). The ESMF hierarchical, component-based architecture facilitates the systematic construction of very 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.

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.

In FY05 the ESMF project completed its first round of funding, development, and deployment; defined a long-term technical vision and multi-agency organizational structure; and began implementation of its next phase. The project also completed a set of “interoperability experiments” that demonstrated new, interagency couplings of Earth system model components enabled by the ESMF software. The ESMF

team used Jazz to run exhaustive nightly unit and system tests and examples, with a variety of the Jazz compilers. These tests were instrumental in ensuring that the ESMF software was robust and portable. The ESMF team also used Jazz as a development platform. Practical additions to the ESMF during FY05 included the ability of components to execute concurrently as well as sequentially, and the ability to run components either as single executables or as multiple executables.



**Figure 10: Experiment performed by UCLA in which two different ocean models were run with the UCLA AGCM and the results compared. ESMF was used as the underlying interoperability framework, with the UCLA AGCM, the POP ocean, and the MITgcm ocean all running as ESMF components. This work is representative of the kinds of coupling experiments and evaluations that ESMF facilitates.**

## Fast Code Development for Large Computed Tomography Data Sets (FASTCTDEV)

PIs: Chris Deemer and Eugene Koehl, Energy Technology

We are addressing issues related to computed tomography from x-ray data sets. The data is obtained from large, flat-plate detectors and wide, line detectors. Flat-plate detectors can image engineering samples as large as 14 inches square with better than 200 micron resolution. Line detectors can image samples as wide as 30 inches with better than 83 micron pixel resolution. The issues are

- Producing volume images from the data sets within 30 minutes of acquisition,
- Preserving the 16-bit resolution and image size, and
- Handling very large data sets (~ 20 GB per set).

The use of massive parallel processors such as Jazz has allowed a significant reduction in real-world time required to reconstruct a volume from ~20 GB data sets. A typical engineering workstation using dual, 3.0 GHz, Intel Zeon processors with 1 GB RAM requires about 1-1/2 hours to calculate a single slice from a 2000 slice volume. A smaller, parallel processor system using 25, 2.4 GHz, Intel P4 processors and 512 MB RAM reduces this time to 15–20 minutes per slice. The use of 50 large-memory nodes on the Jazz system reduces the reconstruction time to less than 5 minutes per slice. Generally, the use of systems such as Jazz allows the acquisition of large, real-world engineering data sets from the factory floor and visualization of reasonable volumes in near-real time (see Figure 11).

The software used to reconstruct the volume images is currently a Beta version ported from smaller systems. It is the first version to run on Jazz. We will be looking at ways to optimize this version to reduce reconstruction times.

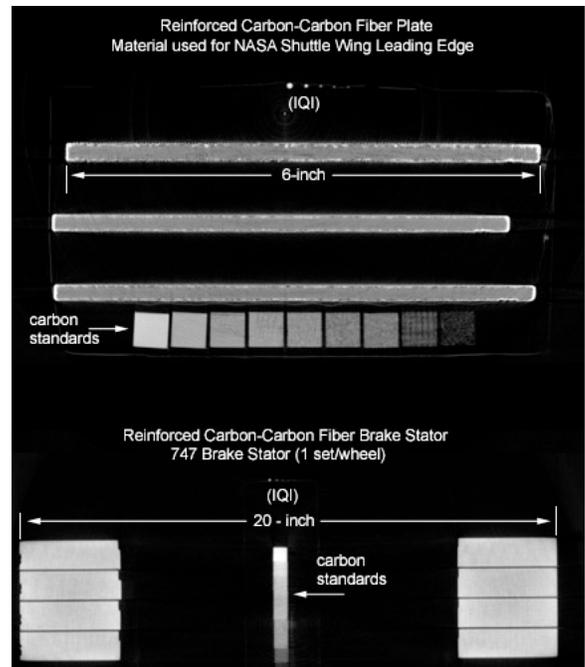
## Global Climate Modeling with the Fast Ocean Atmosphere Model (FOAM)

PIs: Robert Jacob and Yannick Donnadieu, Mathematics and Computer Science

We are trying to understand how the interactions between the atmosphere, ocean and cryosphere function to produce the climate of the present and the climates of the past. We use a coupled climate model called FOAM, Fast Ocean Atmosphere Model. The main features of the model are a low-resolution model of the global atmosphere and an efficient model of the global ocean.

Several new computational experiments were performed on Jazz in FY2005. The first study concerned the quantification of the effect of changing geography over the Mesozoic period (roughly 250-60 Million years ago (Ma)) on the atmospheric CO<sub>2</sub> content. The goal is to examine how the continental drift could have controlled the long-term atmospheric CO<sub>2</sub> and climate variations over the Mesozoic by focusing on 8 typical times during the Pangea breakup process. The second study investigated modes of behaviour of the climate system quite different from the present which occur during the Cretaceous period (~140–160 Ma): a period characterizes by low pole-equator temperature gradients and clement winters (see Figure 12). A third study used FOAM to examine the effect of the pole-to-equator temperature gradient on the poleward transport of energy under ideal “aquaplanet” conditions. Jazz was crucial to performing the simulations. We also used Jazz to maintain and develop FOAM.

Our study of the tectonic-climate relationship our work is in progress, but we are now able to provide a preliminary CO<sub>2</sub> curve for the Mesozoic period, which reveals that the continental drift may have paved the way for a relatively low CO<sub>2</sub> world from the Jurassic period. Such a result has potential implications



**Figure 11: Reinforced carbon-carbon fiber aging plates used on the leading edge of the NASA shuttle wings (top). Carbon-carbon fiber brake stators used on a Boeing 747 aircraft 20-inch diameter, 1-inch thick stack of four (bottom). Both images show nine-carbon density standards and five-carbon, image-quality indicators.**

for the evolution of life as one of the main calcareous producers (i.e., the coccolithophorides) is believed to have appeared at the Trias-Jurassic boundary. There may have been a correlation between the huge CO<sub>2</sub> decrease occurring at the T-J boundary and the appearance of this species.

We also used FOAM to investigate the impact of paleogeography on the global climate, using an Early, Mid-, and Late Cretaceous continental configuration. We found that changes in geography from the Early to Mid-to-Late Cretaceous cause a large decrease of the seasonal cycle. Our study also suggests a mechanism that can weaken the correlation between CO<sub>2</sub> and climate changes during the Cretaceous. This suggests that the paleogeography may affect the relation between pCO<sub>2</sub>.

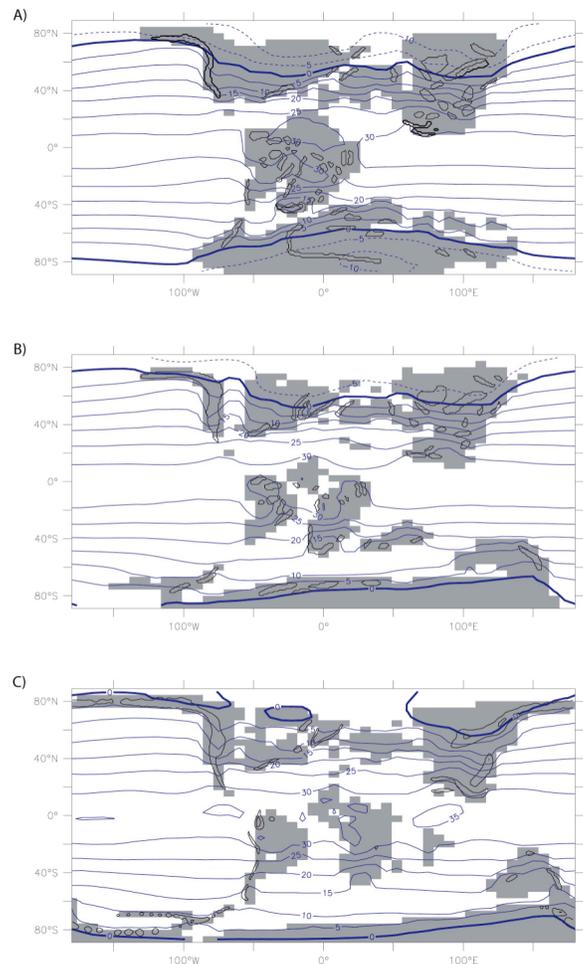
New software developments in FY05 included the ability to output components of the atmosphere momentum, heat, and freshwater budgets and the ability to read and write data files in NetCDF format. We also worked with members of the GriPhyN project to use Grid-based tools for performing ensemble simulations with FOAM.

## High-Throughput Genome Analysis (GADU-GNARE)

PI: Alexis Rodriguez, Mathematics and Computer Science

The GADU-Gnare project is part of a system (PUMA2) that addresses the problem of annotating protein sequences automatically by means of protein comparisons with existing, well-annotated protein sequences from a list of several organisms from different kingdoms of life. Millions of protein sequences need to be compared and analyzed through homology comparison tools. GADU-Gnare uses a variety of tools such as BLAST, BLOCKS, and TMHMM to make sequence homology computations (see Figure 13). The amount of time it takes to run these tools has been significantly reduced because of the use Jazz. The results are then used in conjunction with the results from other analyses to make an educated prediction of the function of a novel protein. To date, we have obtained important results regarding the functions of new protein sequences. We also converted the execution of tools in the form workflows and automatically execute the workflows on high-performance clusters using Condor-G.

In addition to biological questions, through the development of GADU-Gnare we are also helping other groups, such as GriPhyN and the Open Science Grid, through the development of an automated mechanism for controlling job submissions to Grid environments (e.g., the TeraGrid), specifically by checking what Grid site clusters are available and ready to receive a work load. Currently, GADU-Gnare



**Figure 12: Mean annual surface temperature (C) as simulated for 3 parts of the Cretaceous period: (A) Aptian, (B) Cenomanian, and (C) Maastrichtian. Gray shading indicates Cretaceous continents.**

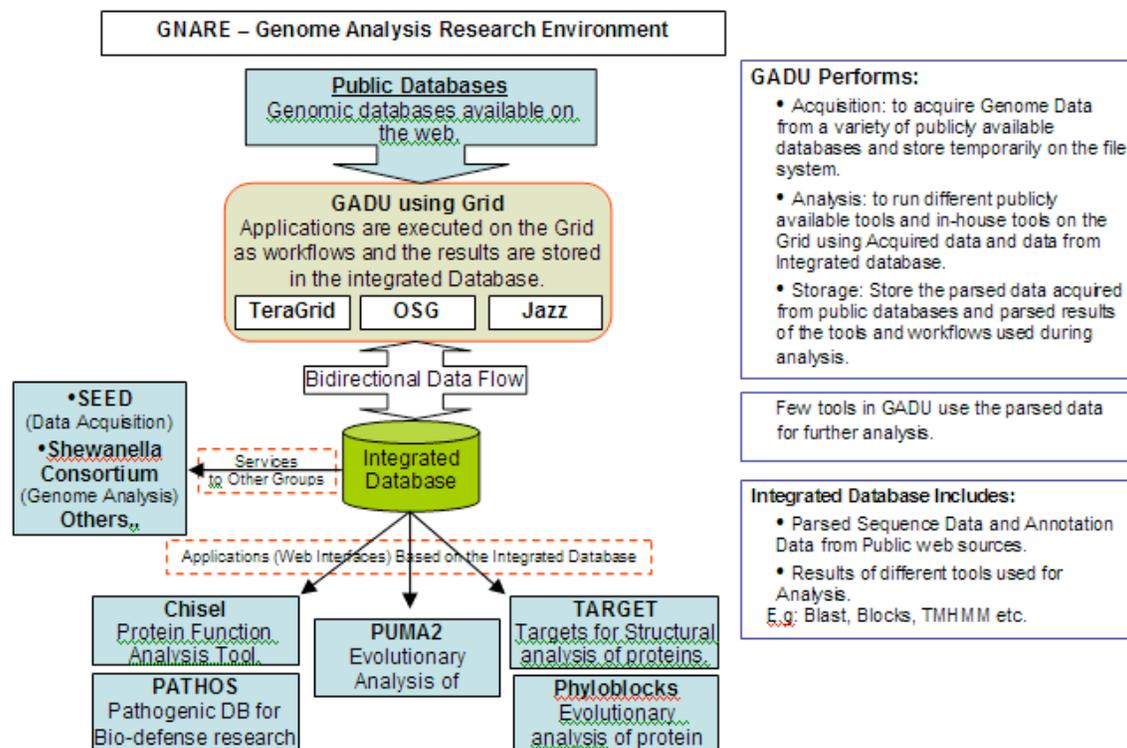


Figure 13: Schematic view of Gnare (Genome Analysis Research Environment).

is one of only a few systems that can submit effortlessly to different Grid clusters, without worrying about which site is available. Another important aspect is that the job will not monopolize a cluster; in other words, a job can request a lesser number of nodes from each Grid cluster, instead of asking for a large number of nodes from one cluster.

## Discharge-Produced Plasma Hydrodynamics and Radiation Transport for EUV Lithography (HEIGHTS-EUV)

PI: Vitali A. Morozov, Mathematics and Computer Science

Extreme ultraviolet lithography (EUVL) at wavelength near 13.5 nm is considered by many as the strongest candidate for large-scale manufacturing of integrated circuits. However, the EUV radiation source has been identified as the largest obstacle toward successful implementation of EUVL because no source technology is currently available to meet all the requirements for a production tool. Several concepts are now under intense development, which include electrically driven plasmas (DPPs) and laser-produced plasma (LPPs). Despite noticeable progress during recent years, the main limitation of the current designs is insufficient total in-band ( $13.5 \pm 2\%$  nm) power and, correspondingly, the low conversion efficiency of the sources.

Our team has been intensively developing a comprehensive computer simulation package, called HEIGHTS, for modeling the properties and radiation output of both DPP and LPP EUVL sources. The general purpose of the development is to provide the leading source manufacturers with a powerful and

flexible research tool to optimize operational regimes for their devices, and/or suggest alternatives with higher stability and efficiency. During FY2005, we developed the core of the HEIGHTS package, which includes magneto-hydrodynamics in a two-temperature approximation and Monte-Carlo-based radiation transport for 2-D cylindrical geometry. We have carried out preliminary computations on Jazz by varying the parameters of the devices (see Figure 14); however, additional study is required to make any conclusions on their efficiency and optimized parameters.

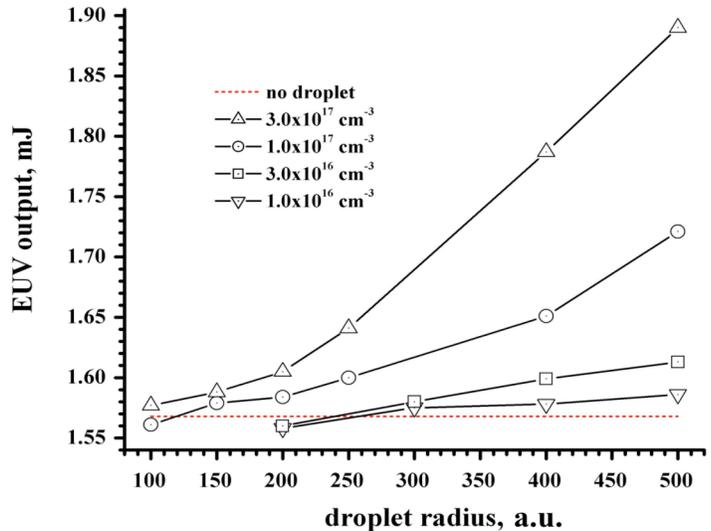


Figure 14: Xenon-driven Z-pinch device: the influence of conversion efficiency of the device from density of droplet

The leading manufacturers of integrated circuits are approaching the time when a final choice will be made for construction of the alpha tool, the prototype of the perspective EUV source. While the international microlithography community has already generated considerable data regarding the various competing approaches, no technology can yet satisfy all requirements. Our simulations with the HEIGHTS code is directed to provide an integral and unbiased comparison of the perspective techniques (LPP vs. DPP, xenon vs. lithium vs. tin, droplet vs. plate laser target, prepulse vs. pulse, and so on), while trying to additionally suggest the ways to improve the overall stability, efficiency, and brightness of the source.

### Publications/Presentations

1. A. Hassanein, Modeling of laser produced plasma in EUV lithography devices, EUV Source Modeling Workshop, San Jose, February 26, 2005.
2. A. Hassanein, V. Sizyuk, V. Morozov, I. Konkashbaev, T. Sizyuk, B. Rice, and V. Bakshi, Dynamic simulation of discharge and laser produced plasmas for EUV lithography devices, ICOPS - 2005, Monterey, Calif., June 18–23, 2005.
3. A. Hassanein, V. Morozov, V. Sizyuk, T. Sizyuk, and I. Konkashbaev, Discharge and laser produced plasma in EUV lithography devices and similarity to fusion plasma facing component lifetime, in *Proceedings of the European Congress in Advanced Materials and Processes — EUROMAT 2005*, Prague, Czech Republic, September 5–8, 2005.
4. V. Sizyuk, A. Hassanein, V. Tolkach, V. Morozov, T. Sizyuk, and B. Rice, Numerical simulation of laser-produced plasma devices for EUV lithography using the HEIGHTS integrated model, *Numerical Heat Transfer*, to appear.

## Lattice Quantum-Chromodynamics in Extreme Environments (LATTICE-QCD)

PI: Donald Sinclair, High Energy Physics

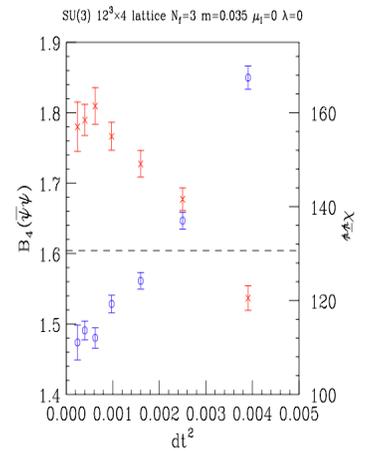
We are interested in quantum-chromodynamics (QCD) at finite baryon-/quark-number density and temperature, in regard to its phases and transitions. These phases include hadronic and nuclear matter

and the quark-gluon plasma. Studies of these properties are relevant to the physics of the early universe, neutron stars and relativistic heavy-ion collisions.

We simulate QCD on a discrete space-time lattice (lattice QCD). This quantum field theory is mapped onto a problem of classical fields on the sites and links of the lattice, evolving in a fictitious “time.” Hamilton’s equations describing this system are integrated numerically. Periodically this system is brought into contact with a heat bath to ensure ergodicity. Finite density is imposed by using a chemical potential.

Because of sign problems at finite quark-number density, we are simulating at finite isospin density, in the neighborhood of the finite temperature transition from hadronic matter to a quark-gluon plasma. Here the physics of small quark-number density and small isospin density are believed to be very similar. We are searching for the critical endpoint where the transition ceases to be a mere crossover and becomes a first-order transition. Such behavior might be accessible to relativistic heavy-ion colliders.

Our work on Jazz (and other clusters) in FY2005 was dedicated to studying 3-flavour QCD. Not only is this close to the real world, but it was believed that one could tune the critical endpoint to be as close to zero chemical potential as one desired by choosing a quark mass close to its critical value (the value at which the zero density transition ceases to be first order). We discovered that the fluctuation quantities (Binder cumulants; see Figure 15), which are used to determine the nature of the transitions, depend strongly on the “time” increment used in the numerical integration of the equations of motion. This fact had caused all groups, who had previously estimated the critical mass, to overestimate its value by at least 20%. We have not found the critical endpoint and have called into question all prior claims to have observed such a point. Jazz was especially useful in providing needed production time while NCSA’s Tungsten cluster was yet to become a stable production environment.



**Figure 15: Dependence of Binder cumulants on time increment.**

Because of our new determination of the critical mass, we will now continue our simulations at a lower quark mass, closer to the newly found value of critical mass. We are also converting our simulations to use a newly developed algorithm (rational hybrid Monte Carlo) that produces results independent of the “time” increment, used for numerically solving the equations of motion. Preliminary reports of our results caused one of the other groups in the field, who are using different techniques for surmounting the sign problem, to reexamine their earlier results. They are now reporting results that confirm our observations.

### Publications/Presentations

1. J. B. Kogut and D. K. Sinclair, Lattice simulations of Born-infeld non-linear QED, Argonne preprint ANL-HEP-CP-05-76 (2005).
2. J. B. Kogut and D. K. Sinclair, 3-flavour lattice QCD at finite density (QCD at finite isospin density and temperature revisited), Argonne preprint, ANL-HEP-CP-05-77 (2005).
3. J. B. Kogut and D. K. Sinclair, Finite dt dependence of the Binder cumulants for 3-flavor QCD at finite temperature and isospin density, [arXiv:hep-lat/0504003].
4. G. T. Bodwin, J. Lee, and D. K. Sinclair, Spin correlations and velocity-scaling in color-octet NRQCD matrix elements, *Phys. Rev. D* 72, 014009 (2005), [arXiv:hep-lat/0503032].

5. G. T. Bodwin, J. Lee, and D. K. Sinclair, Spin correlations and velocity-scaling in NRQCD matrix elements, in *AIP Conf. Proc.* 756, 384 (2005) [arXiv:hep-lat/0412006].
6. J. B. Kogut and D. K. Sinclair, Simulating lattice QCD at finite temperature and zero quark mass, [arXiv:hep-lat/0408003].
7. J. B. Kogut and D. K. Sinclair, The finite temperature transition for 3-flavour lattice QCD at finite isospin density, *Nucl. Phys. B* (Proc. Suppl.) 140, 526 (2005).

## CFD Modeling and Computational Science Studies Model Simulation, Comparison, and Testing in Urban Boundary Layer Applications (MANHATTAN)

PI: Michael Lazaro, Environmental Science

In collaboration with EPA scientists, we are exploring the possibility of developing or adapting the products from computational fluid dynamics simulations to support rapid exposure and risk models to guide urban emergency response and emergency management for chemical, biological, or radiological attacks and accidents. We are also exploring use of advanced, multidimensional, platform-portable stereo visualization technologies and visualization software to render stereo animations of complex urban-canyon fluid dynamic computations. Such visualizations promise to greatly enhance understanding of surface roughness layer-generated turbulence and the 3-D tracer flow fields through street canyons and around tall buildings (Figure 16). This work is expected to provide opportunities for collaboration with the Department of Homeland Security's New York City Urban Dispersion Program.

This program will be able to use our CFD applications in ongoing air monitoring strategy and intensive field measurement studies. The CFD applications will also support development of simple, reliable models to improve and provide practical tools for emergency first responders. Development and completion of CFD simulations supporting the DHS New York City Urban Dispersion project would not have been possible without use of Jazz. The developments during FY05 were a major step toward developing operation use of CFD. During FY06, we will focus on increasing the efficiency of simulations as well as running a large number of application scenarios. This work is already providing

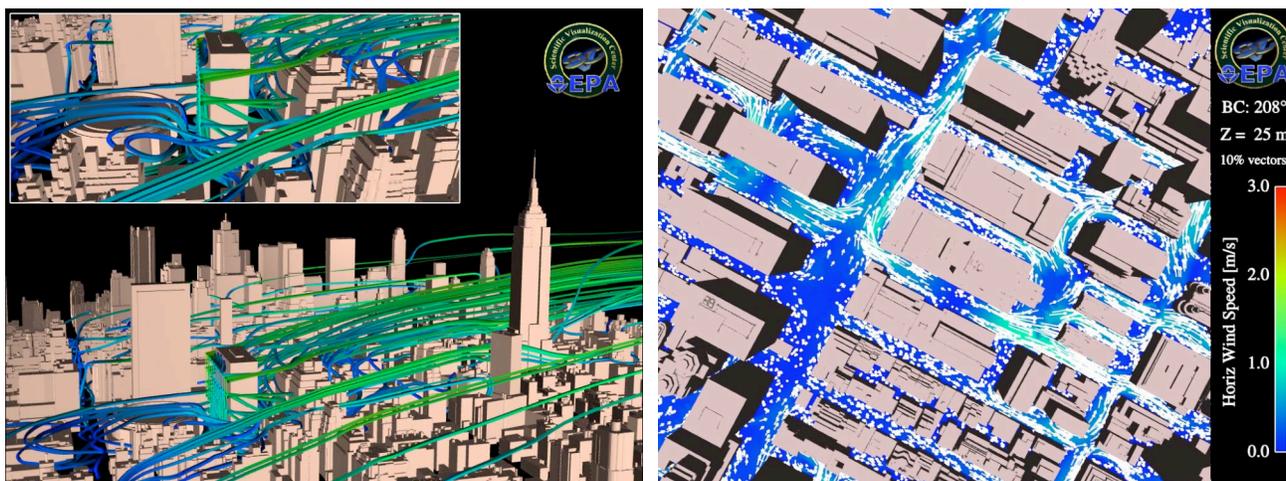


Figure 16: Visualization of flow fields through street canyons and around tall buildings.

opportunities for application of advanced visualization of boundary layer physics using Argonne's recently installed GeoWall.

### Publications/Presentations

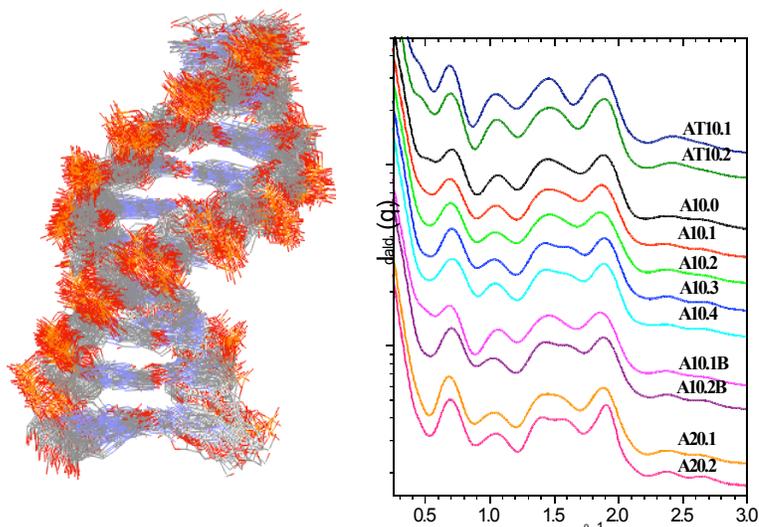
1. Presentations at working group meetings for the DHS UDP program.
2. Presentation at the Eighth Annual GMU Transport and Dispersion Modeling Conference, George Mason University, July 13-15, 2004.

## Validation of Molecular Dynamics Simulations for DNA by Solution X-ray Diffraction (MD\_FOR\_SXD)

PI: David Tiede and Xiobing Zuo, Chemistry

In situ characterizations of DNA conformation and dynamics in solution are critical for achieving a fundamental understanding of DNA function at the molecular level and for achieving the predictive design of DNA-based materials with applications ranging from nanoscience to next-generation pharmaceuticals. Molecular dynamics (MD) simulations are widely used as the primary tool for characterizing the conformational landscapes of biological macromolecules in solution and for predicting DNA conformation, DNA conformational transitions, and DNA-drug interactions.

Further, MD simulations and the associated force fields underlie structural determination using solution nuclear magnetic resonance (NMR) techniques. Up to now, however, there has been no direct, independent method for testing the accuracy of supramolecular structure and dynamics simulations in solution and other condensed-phase noncrystalline media or for testing the appropriateness of the underlying force fields, initial conditions, and simulation parameters. In this program we are developing methods for quantitatively testing the accuracy of MD simulations to represent conformational landscapes of DNA in solution. Fourier transforms are used to produce reciprocal space "fingerprints" of atomic pair distance correlations from MD simulation and to make direct, quantitative comparison with experimental solution X-ray diffraction (SXD) measurements. This program will enable more realistic, experimentally verified molecular force fields to be developed that take into account weak, sequence-specific, long-range molecular forces. Improvements in the accuracies of supramolecular force fields cannot be achieved by traditional crystallographic approaches alone. This program will be significant for making MD simulation accurate for a range of real-world, in situ applications.



**Figure 17: MD simulation results: 100 out of 2000 conformers simulation for a 10 base pair DNA sequence, and reciprocal space "fingerprints" for series of MD simulations that can be quantitatively compared to solution X-ray diffraction experiments.**

In FY2005 we carried out over 20 MD simulations using AMBER 8 running on Jazz for a series of DNA sequences that SXD and NMR experiments have shown exist in different conformations in solution. The simulations tested the effects of DNA nucleotide base sequence, length (containing up to 20 base pairs), and range of simulation parameters on the resulting MD ensemble. The MD simulations included explicit solvent and counter ions and involved over 20,000 atoms. In contrast to experiment, MD simulations were found to be consistently skewed toward a single DNA conformer (so-called B-form conformer with 10.0 base pairs per helix turn), although other conformers were found to be present to various extents as minority species within MD ensembles. Reciprocal space fingerprints proved useful for efficiently comparing simulation to experiment and for searching conformational ensembles to identify conformational subsets that provide a closer match to experiment than the ensemble average. Future work will extend these approaches for evaluating MD simulations for other biopolymers, and for developing reciprocal space fingerprinting as a means for developing optimized supramolecular force fields.

## Multimethod Linear Solvers in Terascale PDE-based Simulations (MULTIMETHOD\_SOLVERS)

PIs: Boyana Norris and Lois Curfman McInnes, Mathematics and Computer Science

Many large-scale scientific simulations involve the parallel solution of time-dependent or nonlinear partial differential equations. Overall simulation time is often dominated by the parallel solution of large-scale, sparse linear systems. Typically, application developers select a particular algorithm to solve a given linear system and keep this algorithm fixed throughout the simulation. However, it is difficult to select a priori the most effective algorithm for a given application.

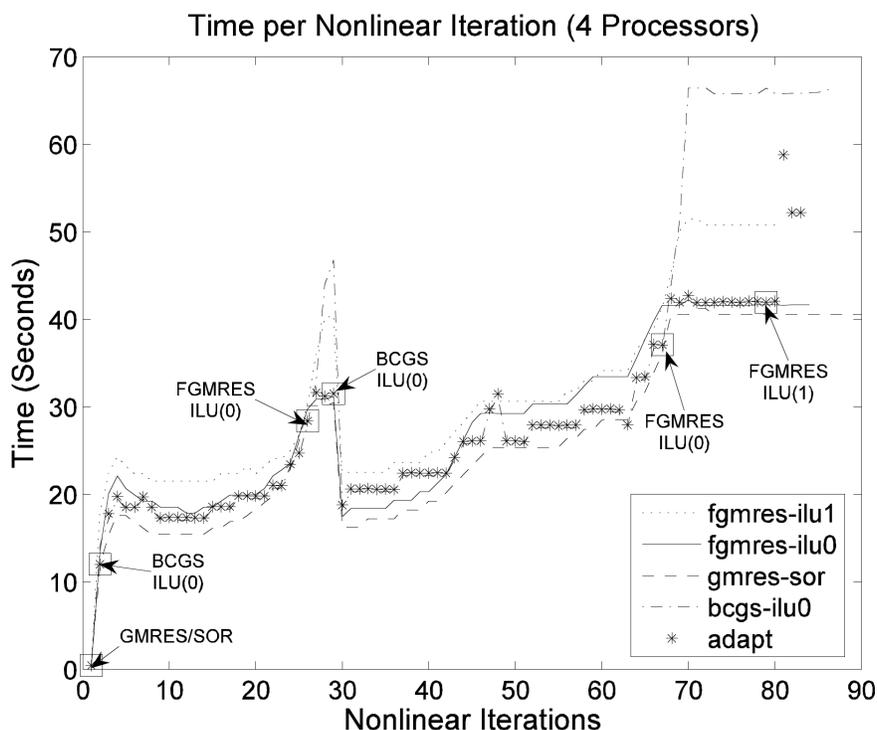


Figure 18: Execution time on Jazz vs. number of nonlinear iterations.

Thus, we are exploring polyalgorithmic multimethod linear solvers in the context of several parallel applications in computational fluid dynamics, including flow in a driven cavity and compressible Euler flow, to potentially improve the execution time and reliability of linear system solution. We are developing composite solvers that 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.

Our work on Jazz during FY2005 focused on developing an adaptive, polyalgorithmic approach for parallel linear solvers in the context of a 3-D transonic Euler flow using PETSc-FUN3D, an unstructured mesh code for solving the compressible and incompressible Navier-Stokes equations, which won a Gordon Bell prize at Supercomputing 1999. This application employs pseudo-transient Newton-Krylov methods for a fully implicit solution. We used Jazz to help develop a technique for adaptively selecting the parallel linear solver methods to match the numeric properties of the linearized Newton systems as they evolve during the course of the nonlinear iterations. Our approach combines more robust, but more costly, methods when needed in particularly challenging phases of the solution, with faster, though less powerful, methods in other phases.

### **Publications/Presentations**

1. S. Bhowmick, D. Kaushik, L. McInnes, B. Norris, and P. Raghavan, Parallel adaptive solvers in compressible PETSc-FUN3D simulations, Argonne National Laboratory preprint ANL/MCS-P1279-0805.
2. B. Norris, L. McInnes, and I. Veljkovic, Computational quality of service in parallel CFD, Argonne National Laboratory preprint ANL/MCS-P1283-0805.
3. L. McInnes, High-performance numerical components and common interfaces, presentation at Joint ORNL/Indiana University Workshop on Computational Frameworks for Fusion, Oak Ridge, TN, Jun 2005.
4. L. McInnes and P. Raghavan, organizers, Minisymposium and presentation on Large-Scale Nonlinear PDE-Based Applications, SIAM Computational Science and Engineering Conference, Feb. 2005.
5. B. Norris, organizer, Minisymposium and presentation on Performance Evaluation Challenges and Adaptive Numerical Approaches in Scientific Software, SIAM Computational Science and Engineering Conference, Feb. 2005.
6. P. Raghavan, M. J. Irwin, L. C. McInnes, and B. Norris, Adaptive software for scientific computing: Co-managing quality-performance-power tradeoffs, in *Proceedings of the IEEE International Parallel & Distributed Processing Symposium 2005* (CDROM), IEEE Computer Society Press, 2005 (also a presentation at the conference).

## **Computational Nanocatalysis (COMPANO)**

PIs: Peter Zapol, Chemistry, Materials Science, Center for Nanoscale Materials

Computational nanocatalysis projects involving density functional theory, molecular orbital theory, and tight-binding methods were performed at the LCRC facility this year. Theoretical studies of reactivity in these types of nanoporous materials are an important complement to experiment because they can provide information on adsorption energies and activation barriers for insight into the catalytic reaction mechanisms such as for selective catalytic oxidation of hydrocarbons. The following paragraphs summarize our achievements in simulations of nanoporous catalysts.

## Molecular Dynamics Simulations of Amorphous Alumina Nanopores (S. Adiga, P. Zapol)

Nanostructured membranes, based on a combination of anodic aluminum oxide and atomic layer deposition of a metal oxide, act as supports for ultra-uniform catalysts. Studies of the dependence of structure and properties of anodic aluminum oxide (AAO) pore surfaces as a function of the pore diameter and surface composition have been continued. The DL\_POLY computer code for molecular dynamics studies using many-body potentials was used to carry out AAO surface structure studies on Jazz with 32 to 48 PEs for about 50,000 atom calculations. The optimized structure of bulk amorphous alumina with the density of  $3.125 \text{ g/cm}^3$  was used to create the surfaces. Radial distribution functions and other structural properties of AAO are shown in Figure 19. The subsurface Al enrichment was predicted and is currently being searched for by experimental techniques. The simulations are being performed for amorphous alumina surfaces of nanostructures from 1 nm to 10 nm with positive and negative curvature.

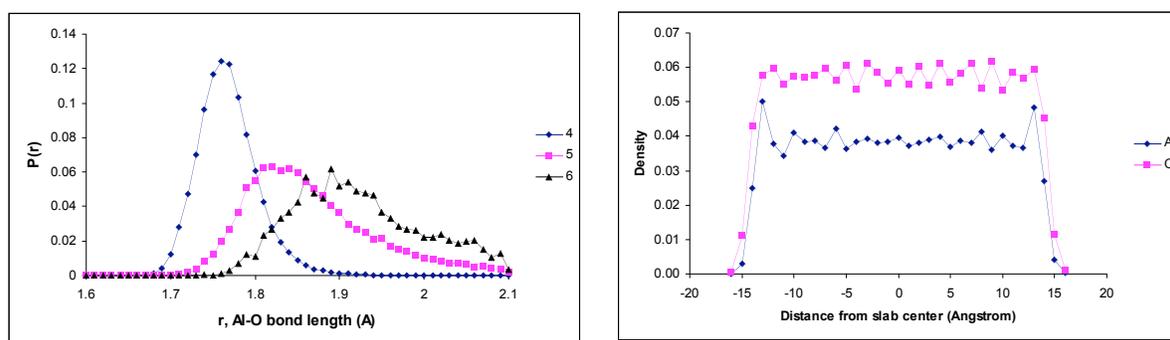


Figure 19: (a) Radial distribution functions for 4, 5, and 6 coordinated aluminum atoms, and (b) concentration profiles as a function of distance from the surface.

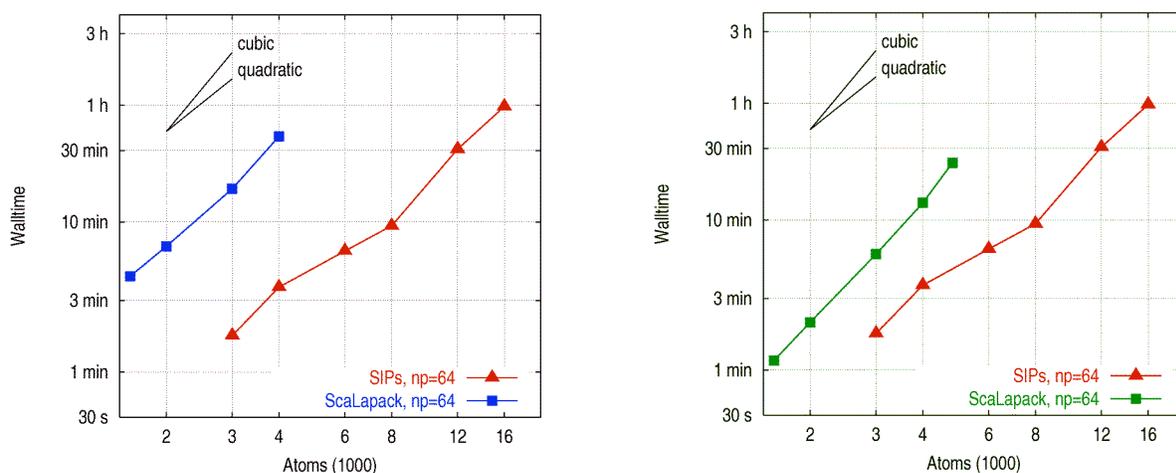
## Catalytic Sites and Reaction Mechanisms (S. Adiga, P. Redfern, M. Sternberg, P. Zapol, L. Curtiss)

The Mars-van Krevelen mechanism of oxidative dehydrogenation of propane on the (010) surface of  $\text{V}_2\text{O}_5$  was studied by using a hybrid density functional study of mechanisms for oxidative dehydrogenation of propane. The potential energy surface was found to involve a singlet/triplet state curve crossing with very high barriers. The highest energy on the potential energy surface at the B3LYP/6-31G(\*) level of theory corresponds to formation of an oxygen vacancy after water elimination and is about 80 kcal/mol above the energy of the reactants. Subsequent addition of an oxygen molecule to fill the vacancy is predicted to be energetically downhill. The reactions of propane at a bridging oxygen site and at a vanadyl site have similar energies, and water elimination occurs at a bridging site. The periodic calculations are used to validate key energies obtained by using the cluster models. Further studies of vacancies with periodic methods are under way.

## DFTB Method Development (M. Sternberg, Kedziora, P. Zapol, L. Curtiss)

We worked on development of an efficient and massively parallel eigensolver for the Density Functional Based Tight Binding code for the determination of electronic energies and other quantities of relevance to nanoparticle and nanoparticle/molecule interactions such as those described above. The new package, called SIPs, implements a shift-inverted eigensolver and is built on top of SLEPc and the PETSc toolkit developed by researchers in Argonne's Mathematics and Computer Science Division. It is designed to handle large sparse matrices, when about 60% of eigenvectors are required.

The performance of the SIPs package was tested on a number of cases with varying sparsity (7% to 50%) depending on the dimensionality and structure of physical problem. For a 7% sparse problem, the new package outperforms ScaLAPACK in both absolute time and scaling, requires much less memory and scales very well with the number of processors. We studied several model systems, with the largest system containing 16,000 atoms. For the densest system, the new package performs as well as the conventional diagonalization package (ScaLAPACK) using slow interconnect (Ethernet, Figure 20, left) but is somewhat slower using fast interconnect (Figure 20, right). However, it scales better with the system size and number of processors and will perform very well in all cases when it is deployed on a massively parallel platform and for larger problems that are inherently sparser. Currently, calculations on physically relevant applications are under way to obtain new information on chemical and physical properties of nanotubes and nanowires interacting with molecules.



**Figure 20: Performance of SIPs as compared to ScaLAPACK using Ethernet (left) and Myrinet (right) for a test case of a carbon nanotube. The matrix size of 64,000 corresponds to 16,000 atoms. Note that the performance of SIPs does not depend on communication speed.**

## Computational Nanophotonics (NANOPHOTONICS)

PI: Stephen Gray, Chemistry

Nanophotonics is a rapidly growing area of nanoscience that involves light or photons interacting with nanoscale objects. The electrons near the surfaces of nanostructured metallic systems, in particular, can resonantly interact with light in the form of surface plasmons. Surface plasmons can be highly localized and intense and are of potential use for diverse practical applications, ranging from chemical and biological sensors to optoelectronic devices. Computational modeling is essential both for interpreting experiments and for suggesting new directions. This project is devoted to the development and application of finite-difference time-domain (FDTD) and related methods for the numerical solution of the relevant Maxwell's equations to generate the electric and magnetic fields due to light interacting with metallic nanostructures. Surface plasmon excitations can involve strong field variations over 1–10 nm scales near the surfaces of much larger, 100–1000 nm scale metallic structures. Such problems require the use of large, dense numerical grids and can consume significant amounts of computer time and memory. Parallel computing approaches are needed, with the simulation of many realistic problems being possible only in a parallel environment.

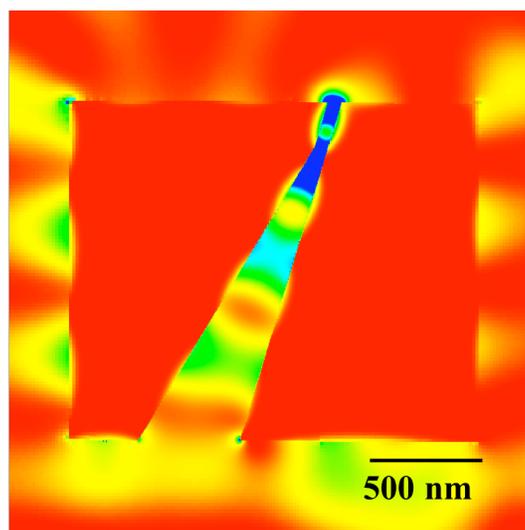
The Jazz cluster has been used intensively during this project. In particular, we carried out several realistic simulations of light interacting with nanoscale holes and slits in metals, and nanowires. New results on the transmission of light through isolated and arrays of nanoholes, as well as the associated near-field patterns, have been obtained. Our nanoscale-hole results have allowed us to explain the origins of the extraordinary transmission of light observed in many experimental studies on such systems. We have predicted novel ways to confine and waveguide light in such structures, and we anticipate that some of our predictions will be verified experimentally.

In the past year we developed and applied a straightforward, parallel implementation of the standard FDTD method in three dimensions. We also developed special reconstruction techniques for improving the accuracy of the numerical solutions of certain types of time-domain simulations.

Further, we developed a parallel adaptive mesh refinement (AMR) finite difference time domain (FDTD) application, called *Shapes*. The present version of the code can be used to study arbitrary nanoparticle shapes and configurations in two-dimensional systems. Numerous tests of *Shapes* have been run; Figure 21 shows an example of nanoscale waveguiding by a tapered slit to yield a plasmonic excitation in the narrow portion of the slit. We are actively developing a more general, 3-D version of *Shapes*.

#### Publications/Presentations

1. S.-H. Chang, S. K. Gray and G. C. Schatz, Surface plasmon generation and light transmission by isolated nanoholes and arrays of nanoholes in thin metal films, *Optics. Express* **13**, 3151–3165 (2005).
2. M. S. Min, T.-W. Lee, P. F. Fischer, and S. K. Gray, Fourier spectral simulations and Gegenbauer reconstructions for electromagnetic waves in the presence of a metal nanoparticle. *J. Comp. Physics*, 2005 (in press).
3. E.-S. Kwak, J. Henzie, S.-H. Chang, S. K. Gray, G. C. Schatz, and T. W. Odom, Surface plasmon waves in large-area subwavelength hole arrays. *Nano Letters* **5**, 1963–1967 (2005).
4. Nanoscale confined light: From metal nanoparticles to nanoholes Invited lecture to the Chemistry Department, University of Barcelona, Barcelona, Spain, March 3, 2005.
5. Nanoscale confined light: From metal nanoparticles to nanoholes. Invited talk at the Spring National Meeting of the American Chemical Society, San Diego, March 13, 2005.
6. Electrodynamics simulations of surface plasmon behavior in metallic nanostructures. Invited talk at Optics and Photonics (a SPIE Meeting), San Diego, July 31, 2005.



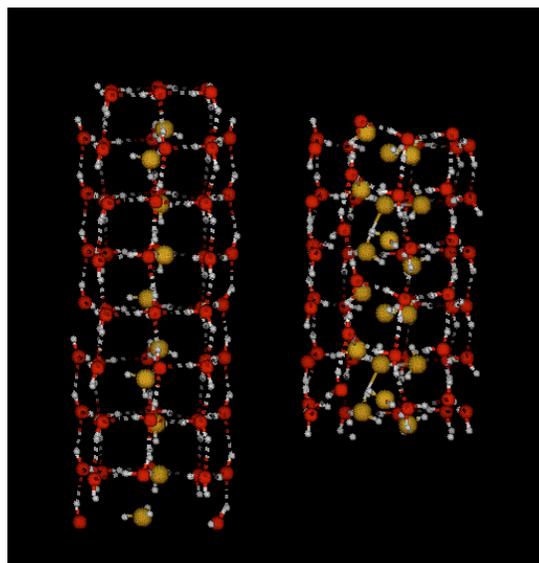
**Figure 21:** Snapshot of the electric field as light is exposed to a slanted, tapered nanoscale slit structure in a block of silver. Low to high intensities range from red to blue. This result was obtained with the AMR-FDTS code *Shapes*, developed in this project.

## Structural and Dynamical Properties of Water Confined in Nanotubes (NANOTUBES-WATER)

PIs: Alexander I. Kolesnikov, Intense Pulsed Neutron Source Division; Christian J. Burnham, Department of Physics, University of Houston

Researchers have expressed increased interest in the formation of crystalline water in carbon nanotubes at low temperatures. In a recent study, we showed that this “nanoice” has remarkably different properties compared to the bulk behavior. Most notably, neutron scattering has revealed that in a 14 Å diameter nanotube, the proton motions involve anomalously large mean squared displacements, several times larger than observed in bulk ice at the same temperature.

In the original study, we were able to show through molecular dynamics (MD) simulation that a convincing atomic model for the nanotube water consisted of (i) an outer cylindrical “shell” of water molecules at around 3 Å inside the nanotube, in which the waters are H-bonded together in a square lattice wrapped into a cylinder, and (ii) an inner “chain” arrangement of waters running down the central axis of the nanotube, in which the waters are H-bonded to form a quasi one-dimensional linear chain (Figure 22). It was found that these chain waters are responsible for the observed large mean square displacements that are a result of their low coordination and weak bonding to the outer shell. This result is of considerable interest as the motion of the quasi-one-dimensional chain can be seen as an analogue to the movement of water through aquaporin channels across membranes, which also involve single-file transport of waters through not dissimilar radii.



**Figure 22: Structure of water in single-wall carbon nanotubes at ambient pressure (left) and at 0.37 GPa (right).**

For the past six months we have been using Jazz to perform more comprehensive simulations of water behavior confined in nanotubes. We have employed parallelizable algorithms, most notably a parallel tempering molecular dynamics hybrid algorithm. This algorithm is suited to finding the equilibrium structural properties as a continuous function of temperature over a temperature range. Instead of performing one long trajectory, the algorithm spawns multiple trajectories running in parallel on different processors, where each trajectory has a unique temperature, in our case a value between 100 and 350 K. The algorithm then allows occasional crossover of structures between two different temperatures so that an individual trajectory can heat up or cool down over the course of the simulation.

Not only does this allow us to span the desired temperature range, but it also overcomes undesirable trapping in local minima (the ergodicity problem), so helping the structures to reach equilibrium faster. The equilibrium results are collected from all temperatures, and using statistical methods for entropy estimation, we can transform the data into a continuous function of temperature.

We have employed the above methods to study equilibrium behavior of nanotube confined water across a range of temperatures and different-sized nanotubes. We have been able to locate the temperatures at which phase transitions occur in which the nano-ice melts into a diffusive, waterlike structure. We have

also discovered that the presence of chain molecules is astonishingly sensitive to the radius of the carbon nanotube: below 14 Å the chain waters entirely disappear from the equilibrium distribution. Also, we have recently implemented the ability to apply an external pressure into the algorithm, which has allowed us to observe the behavior of water in nanotubes under pressure. We have observed a phase change with increasing pressure to a new crystalline structure at 0.37 GPa in which the central chain of waters has been replaced with a denser higher coordinated inner cylinder of waters (see Figure 22). Dynamical calculations using this structure have shown promising agreement with neutron scattering measurements.

### **Publications/Presentations**

1. Kolesnikov, M. Zanotti, C. K. Loong, P. Thiyagarajan, A. P. Moravsky, R. O. Loutfy, and J. Burnham, Anomalously soft dynamics of water in a nanotube: A revelation of nanoscale confinement, *Phys. Rev. Lett.*, 93 (2004) 035503

## **Neocortical Seizure Simulation (NEOCORTEX\_SIM)**

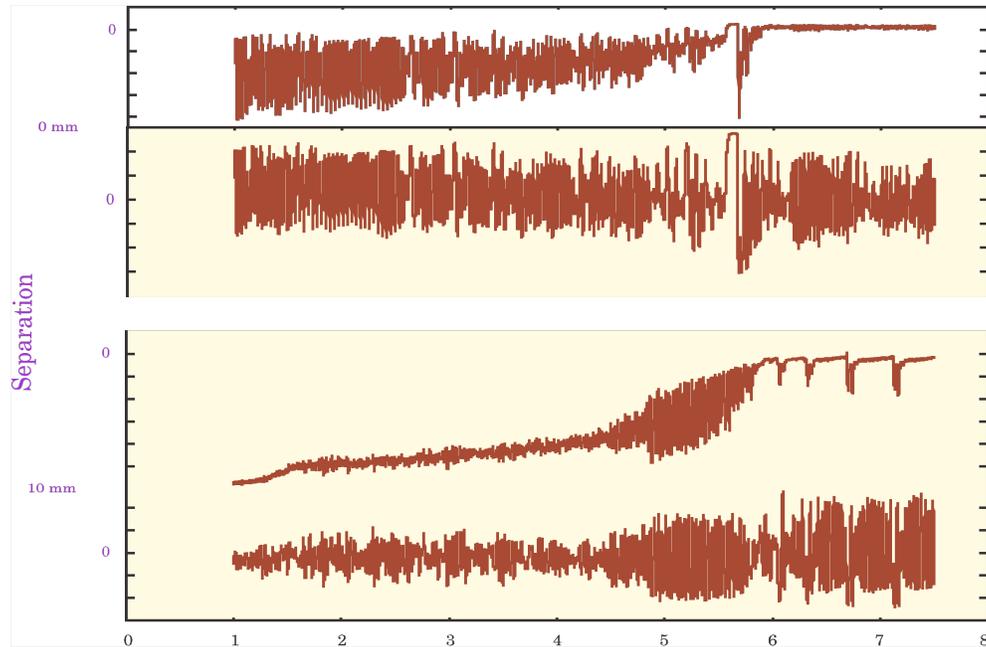
PIs: Mark Hereld, Rick Stevens, Mathematics and Computer Science; Wim van Drongelen, Hyong E. Lee, University of Chicago

Pathologic activity in the neocortex frequently plays an important role in pediatric epilepsy. At the level of the microcircuitry of the cortex, one might hypothesize that epileptiform discharges are caused by malfunction of the neurons themselves (intrinsic properties), pathology in the neural networks (synaptic), or both. During the past year we studied the small neuronal network embedded in a set of larger populations; this enabled us to describe the propagation of seizure-like activity from a focal point towards the neighboring network (see Figure 23). Our results were presented at an IEEE meeting last May in Minneapolis. We also performed a large set of parameter searches related to the bursting behavior in neurons including a persistent sodium current. This study has duplicated the role of this current in a network (as recorded in neocortical tissue). A combination paper describing the simulation and experimental results is in progress. We are exploring parameter search techniques (simulated annealing, genetic algorithms) in addition to our current brute-force approach.

Our recent efforts are motivated by several key questions. Can epileptic activity in the neocortex be caused by changes from the norm in excitatory and/or inhibitory connection strengths in the neural network? What are some specific conditions (“parameters” in our model) that can cause epileptic seizures? How localized are the generators of epileptiform activity? Answers to these questions can lead to refined or new techniques to curtail seizures in children.

### **Publications/Presentations**

1. Wim van Drongelen, Hyong C. Lee, Mark Hereld, Zheyang Chen, Frank P. Elsen, and Rick L. Stevens, Emergent epileptiform activity in neural networks with weak excitatory synapses, *IEEE Trans. on Neural Systems and Rehabilitation Engrg*, 13:2, pp. 236–241, June 2005.
2. Hyong Lee, Mark Hereld, Rick Stevens, and Wim van Drongelen, Epileptiform activity patterns in coupled neuronal networks, invited paper at Joint Meeting of 5th International Conference on Bioelectromagnetism and 5th International Symposium on Noninvasive Functional Source Imaging within the Human Brain and Heart (BEM and NFSI), Minneapolis, May 2005.



**Figure 23: Overview of compound electrical activity in two interconnected neuronal populations. The data suggest that nearby strongly connected patches protect against epileptiform patterns, whereas remote and more loosely connected areas create a larger risk for emergent seizure-like activity [2].**

3. Mark Hereld, Rick Stevens, Justin Teller, Wim van Drongelen, and Hyong Lee, Large neural simulations on large parallel computers, invited paper at Joint Meeting of 5th International Conference on Bioelectromagnetism and 5th International Symposium on Noninvasive Functional Source Imaging within the Human Brain and Heart (BEM and NFSI), Minneapolis, May 2005.

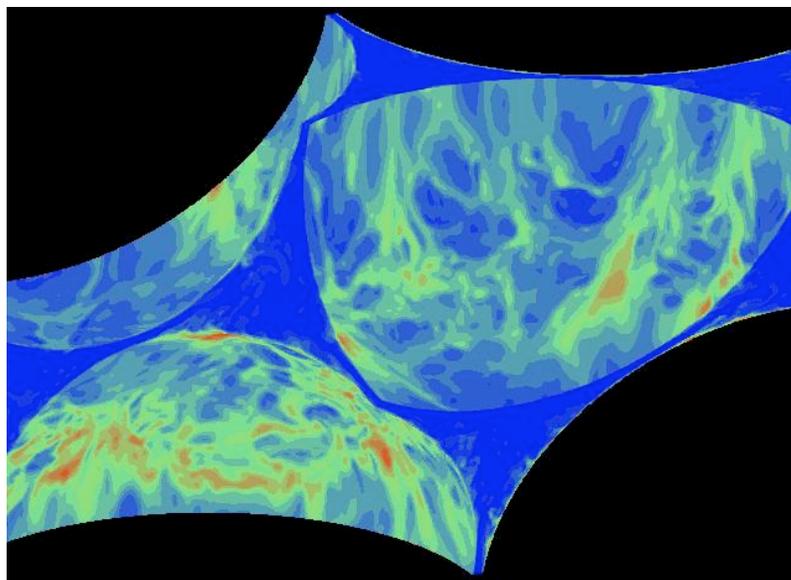
## **Heat Transfer in Pebble Bed Reactors for Next-Generation Nuclear Power (NGNPCFD)**

PIs: Paul Fischer and Gary Leaf, Mathematics and Computer Science

We are investigating a multiscale approach to heat transfer analysis of pebble bed reactors (PBRs) that are being considered for next-generation nuclear power plants in the United States. The PBR design calls for a vertical cylindrical silo containing several hundred thousand spherical fuel pebbles with a diameter of 60 mm. The pebbles are continually moving downward through the silo as pebbles are removed from the bottom at the rate of two per minute, inspected, and recycled to the top or rejected according to the level of fuel within each. High-pressure helium pumped downward through the silo acts as the reactor working fluid by removing the heat from the fuel pebbles.

Our work addresses questions relating to the efficiency of the heat transfer, the required pumping power, and the maximum temperature of the fuel pebbles under standard operating conditions and under scenarios in which external pumping is turned off (Figure 24).

Our multiscale approach is based on a hierarchy of simulations ranging from direct numerical simulation (DNS) of a unit periodic cell in the reactor bed; large eddy simulation of “meso-cells,” which are perturbed aggregates of the unit-periodic cell involving up to ~10 pebbles; and integrated analyses of the entire bed. The simulation domain for convective heat transfer in the PBR comprises the void region surrounding the pebbles and interior to the reactor silo. The heat transfer problem amounts to being able to reliably predict the maximum temperature within PBR to ensure that it stays safely below the critical value of 1600 °C. The high velocities make the flow turbulent with significant fine-scale structure. The random structure of the pebble packing induces a mesoscale that is larger than the turbulence but much smaller than the overall reactor, which constitutes the largest scale in the problem.



**Figure 24: Turbulent heat transfer in an fcc packed-array of spheres subject to unit-flux boundary conditions.**

We are using Jazz for simulations at the finest scale by computing the flow and associated heat transfer through the passageways formed by a periodic array of spheres placed in a close-packed lattice arrangement using DNS of the Navier-Stokes and energy transport equations. Although DNS is too expensive for the simulation of a large domain, preliminary results have shown that it is possible to achieve close to reactor-scale Reynolds numbers for a single unit cell in the periodic lattice. The DNS results will provide important information about maximum pressure drop through the PBR, local temperature fluctuations, and mean temperature variations in a fundamental configuration. These quantities, computed from first principles, will provide important input to macroscopic models based, for example, on Darcy’s law or other similar homogenization approximations. The DNS results will also provide a database for validation of large-eddy simulations. Our computations use the Argonne code Nek5000, which has been developed specifically for the investigation of high-Reynolds number flows in complex geometries.

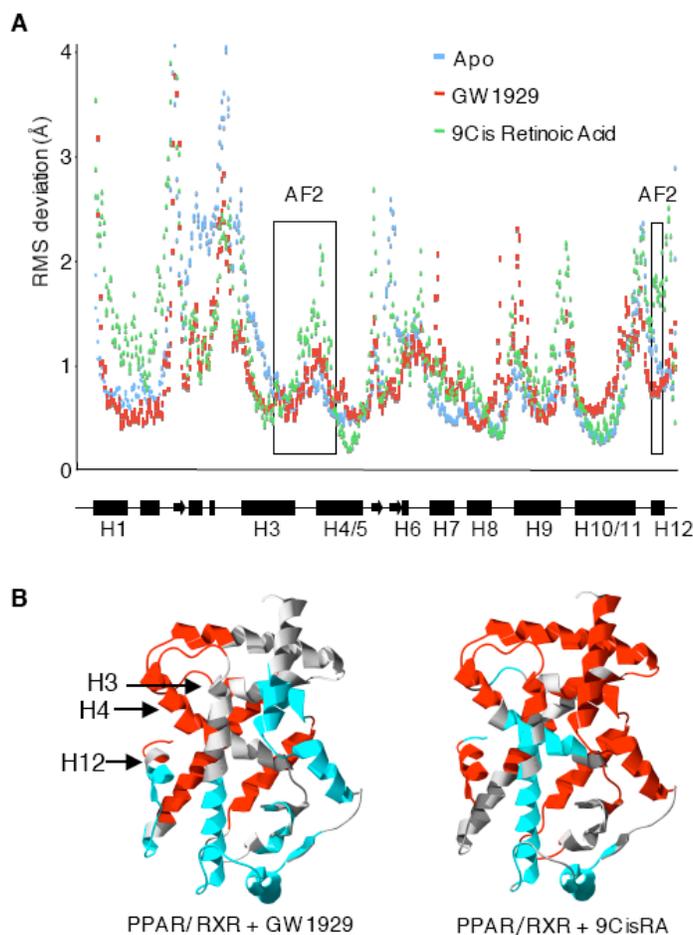
## **Nuclear Receptors (NUCLEARRECEPTORS)**

PIs: Mark Cunningham and Kendall Nettles, Biosciences

The nuclear receptor superfamily of transcription factors is part of the signal transduction machinery used by cells to regulate the transcription of DNA into messenger RNA. The various nuclear receptors respond to different chemical signals including steroid hormones, bile acids, fatty acids, and oxysterols. Nuclear receptors represent primary targets for cardiovascular, metabolic, and endocrine disorders, as well as cancer and the steroid anti-inflammatory drugs. Currently, these therapeutic targets represent 10–20% of the \$400 billion spent worldwide on prescription drugs.

Our work on Jazz has focused on conducting molecular dynamics simulations of different heterodimers, to elucidate the mechanisms that give rise to the observed experimental behavior. We have performed simulations on PPAR/RXR and LXR/RXR heterodimers, with and without ligands and for several different mutations that have been identified experimentally as being important for biological function.

These simulations have proven valuable in illuminating the subtle connections between the dynamical motion of protein atoms and their effect on signaling. For example, an earlier prediction based on x-ray crystal structures suggested that in the PPAR/RXR heterodimer the binding of RXR induced folding of the AF2 coactivator-binding surface in PPAR, either through helix 11 or through the hydrophobic core. This hypothesis was strongly refuted by the molecular dynamics simulations, which demonstrate that RXR induced an *increase* in dynamics of the AF2 surface (see Figure 25). Instead, communication occurred through modulation of coupled motion across the dimer interface. Encouragingly, these results are consistent with recent amide deuterium-exchange experiments, suggesting that the picture of signal transduction developed through our calculations accurately represents the actual behavior of a complex biochemical system.



**Figure 25: Molecular dynamics of the PPAR ligand-binding domain. (A) The RMS deviation of the position of backbone Ca atoms is displayed for three different simulations, with the PPAR/RXR heterodimer bound to different ligands, including a PPAR agonist (GW1929) and an RXR agonist (9-cis retinoic acid). (B) The differences in RMS deviation from the apo receptor are mapped onto the PPAR ligand-binding domain.**

## Optimization of Many-Body Wavefunctions (NUCLEARSTRUCTURE)

PI: R. R. Chasman, Physics

We are exploring the issue of many-body correlations and collective behavior in nuclei. Collective behavior or the coherent behavior of many particles can be addressed at many levels. The simplest is the mean-field level, which is a modification of a one-body potential to incorporate many of the many-body interaction effects. At a more sophisticated level, one constructs many-body wave functions to address the subtler features of many-body correlations. In our project, we deal with many-body effects on both levels to develop an understanding of nuclear structure. Most recently, we have developed many-body wave functions to explore neutron-proton pairing effects in nuclei having almost equal numbers of protons and neutrons. Many nuclei of this type will be studied with the advent of the RIA facility. We have also carried out studies of the heaviest known nuclei at the mean-field level.

We have developed and tested on Jazz a new technique for obtaining accurate energies and wave functions for nuclei in which neutron-proton pairing is important (Figure 26). This approach is accurate for systems in which the correlations are both weak and strong. We have also completed calculations for low-lying states in  $^{249}\text{Bk}$ , one of the heaviest nuclides for which there is good experimental information on proton single particle states. Also, our computations on neutron-proton pairing have provided an explanation of the Wigner energy anomaly.

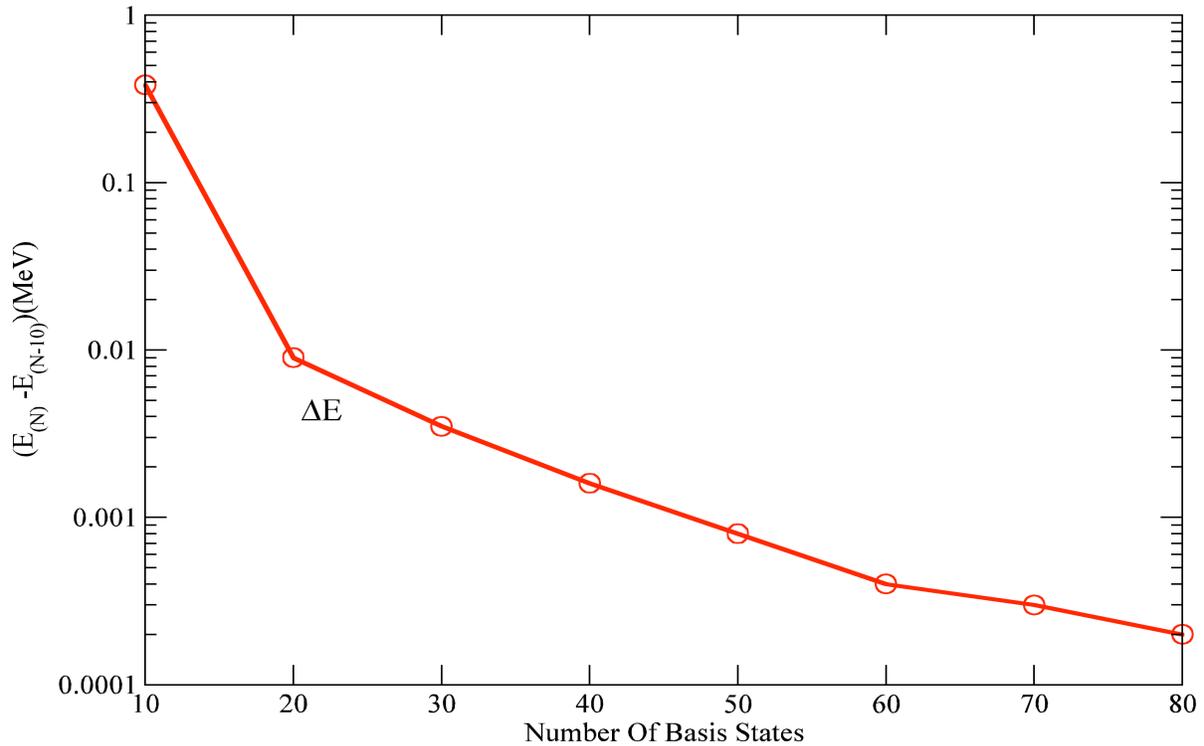


Figure 26: Change in total energy as a function of the number of configurations used in the calculation.

### Publications/Presentations

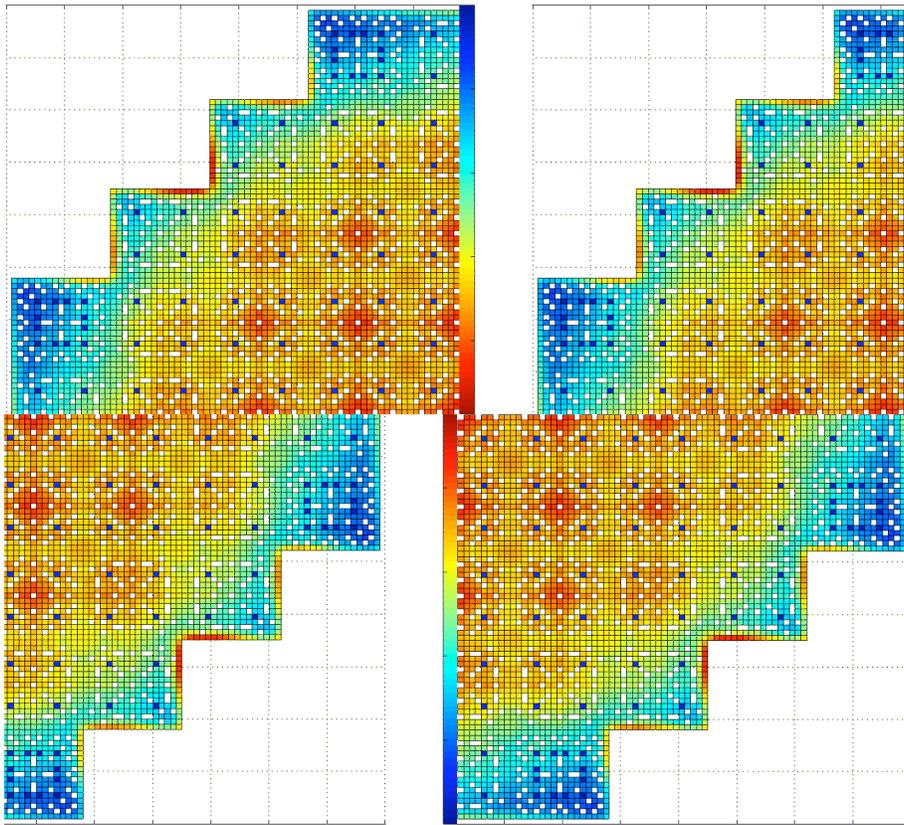
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2. R. R. Chasman, Neutron proton pairing in nuclei, Colloquium Lawrence Berkeley Laboratory, May 26, 2005.

# Integrated 3-D Simulation of Neutronic, Thermal-Hydraulic, and Thermo-Mechanical Phenomena (NUMERICALREACTOR)

PI: Tanju Sofu, Nuclear Engineering

The “Numerical Reactor” project seeks to develop next-generation computational tools to support the design of future nuclear energy systems through high-fidelity, first-principles-based simulations. The integrated analysis of a reactor core has never been implemented at the level of fidelity achieved in this project. The development of first-principles-based models, the availability of massively parallel computing resources, and our demonstration in solving significant-scale design and operational issues on Jazz have now set the stage for radically changing nuclear reactor core simulations (Figure 27).

Based on our interactions with the vendors, utilities, research organizations, and regulators, we believe we are on the threshold of a revolution in the design methodology for the light water reactor nuclear power industry. This is similar to the recent transitions that were accomplished in other areas such as automotive, aerospace, and pharmaceutical industries.



**Figure 27: Pin-by-pin core power distributions for a small pressurized water reactor using the integrated whole-core simulations with intrapin-level thermal feedback.**

## Publications/Presentations

1. T. Sofu, The Numerical Nuclear Reactor – a high-fidelity, integrated neutronic, thermal-hydraulic and thermo-mechanical code, in *Proceedings of Intl Conf. on Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Palais des Papes, Avignon, France, September 12–15, 2005, American Nuclear Society, 2005.

## Parallel Tools (PARALLEL-TOOLS)

PIs: Robert Latham and Robert Ross, Mathematics and Computer Science

The parallel tools project continues to develop and study highly scalable software tools and libraries for parallel applications. Our efforts include a parallel file system (PVFS2), an MPI-IO implementation (ROMIO), and higher-level libraries (Parallel-NetCDF, HDF5). We have made extensive use of Jazz to evaluate several novel approaches for implementing synchronization with MPI-2 one-sided operations. Experiments on Jazz helped us evaluate an implementation of MPI-IO atomic mode, MPI-IO shared file pointers, and byte-range file locking. Jazz’s node count and Myrinet interconnect provided a useful testbed for our experiments.

Also in FY 2005 we developed a “Logistical Networking” driver for ROMIO. We used Jazz to evaluate performance of our driver as we communicated with servers at the University of Tennessee, Knoxville. We also used Jazz to evaluate some early efforts at efficient lock servers, scalability of some bioinformatics-related algorithms, and techniques for better noncontiguous I/O performance.

Recently, we have used Jazz to perform nightly tests of PVFS2; these tests help us catch any regressions in either PVFS2 or ROMIO’s PVFS2 driver. Our results have helped us refine both our analysis and our implementation. In the case of the shared file pointer, byte-range file locking, and atomic-mode experiments, we now have great confidence that we can feasibly implement our algorithms and introduce new features into ROMIO with acceptable additional overhead.

Also, our work on Jazz helped us identify inefficiency in PVFS2 servers (Figure 28). In some write cases, this inefficiency was costing us about 10–15% performance. We have since changed the default PVFS2 behavior to eliminate this overhead.

## Publications/Presentations

1. Robert Latham, Robert Ross, Rajeev Thakur, and Brian Toonen, Implementing MPI-IO shared file pointers without file system support, in *Proceedings of the 12th European PVM/MPI Users’ Group Meeting (Euro PVM/MPI 2005)*, Recent Advances in Parallel Virtual Machine and Message Passing Interface, Lecture Notes in Computer Science, LNCS 3666, Springer, September 2005, pp. 84–93.
2. Rajeev Thakur, Robert Ross, and Robert Latham, Implementing byte-range locks using MPI one-sided communication, in *Proceedings of the 12th European PVM/MPI Users’ Group Meeting (Euro PVM/MPI 2005)*, Recent Advances in Parallel Virtual Machine and Message Passing Interface, Lecture Notes in Computer Science, LNCS 3666, Springer, September 2005, pp. 119–128.
3. Robert Ross, Robert Latham, William Gropp, Rajeev Thakur, and Brian Toonen, Implementing MPI-IO atomic mode without file system support, in *Proceedings of the 5th IEEE/ACM International Symposium on Cluster Computing and the Grid (CCGrid 2005)*, May 2005.

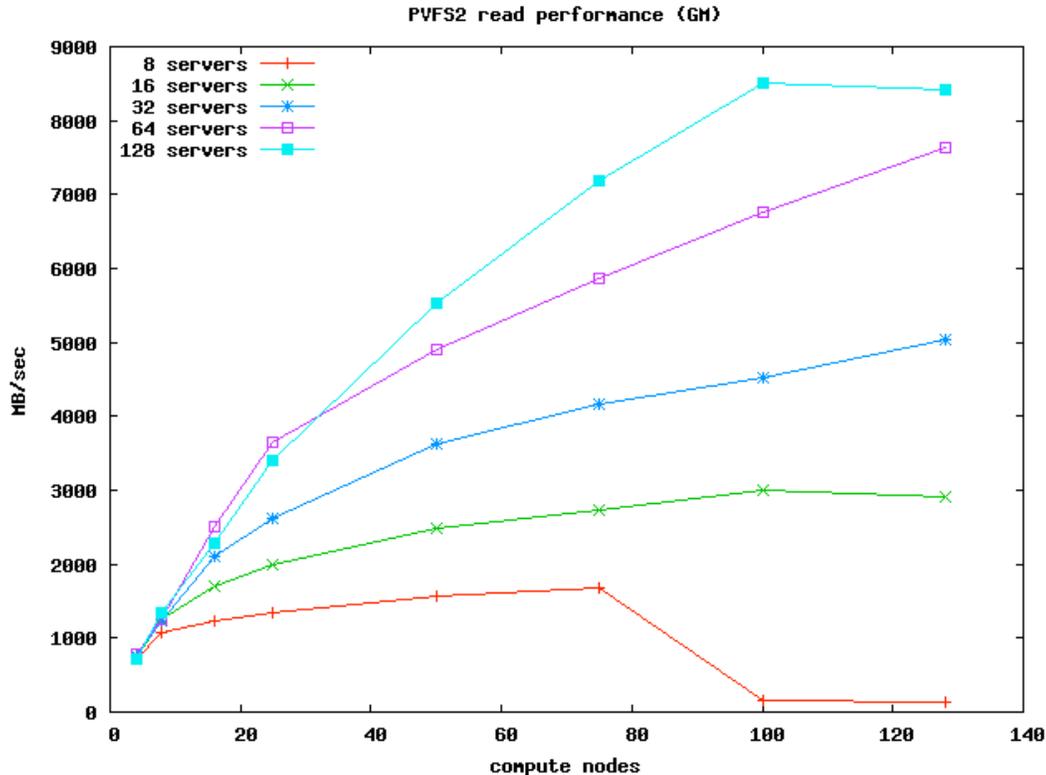


Figure 28: PVFS2 scalability testing, showing performance with variable numbers of clients and servers for a contiguous I/O benchmark. We reach nearly 9 GB/s of aggregate I/O bandwidth using Myrinet and low-end storage devices.

## Quantum Monte Carlo Calculations of Light Nuclei (QMC\_FOR\_NUCLEI)

PIs: Kenneth M. Nollett, Steven C. Pieper, and Robert B. Wiringa, Physics

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

During FY05 Jazz was used for many aspects of this project. The fast turnaround of Jazz makes it the machine of choice (along with Blue Gene) for all but our biggest calculations, which are done at NERSC or Los Alamos. The specific projects this year fell into five categories: (a) GFMC scattering, (b) multiple excited states with the same quantum numbers, (c) unnatural-parity states, (d) spectroscopic factors, and (e) RMS radii of weakly bound nuclei (see Figure 29).

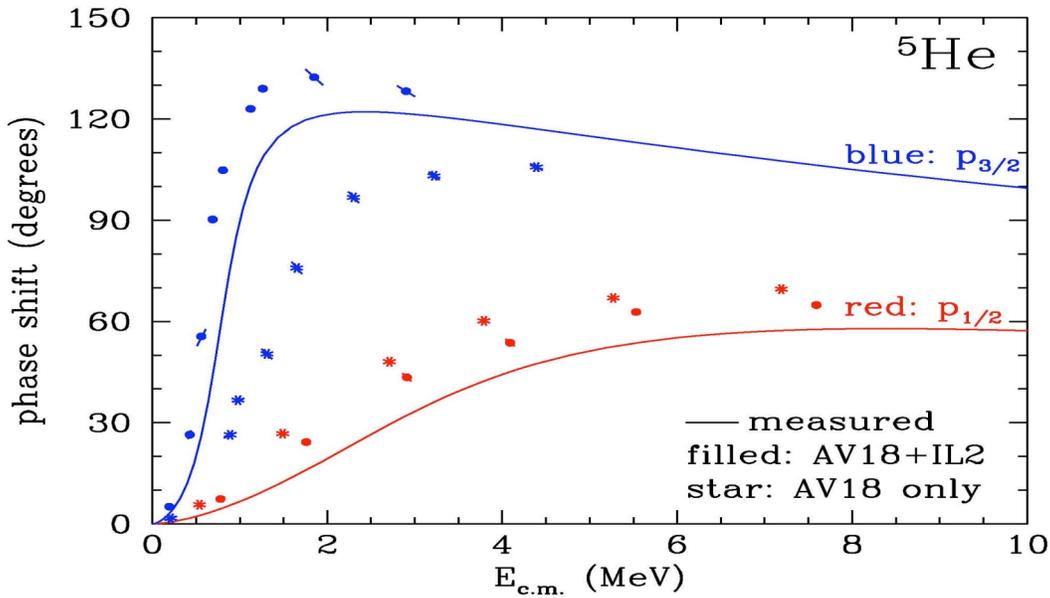


Figure 29: Phase shifts for  $4\text{He}$ -neutron scattering in the  $3/2^-$  (blue) and  $1/2^-$  (red) partial waves.

### Publications/Presentations

1. Steven C. Pieper, R. B. Wiringa, and J. Carlson, Quantum Monte Carlo calculations of excited states in  $A=6-8$  nuclei, *Phys. Rev. C* 70, 05425-1:11 (2004).
2. Steven C. Pieper, Quantum Monte Carlo calculations of light nuclei, in *Proceedings of the 22nd International Nuclear Physics Conference*, Goeteborg, Sweden, June 27 - July 2, 2004, *Nucl. Phys. A* 751, 516c-532c (2005).
3. A. H. Wuosmaa, K. E. Rehm, J. P. Greene, D. J. Henderson, R. V. F. Janssens, C. L. Jiang, L. Jisonna, E. F. Moore, R. C. Pardo, M. Paul, D. Peterson, Steven C. Pieper, G. Savard, J. P. Schiffer, R. E. Segel, S. Sinha, X. Tang, and R. B. Wiringa, Neutron spectroscopic factors in  $9\text{Li}$  from  $2\text{H}(8\text{Li},p)9\text{Li}$ , *Phys. Rev. Lett.* 94, 082502-1:4 (2005).
4. H. Wuosmaa, K. E. Rehm, J. P. Greene, D. J. Henderson, R. V. F. Janssens, C. L. Jiang, L. Jisonna, E. F. Moore, R. C. Pardo, M. Paul, D. Peterson, Steven C. Pieper, G. Savard, J. P. Schiffer, R. E. Segel, S. Sinha, X. Tang, and R. B. Wiringa, Search for excited states in  $7\text{He}$  with the  $2\text{H}(6\text{He},p)7\text{He}$  reaction, *Phys. Rev. C* 72, 061301(R)-1.5 (2005).

## Agent-Based Simulation of Bacterial Chemotaxis (REPAST\_CHEMOTAXIS)

PI: C. Macal, Decision and Information Sciences

Computational simulation of the dynamics of intracellular processes is becoming an important adjunct to laboratory experiments in biology. Signal transduction, the process by which a cell's sensor information is transformed into action lends itself to representation as a network of chemical reactions. A fundamental biological question is how specific cellular behaviors are the direct result of the biochemical processes that occur in the cell at the molecular level. Understanding these connections will provide insight into the basic mechanisms of cellular behavior, growth, adaptability, scalability, and diversity, as well as the factors responsible when these processes go awry. Recent laboratory findings

have provided much information on the details of these processes, in some cases, forming a complete picture of the underlying biochemical processes.

In recent years, single-cell biology has focused on the relationship between the stochastic nature of molecular interactions and variability of cellular behavior. In order to describe this relationship, it is necessary to develop new computational approaches at the single cell level. We have developed AGENTCELL, a multiscale agent-based simulation platform, to model the relationship between intracellular processes in individual cells and the behavior of a cellular population. Agent-based computational approaches have a natural modular architecture, which reflects the modular organization of biological systems. We have used the chemotaxis system of the *E. coli* bacterium to simulate individual molecular interactions within single swimming cells. Internal molecular fluctuations produce temporal variability in the behavior of individual cells. In this approach, each cell is an independent agent equipped with its own chemotaxis network, motors and flagella.

To investigate the relationship between population behavior and the particular phenotype of individual cells, we used AGENTCELL to simulate 2000 *E. coli* cells swimming in a 3-D environment. Simulation runs consisting of 2,000 cells for 120,000 time steps have been successfully run on Jazz over a period of 60 hours. Simulations with only a few cells were also run on laptops and desktops under Linux or Windows. The laboratory results [3] were reproduced exactly through computational experiments using AGENTCELL [2]. Figure 30 illustrates macroscale behavior for a group of cells swimming through an attractant gradient.

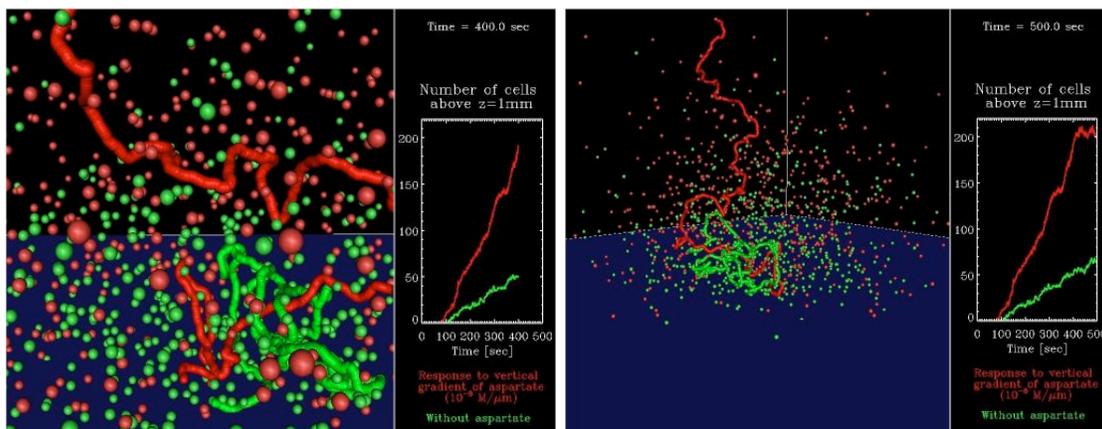


Figure 30: Macroscale behavior of 1,080 cells in a 3-D medium with a vertical gradient of aspartate ( $10^{-8}$  M/micrometer). 540 cells are sensitive to aspartate (green), and 540 cells are not sensitive (red).

### Publications/Presentations

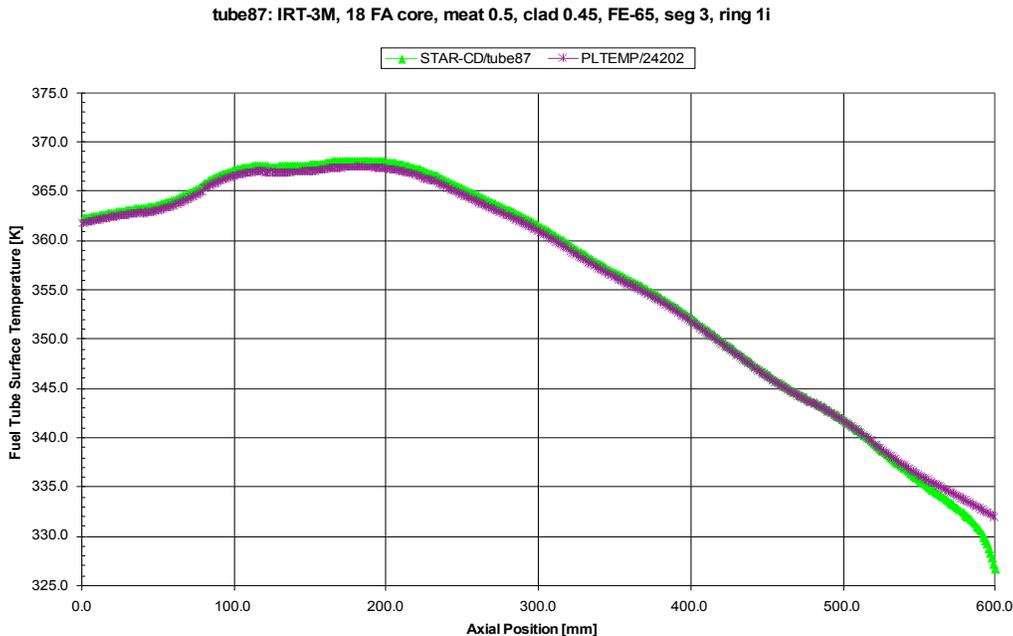
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2. T. Emonet, C. Macal, M. J. North, C. Wickersham, and P. Cluzel, AGENTCELL: A digital single-cell assay for bacterial chemotaxis, *Bioinformatics* 21(11), 2714–2721, 2005.
3. E. Korobkova, T. Emonet, J. M. G. Vilar, T. S. Shimizu, and P. Cluzel, From molecular noise to behavioural variability in a single bacterium." *Nature* 428:574–578, 2004.
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# Use of Computational Fluid Dynamics (CFD) for Analysis of Core Designs under the Reduced Enrichment for Research and Test Reactors Program (RERTR\_CFD)

PI: Patrick Garner, Nuclear Engineering

The redesign of reactor cores to use low-enriched uranium fuel requires a series of nuclear physics and thermal-hydraulics calculations in order to assure that the fuel produces the maximum required power while still being adequately cooled. The spatial variation of heat generation and fluid flow suggests the use of detailed 3-D calculations rather than dealing simply with averages.

In FY2005 we used the STAR-CD software to compute the heat transfer and fluid flow within several fuel assemblies, including one having six concentric square fuel tubes and a one-quarter sector model of an assembly containing 176 twisted, finned, square fuel pins. Simpler models (e.g., partial sector or single pin) were developed on the 80-node Linux cluster in the Nuclear Engineering Division; the models were then expanded to full size and ported to Jazz for final calculations. The results in the concentric tube assembly showed spatial details that were not available in simpler analysis models, for example, velocity peaking in the rounded corners and temperature peaking along the flats. Fuel temperatures for a case having no azimuthal dependence computed by using the k- $\epsilon$  turbulence model for high Reynolds number flow in STAR-CD coincided with results computed by using the Seider-Tate heat transfer correlation in a much simpler code such as PLTEMP, as shown in Figure 31.



**Figure 31: Clad surface temperature for outside of fuel tube 1 calculated by using STAR-CD and PLTEMP (1H=0:Seider-Tate).**

### **Publications/Presentations**

1. P. L. Garner and T. Sofu, Use of computational fluid dynamics (CFD) tools for fuel assembly analysis, presented at the International Meeting on Reduced Enrichment for Research and Test Reactors, Vienna, Austria, November 7–12, 2004.

## **Accelerator and Targets Simulations for the Rare Isotope Accelerator Facility (RIA-RND)**

PI: Brahim Mustapha, Physics

The RIA-RND project addresses mainly accelerator design and optimization through large-scale simulation of design options, comparing their performance and limitations. So far we have applied our new beam dynamics code TRACK [1] to the design and simulation of the Rare Isotope Accelerator driver linac. It could, however, be applied to any future proton or ion accelerator project. In fact, we started performing extensive simulations for the future proton driver project at Fermilab.

During the past year, we introduced many updates to the code TRACK, such as distinguishing between static and dynamic errors and correcting for static errors. We performed several simulations to test the new features of the code. These runs proved the validity of the latest updates, especially the correction of static field amplitude and phase errors in accelerating cavities [2].

We also performed independent benchmarking of our code TRACK by comparing it to well-established beam dynamics code such as IMPACT from Lawrence Berkeley National Laboratory. IMPACT was installed and run successfully on Jazz. The comparison showed excellent agreement between TRACK and IMPACT [3] (see Figure 32). With the updated and benchmarked version of TRACK, we expect to move forward in the design optimization and simulation of both the RIA driver linac and the Fermilab proton driver linac.

### **Publications/Presentations**

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2. B. Mustapha, V. N. Aseev, and P. N. Ostroumov, Error simulations and beam loss studies in the RIA driver linac using the code TRACK, in *Proceedings of HPSL (High Power Superconducting Linacs) Workshop*, Naperville, Illinois, May 22–24, 2005.
3. B. Mustapha, V. N. Aseev, P. N. Ostroumov, J. Qiang, and R. D. Ryne, RIA beam DYNAMICS: comparing TRACK to IMPACT, in *Proceedings of PAC-05 Conference*, Knoxville, Tennessee, May 16–20, 2005.
4. P. N. Ostroumov, V. N. Aseev, and B. Mustapha, Beam loss studies in high-intensity heavy-ion linacs, *Phys. Rev. ST. Accel. Beams*, 7, 090101, 2004.

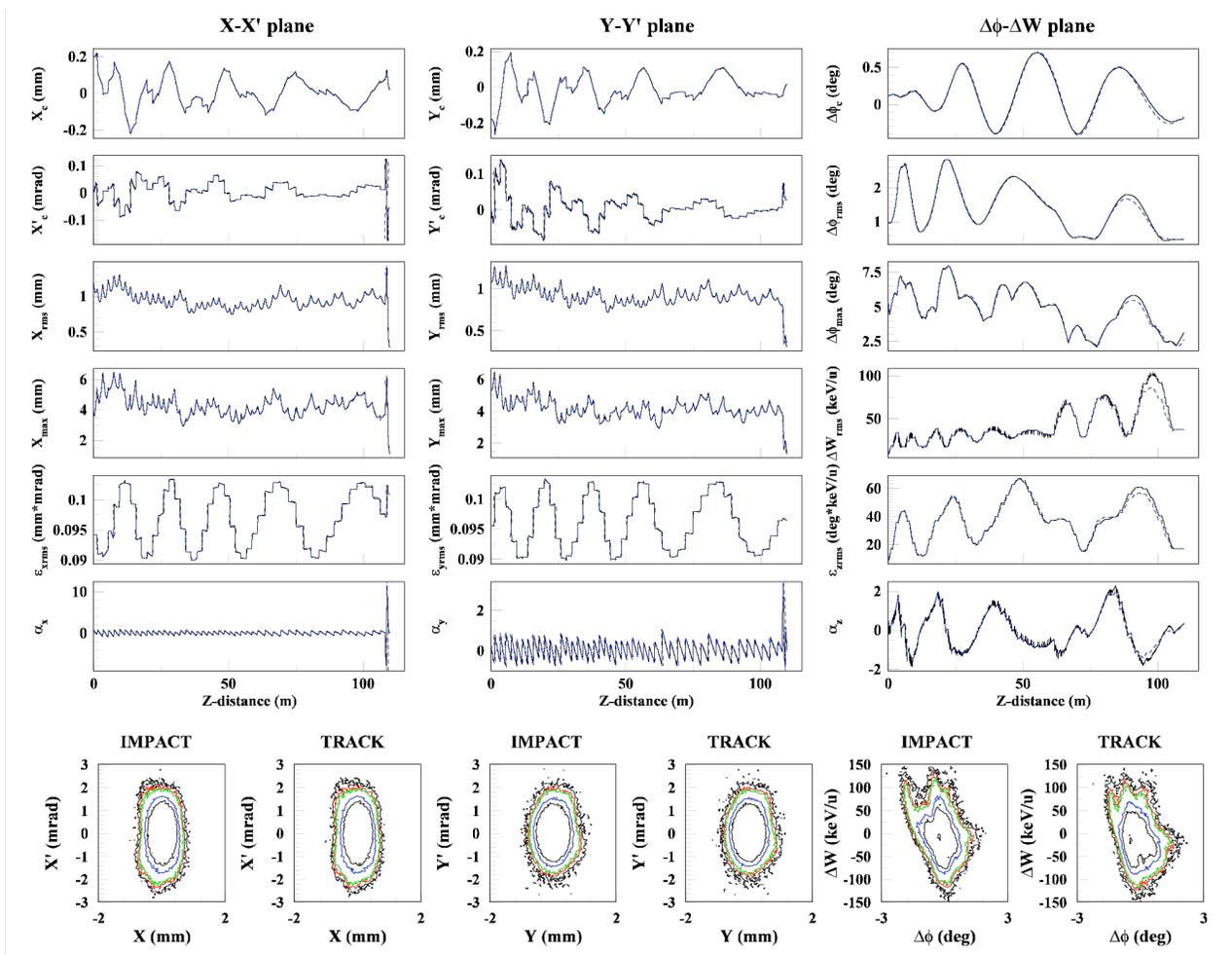


Figure 32: Comparison of IMPACT and TRACK simulations for the second linac section of the RIA driver linac for a five-charge-state uranium beam ( $Q=72,73,74,75,76$ ).

## Sediment Transport (SEDIMENT)

PIs: Paul Fischer and Gary Leaf, Mathematics and Computer Science; Juan Restrepo, University of Arizona

Particle transport is a process common to many physical systems. One aspect of such transport involves particles in suspension in oscillatory flows as, for example, wave-generated sediment transport. The principal factors in this process are the lift and drag on the particles in the presence of such flows. The numerical approach is attractive here, not only because it overcomes several experimental challenges, but also because our calculations are full direct numerical simulations of the Navier-Stokes equations in time and 3-D space.

In our ongoing study of particle transport, we have systematically quantified and analyzed the lift and drag on an increasing array of parameters. For the lift in an oscillatory flow, we have been able to determine two distinct subregions in the parameter space where the lift is dominated by different effects. In the large-gap short-period regime the lift is dominated by its viscous contribution, whereas in the

small-gap long-period regime, the lift is dominated by the pressure. Moreover, if either parameter is held fixed while the other is increased, the lift decays to zero.

The numerical simulations of the 3-D periodically forced flow were based on approximating a non-dimensional Navier-Stokes equation with our spectral element code Nek5000, which achieves linear scaling to at least 64 processors for the problem sizes required for this project. The core kernel of Nek5000 (>95% of all operations) is a highly tuned matrix-matrix product routine that attains in excess of 800 Mflops on each node of Jazz for noncached data.

### Publications/Presentations

1. P. Fischer, J. M. Restrepo, and G. K. Leaf, Forces on particles in oscillatory boundary layers, *J. Fluid Mechanics*, 468, 327–347, 2002.
2. P. F. Fischer, G. K. Leaf, and J. M. Restrepo, Influence of wall proximity on the lift and drag of a particle in an oscillatory flow, *J. Fluids Engineering*, 127, 583–594, 2005.

## Simulated Maximum Likelihood Estimation of Returns to Schooling (SIMAXLIKE\_SCHOOLING)

PI: Gale Boyd, Decision and Information Sciences

Differences in educational outcomes represent one of the main mechanisms that produce inequality. While the sources of these differences have been intensively studied for many years, social scientists still lack a full explanation as to why some groups (classified by race, gender, etc.) go to school more than others. The differences in years of schooling between blacks and whites is especially intriguing given the increasing labor premium for education (in particular for college attendance), a premium that is greater for blacks than for whites. While different authors have attributed this gap to individual background, family income, credit constraints, preferences, and a host of other explanations (see, for example, Figure 33), there is still no consensus on the question. The goal of this research is to analyze fully specified behavioral models that can account for all these possible explanations and thereby adjudicate the importance of different factors.

We obtained estimates for models of schooling choice that account for some of the possible causes mentioned before. In particular, focusing on white males, we were able to establish that there is relatively little uncertainty in schooling choices that ability and preferences play a predominant role in deciding whether to attend college and that tuition policies (i.e., reducing tuition) seem ineffective in increasing college attendance among white males. We have used Jazz to do massive parallel computations, thereby cutting computation time from months to days.

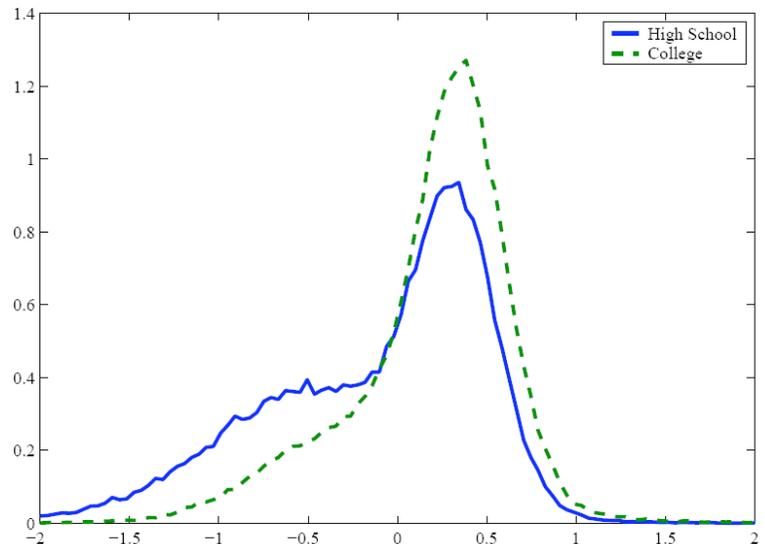


Figure 33: Distribution of cognitive ability in the population is lower for people with a high-school education than that for people with a college education.

Our computations have sparked a debate on whether tuition or other longer-term factors (what we call early interventions) are the main determinants of college attendance. We have also raised the question of whether the increased observed variability in earnings is due to an increase in uncertainty about future earnings or an increase in unobserved (to the analyst) agent heterogeneity. Our computations challenge the conventional wisdom that there is great uncertainty about future earnings when making schooling decisions. This result is of great importance because the implications in terms of the need to implement “insurance” mechanisms against uncertain events are completely different depending on whether variability is due to uncertainty or heterogeneity.

### **Publications/Presentations**

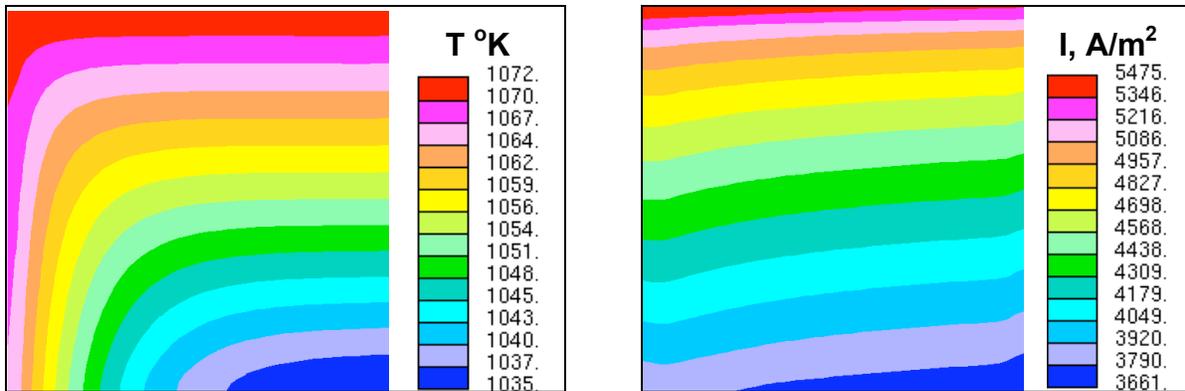
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2. G. Boyd, Counterfactual analysis of inequality and social mobility, in *Mobility and Inequality: Frontiers of Research from Sociology and Economics*, ed. G. Fields, D. Grusky, and S. Morgan, forthcoming.
3. G. Boyd, Understanding schooling: Using observed choices to infer agent’s information in a dynamic model of schooling choice when consumption allocation is subject to natural borrowing constraints, working paper, 2006.
4. Presentations: at the World Congress of the Econometric Society, August 2005; at the Institute for Computational Economics at Argonne, July 2005; and at workshops in Yale University, Boston University, University of Wisconsin-Madison, New York University, University of Illinois at Urbana-Champaign, University of Southern California, and Stanford University, between February and March 2005.

## **Thermal-Fluid and Electrochemical Modeling and Performance Study of a Planar Solid-Oxide Electrolysis Cell (SOEC-EC)**

PI: Bilge Yildiz, Nuclear Engineering

High-temperature electrolysis (HTE) is an environmentally acceptable and effective candidate process for hydrogen production in evolving hydrogen markets. The currently considered HTE system concepts and demonstrations are based on solid-oxide electrolysis cells (SOECs) that are similar to those used for solid-oxide fuel cells (SOFCs). The thermal and electrical energy needed for the HTE can be provided by a nuclear reactor. One of the major challenges facing the commercialization of this technology is the durability of the SOECs with high efficiency in operation. The goal of this project is to develop a model that can guide the performance optimization of HTE systems.

The SOECs operate with an applied potential to electrocatalytically split steam into  $H_{2(g)}$  and  $O_{2(g)}$ . There is limited knowledge about the intermediate reaction steps that define the phenomenological behavior of solid oxide electro-chemistry, especially for the less-investigated SOEC mode of operation. Several electrochemical and thermal-fluid dynamics models have been developed for SOFCs. However, none has been built for SOECs based on the first principles of the governing electrochemical mechanisms. The model developed in this work appropriately combines the governing electrochemical mechanisms to the heat transfer and fluid dynamics in the operation of SOECs for the first time. The computed results indicate the large margin for improving the thermal gradients of the SOECs at high current densities (Figure 34). These results will influence the choice for the operating conditions of the planar solid-oxide fuel cells being tested at Idaho National Laboratory.



**Figure 34: Simulated profiles for (a) temperature in the electrolyte, (b) current density for the cross-flow configuration SOEC. Inlet conditions: 800°C and 1 atm, V applied: 1.3 V, with 0% of H<sub>2</sub> and 50% N<sub>2</sub> at the cathode inlet.**

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## Large-Scale Parallel Simulation of Subduction Zone Geodynamics (SUBDUCTION)

PIs: Mathew Knepley, Mathematics and Computer Science; Richard Katz, Columbia University

We are interested in the general dynamics of the coupled magma/mantle system and applications of these dynamics to models of volcanic source regions in tectonic subduction zones. The source regions of volcanoes control the characteristics of erupted lavas; however, they are inaccessible to direct observation. Models are thus essential for developing a general knowledge of the behavior of the coupled magma/mantle system. This system is described by a set of conservation equations for mass, momentum, energy and composition of two interpenetrating fluid phases of vastly different viscosity (magma  $\sim 1$  Pa-s, mantle  $\sim 10^{19}$  Pa-s). Solutions to these equations can provide useful information to geochemists who study the long-term chemical evolution of the planet, as well as geophysicists trying to understand the current structure and composition of the deep Earth.

We investigated two instabilities in the magma/mantle system. The first is a chemical instability that arises when hydrous fluids react with mantle rock in subduction zone, leading to the production of hydrous silicate magma (Figure 35). This system undergoes a spontaneous localization of magmatic flux from diffuse porous flow to highly channelized porous flow with implications for rates of melt transport and magma chemistry. The second instability arises from a mechanical interaction between magma and the mantle. Our calculations suggest that localization and channelization of magma should be an expected feature of volcanic source regions. This hypothesis has testable implications for the predicted seismic properties of the mantle and the predicted geochemical signature of lavas.

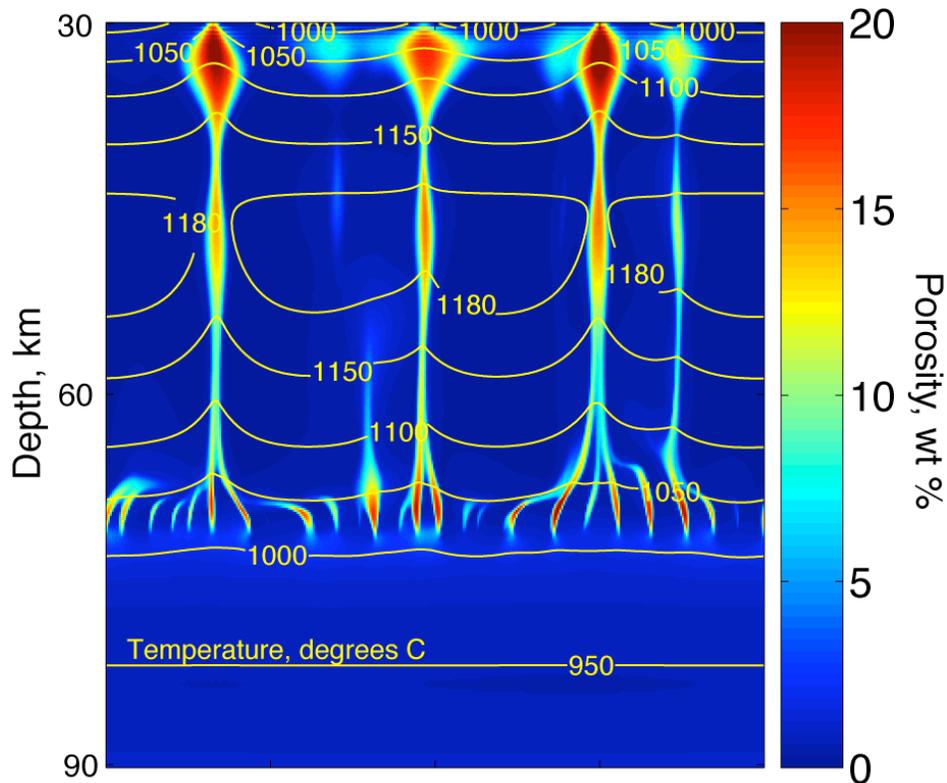


Figure 35: Chemical instability of magma/mantle system

We have used Argonne's PETSc system in all the calculations performed on Jazz during FY2005. Our codes couple up to 7 degrees of freedom per node in two-phase fluid dynamics simulations with non-Newtonian viscosity, chemical reactions, phase changes, localization, and solitary waves. Furthermore, we have extended PETSc with a parallel version of a characteristics-based advection scheme (semi-Lagrangian) that uses MPI and dynamic queues to efficiently communicate particle trajectories between processors.

### Publications/Presentations

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2. M. Knepley, Progress towards an integrated model of magma genesis and transport in subduction zones, invited talk at the fall 2004 meeting of the American Geophysical Union, 2004.
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# Cosmological Properties of Supersymmetry (SUSYCosMO)

PIs: Csaba Balazs and Carlos E. M. Wagner, High Energy Physics

In the past few years, the exceptionally precise measurements of the Wilkinson Microwave Anisotropy Probe made it obvious that ordinary matter (atoms and radiation) makes up only about one-sixth of the matter content of the universe. The rest, called dark matter, is a new type of nonluminous matter. The leading particle theory candidate providing new type of matter is supersymmetry, which has the potential to explain the origin of all matter, dark and luminous alike.

The SUSYCosmo project encompasses the heavy numeric calculations necessary to determine the range of supersymmetric models that can produce the measured amount of luminous and dark matter of the universe. We have shown that in one of the simplest yet experimentally and theoretically most motivated supersymmetric theories, the measured amount of matter and dark matter can be produced simultaneously.

If this model is confirmed by direct detection or production of dark matter at particle colliders, that result will imply the supersymmetric origin of all matter in the universe.

Calculations of the dark matter density in this model were performed on Jazz (Figure 36). The results led to the conclusion that the supersymmetric model is a viable candidate to explain all the matter content of the universe. Direct detection prospects were also evaluated by using Jazz. These results show that experiments will start to probe this model in the near future and might discover or exclude it by the end of the decade. Similar conclusions can be drawn for the collider searches [2], which are also done using Jazz.

## Publications/Presentations

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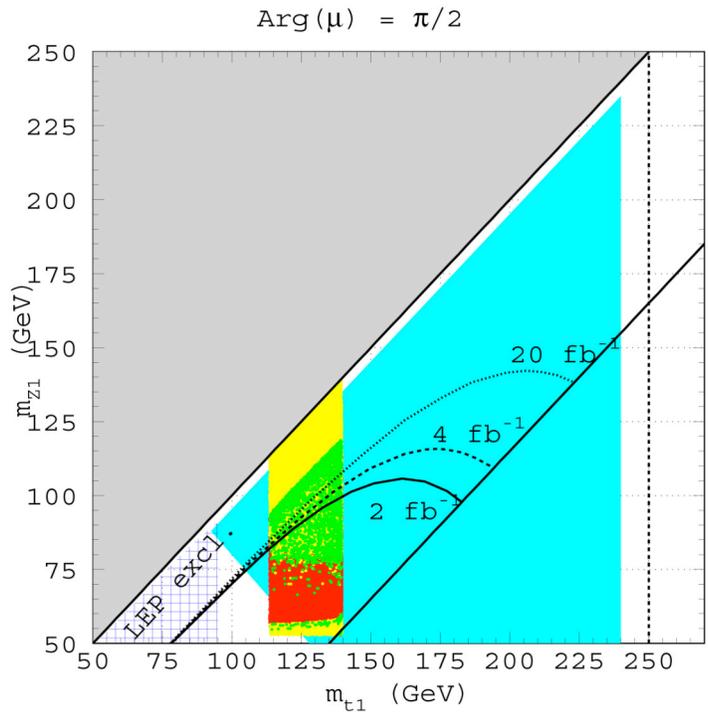
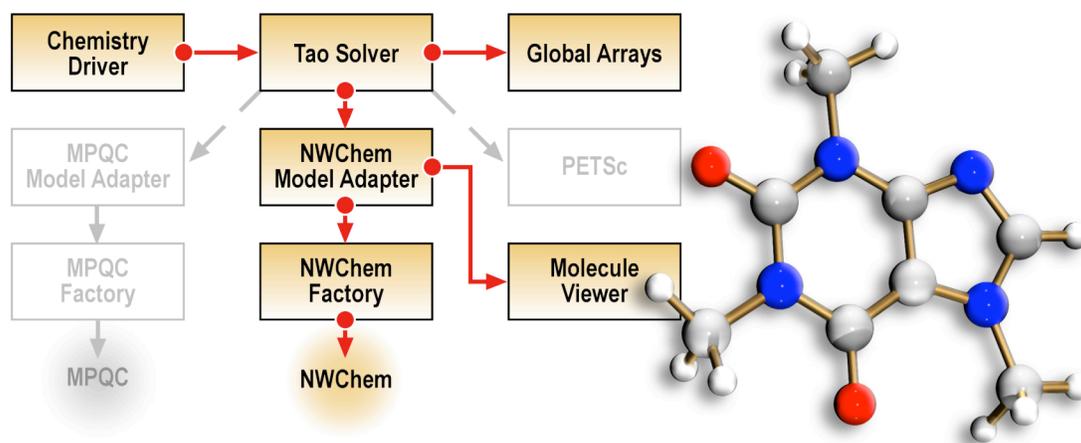


Figure 36: Dark matter density calculations.

## Toolkit for Advanced Optimization (TAO)

PIs: Steven Benson, Mathematics and Computer Science

Molecular geometry optimization is a fundamental problem in computational chemistry. The function of a molecule is often determined by its shape. Each shape, or geometry, of a molecule has an energy associated with it, and stable geometries coincide with a state of least energy. Adopting the methodology and tools of the Common Component Architecture Forum, we have developed a component architecture for molecular structure optimization and used the technology in large applications (Figure 37).



**Figure 37: Molecular geometry optimization using CCA-compliant electronic structure components based on NWChem (PNNL) and MPQC (SNL), optimization components based on TAO (ANL), and linear algebra components based on PETSc (ANL).**

Six molecular structures were optimized at the RHF/6-31G level of theory by using a starting structure obtained at the RHF/STO-3G level of theory. In each example, the optimization solvers in the Toolkit for Advanced Optimized (TAO) required fewer function evaluations than did the NWChem solver. In the case of the cholesterol molecule, the TAO solver converged to a solution while the NWChem solver could not. Furthermore, parallel scalability was maintained for the larger examples. The data adds to the extensive discussion in [1].

The collaborative effort enables research chemists to leverage current developments in the area of computational chemistry and numerical optimization without duplicating the efforts of experts in the field.

### Publications/Presentations

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# The Seed Project (THE\_SEED)

PIs: Robert Olson and Ross Overbeek, Mathematics and Computer Science

The SEED project is implementing a system to support comparative analysis of genomes. In the process we find it important to compute similarities between protein and DNA sequences, detection of motifs, and so forth. These are computationally intensive, but straightforwardly parallelized, computations. The Jazz cluster provides needed cycles to support the large amount of computation required to maintain the all-to-all similarities database for the SEED.

Up-to-date similarities computations form the foundation for many higher-level computations within the SEED environment. These include the determination of functional coupling on the prokaryotic genome, which provides key insights into determining the function of genes, and the calculation of bidirectional best hits, a much more compact form of similarity data. This is a key component of the National Microbial Pathogen Data Resource, an NIH-funded project to curate a number of pathogenic bacterial genomes (Figure 38).

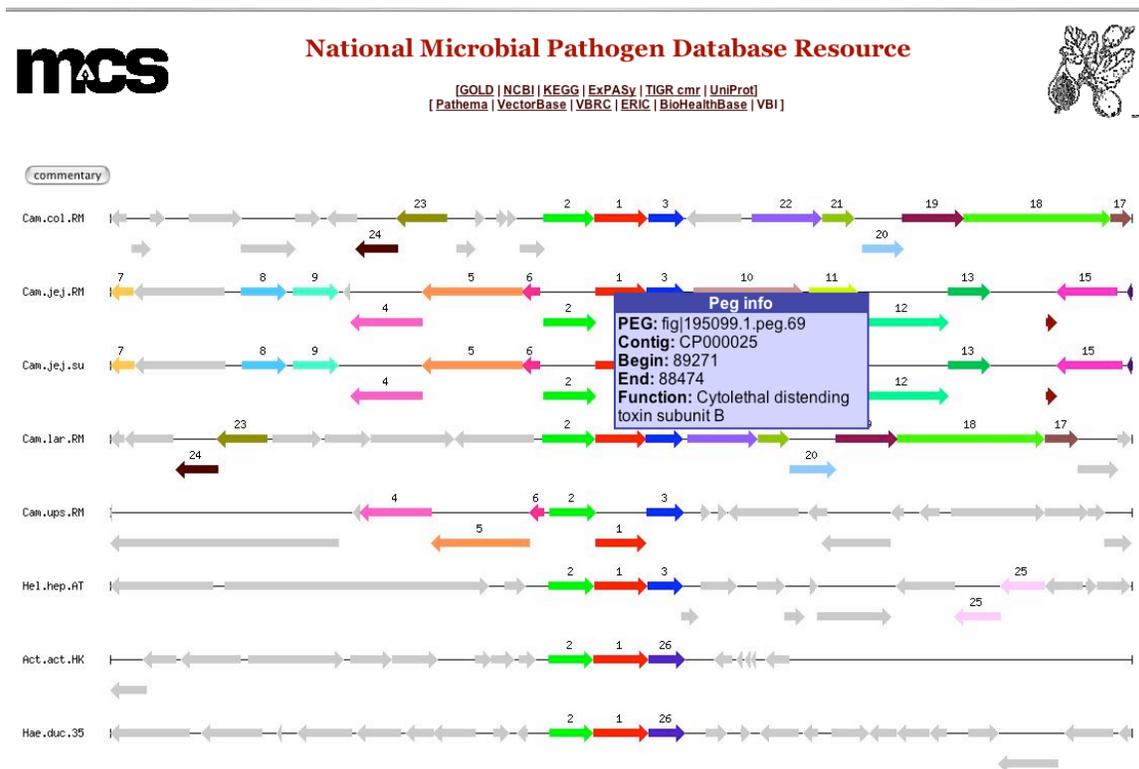


Figure 38: Screen shot from the NMPDR website.

## Publications/Presentations

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# Phase Diagram of Vortex Chains in Layered Superconductors (CHAIN3DAG.F)

PI: Alexei Koshelev, Materials Science

Layered high-temperature superconductors have a very rich vortex phase diagram in tilted magnetic field. Small magnetic field applied at a finite angle with respect to crystal axes generates isolated vortex chains. The chains have quite rich internal structure depending on the magnitude and tilt angle of the magnetic field and the temperature. Typically, at small temperatures and large tilt angles the vortex chain is composed of two perpendicular sublattices: a chain of Josephson vortices, oriented along the layers, and a chain of point (pancake) vortices, oriented perpendicular to the layers. We computed the ground state configurations at different parameters and constructed the phase diagram of an isolated vortex chain.

We developed a code that minimizes the energy with respect to the 3-D distribution of the superconducting phase and the coordinates of the point vortices within the chain unit cell. The most CPU-time-consuming part is calculation of the phase field. Realistic simulation typically requires  $256 \times 512$  grid in each layer and 5 to 10 layers. Typically, exploration of temperature evolution at one fixed magnetic field requires 2–5 days of CPU time on a 2 GHz Linux workstation. We have used Jazz to significantly advance our theoretical understanding of the vortex chain phase diagram. The key parameter that determines the chain structure at fixed magnetic field is the ratio of the two typical lengths: the London penetration depth ( $\sim 200$  nm at low temperatures) and the Josephson length ( $\sim 800$  nm). As this ratio increases with temperature, the chain structure also varies with temperature. Numerically exploring chain configurations, we found that the chain phase diagram is very rich. In general, the chain structure depends on three parameters: pancake separation along the chain, separation between Josephson vortices and ratio. We explored in detail the evolution of chain structures with increasing c-axis field at fixed temperature and in-plane field. An important feature of the phase diagram is *pancake density jumps*, which are due to the attractive interaction between the deformed pancake stacks located on the Josephson vortices. In the region of intermediate values we found two different scenarios of chain structure evolutions with increase of c-axis field:

1. In the range  $0.4 < \alpha < 0.5$  and large  $N$ , the small c-axis field first penetrates in the form of chains of pancake stacks located on Josephson vortices. Because of attractive coupling between deformed stacks, their density jumps from zero to a finite value, which depends on  $\alpha$  and the number of layers between Josephson vortices  $N$ . With further increase of the c-axis field the chain structure first evolves into modulated tilted vortices, which then transform via a second-order phase transition into tilted straight vortices. The chain phase diagram for  $\alpha = 0.5$  is presented in the top panel of Figure 39.
2. In the range  $0.5 < \alpha < 0.65$  (smaller anisotropies) we found even richer behavior. The small c-axis field first penetrates in the form of kinks, creating kinked tilted vortices. With increased c-axis field this structure is replaced via a first-order phase transition by the chain of pancake stacks, which are typically strongly deformed.

This transition is accompanied by a large jump of pancake density. Further evolution of the chain structure is similar to the higher anisotropy scenario: the structure first transforms into modulated tilted vortices and then, via second-order phase transition, into tilted straight vortices. Exact values of the

ratio  $\alpha$  separating the two scenarios depend on the spacing between the Josephson vortices. The chain phase diagram for  $\alpha = 0.6$  is presented in the lower panel of Figure 39.

**Publications/Presentations**

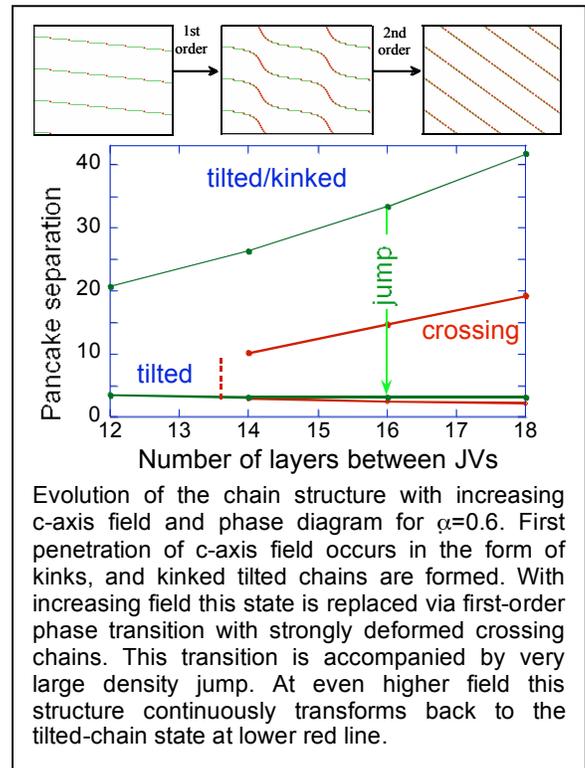
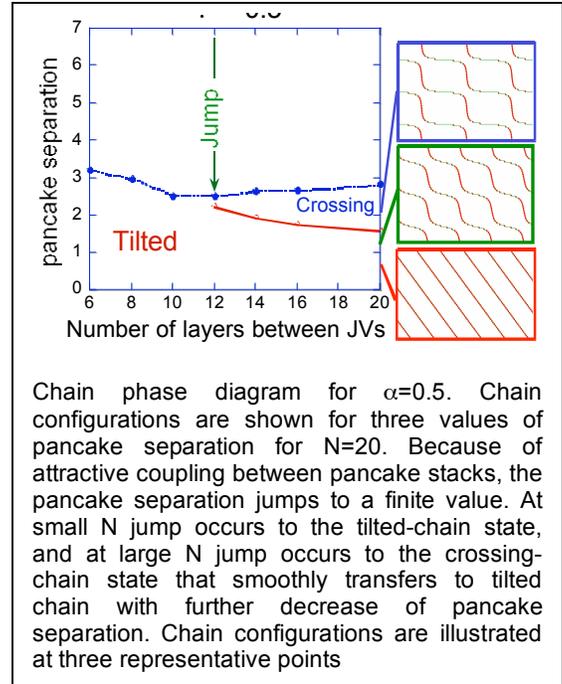
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**CHAOS (NEK5000)**

PI: Paul Fisher, Mathematics and Computer Science

Spatiotemporal chaos is an important field of study, both for its contributions to chaos and bifurcation theory and for its applications to a variety of problems such as chemical reaction-diffusion equations and ventricular fibrillation in a human heart. Nevertheless, many of the basic characteristics of spatiotemporal chaos remain poorly understood. Our calculations of the sensitivity to initial conditions and dimensions of the attractor via the Lyapunov exponents seek to quantify the complexity of the dynamics and how it increases as system size and driving strength are increased. The simulations of Rayleigh-Benard convection, for which the basic underlying equations are well understood and on which precise experiments are ongoing in various labs, provide a well controlled laboratory for developing understanding of these basic issues.

We have successfully modified our Nek5000 code to evolve multiple copies of the linearized perturbation equations simultaneously with the full solution. Numerous convergence and consistency tests have been performed to make us fully confident of our



**Figure 39: Chain structure evolution with increasing c-axis field.**

results. The largest Lyapunov exponents and their corresponding Lyapunov eigenvectors have been computed, for the first time, for various parameters.

For aspect ratio 5, the largest Lyapunov exponent is indeed positive, confirming that the turbulent state is truly chaotic. The Lyapunov eigenvector seems to be most localized in regions where defects are present. A systematic exploration of the correlation between Lyapunov eigenvalues and defect nucleation/annihilation has been performed on these small aspect ratio cells. We have found that while there are large fluctuations in the largest Lyapunov eigenvalue when a defect is nucleated/annihilated, there is no overall contribution to the long-time Lyapunov exponent. Instead, the deviations from periodic behavior contribute most significantly to the largest Lyapunov exponent.

Lyapunov exponents and eigenvectors have also been computed for aspect ratio 40 domain chaotic states in rotating cylinders. We have found that the largest Lyapunov exponent increases linearly with the control parameter. Moreover, for exactly the same parameters, the Lyapunov exponent increases as the aspect ratio increases from 10 to 40. We are also investigating the behavior of the Lyapunov eigenvector for domain chaos and its correlation with defect motion and domain wall motion. We plan to continue this research and eventually compute all the positive Lyapunov exponents for our systems.

We have also resolved the long-standing discrepancy between experiment and theory for rotating Rayleigh-Benard convection, by performing simulations for the exact parameters as the experiments. These are the aspect ratio 40 cells, which were also used for studying the Lyapunov exponents. The experiments found that time and length quantities have a different control parameter scaling from what the theory predicts. We have found that when only the Coriolis force is included, the scaling laws for our numerical simulations agreed better with the theory. However, when the centrifugal force is included as well, we found agreement with the experiments.

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2. J. Scheel and M. Cross, Scaling laws for rotating Rayleigh-Benard convection, submitted to *Phys. Rev. E* (June 2005)

## **Physics of the High-Temperature Gas-Cooled Reactor (HTGR)**

PI: Taek K. Kim, Nuclear Engineering

The very high temperature gas-cooled reactor (VHTR) is an important element in the DOE program to revitalize nuclear power in the U.S. suite of energy generation options. Two VHTR options were evaluated during FY2005. First, preliminary neutronic studies were performed in order to provide guidelines to the design of the salt-cooled VHTR (LS-VHTR) using  $\text{Li}_2\text{BeF}_4$  as coolant and a solid cylindrical core. Evaluation of the lattice codes revealed that their accuracy was similar to the Monte Carlo MCNP4C code for the prediction of the fuel element multiplication factor ( $k_{\text{inf}}$ ) and the double heterogeneity effect of the coated fuel particles in the graphite matrix. Second, a systematic assessment of the deep burn transmutation in VHTR (DB-MHR) was performed. Preliminary benchmarking of deterministic physics codes was done by comparing code results to those from MONTEBURNS calculations. Detailed fuel cycle analyses were performed in order to provide an independent evaluation of the physics and transmutation performance of the deep-burn concepts. Key performance parameters such as transuranic consumption, reactor performance, and spent fuel characteristics were analyzed. This

effort has been undertaken in close collaboration with the General Atomics design team and Brookhaven National Laboratory evaluation team.

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## **Terascale Simulation Tools and Technologies (TSTT)**

PI: Paul Fischer, Mathematics and Computer Science

The Terascale Simulation Tools and Technologies (TSTT) project is part of DOE's Scientific Discovery through Advanced Computing strategic initiative. The goal of TSTT is to provide cross-cutting technologies for large-scale simulation-based science projects such as climate modeling, fusion reactor design, accelerator design, and magnetohydrodynamics of stellar atmospheres.

We have used Jazz to further develop our incompressible MHD capabilities. This effort has resulted in the receipt of for 2 million node hours at NERSC as one of three DOE INCITE Awards for the study of momentum transport in accretion disks. We have successfully used Jazz to demonstrate the feasibility of direct numerical simulations of turbulent heat transfer in the interstitial space within a packed array of spheres that model pebble bed configurations that are under consideration for next generation nuclear power reactors. This work is a preliminary step toward a multiscale analysis of the reactor. Jazz has also been used to do development work for direct numerical simulation of turbulence in particulate flows, in collaboration with UIUC.

Using Jazz, we have also been able to develop and test several nonhydrostatic simulations of gravity driven density currents in the ocean, as part of an NSF-funded project, and to develop and test simulations of turbulence in arteriovenous grafts as part of an NIH-funded project.

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3. L. Zeng, S. Balachandar, and P. Fischer, Wall-induced forces on a rigid sphere at finite Re, *J. Fluid Mech.* 536:1–25, 2005.
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**Argonne National Laboratory**

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