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in affiliation with the Departments of

**Computer Science and
Applied Mathematics and Statistics
State University of New York at Stony Brook**

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1. MISSION

CDIC was established to provide state-of-the-art computational and computer science for the Laboratory and for the broader DOE and scientific community.

We achieve this goal by performing advanced scientific computing research in the Laboratory's mission areas of High Energy and Nuclear Physics, Basic Energy Sciences, and Biological and Environmental Research. We also assist other groups at the Laboratory to reach new levels of achievement in computing.

We are "data intensive" because the production and manipulation of large quantities of data are hallmarks of scientific research in the 21st century and are intrinsic features of major programs at Brookhaven.

An integral part of our activity to accomplish this mission is a close collaboration with Stony Brook University.

2. OVERVIEW

Modern science is critically dependent on computers and computing. A mix of capabilities is required, which range from advanced hardware to high-level and focused software efforts to high-speed networking - all aimed at the solution of forefront scientific problems which are consistent with our missions in High Energy and Nuclear Physics, Biology and Medicine, Materials and Chemical Sciences, Energy, Environmental Science, and National Security.

National plans for Information Technology in the early 21st century call for computing at the level of 100 teraflops and data storage in the petabytes. However, because this computational power will be obtained from massively parallel architectures, there is no guarantee that scientific and engineering codes will actually achieve these speeds. This issue is central to the Department of Energy's five-year program "Scientific Discovery Through Advanced Scientific Computing" (SciDAC). It is central to planned large-scale development of parallel nodes, each with high-speed vector processing. CDIC plays a prominent role in the SciDAC program through TSTT - Terascale Simulation Tools and Technologies. TSTT is a multi institutional effort to develop interoperable adaptive grid and meshing tools for a wide variety of scientific problems. Targeted applications include accelerator design, fusion, and fluid dynamics. In addition, large-scale computational physics codes aimed at studying the fundamental properties of quarks and gluons (lattice quantum chromodynamics) are planned to run at tens of teraflops.

Requirements for storage of experimental and observational data will reach hundreds of petabytes. Examples at BNL include RHIC, the Relativistic Heavy Ion Collider; US-ATLAS, one of the detectors planned for the Large Hadron Collider at CERN; climate modeling and simulation; brain imaging; protein structure and function; and computational fluid dynamics.

To be useful, this data must be processed, visualized, analyzed, and understood, as well as stored. Ultimately, data achieves value through its influence on some human decision. Increasingly,

decisions will be made on a computer-assisted basis. For this reason, the modern theory of data management goes beyond sheer volume to data intelligence.

CDIC will mount a research program in computational science to develop fundamentally new approaches to the management of large-scale, highly complex data and to assess uncertainties inherent in their use.

CDIC is closely linked with the Department of Applied Mathematics and Statistics and with the Computer Science Department at Stony Brook University, as well as with the Information Technology Division at BNL. The Center Director and one of the staff members hold joint SBU appointments. One staff member has a joint Columbia University appointment. Nine SBU faculty are CDIC Affiliates, and 10 graduate students contribute to CDIC projects. This arrangement adds critical strength to the Center.

Research in these areas provides a close link to Brookhaven's scientific programs. The Center will promote excellence, Laboratory wide, in scientific computing. CDIC will contribute to progress and productivity at BNL in a broad sense with special emphasis on:

- **High Energy and Nuclear Physics**
- **Biological and Environmental Science**
- **Basic Energy Sciences**
- **Advanced Scientific Computing**

3. PERSONNEL

The Director of the Center for Data Intensive Computing (CDIC) is James Glimm; James Davenport is the Associate Director, and the Staff Assistant is Claire Lamberti. CDIC is located in Building 463, Room 255, at Brookhaven National Laboratory, Upton NY 11973-5000.

CDIC, established in 1999, presently has a staff of ten, which is expected to approximately double over the next four years. As part of an active, ongoing collaboration with graduate students from Stony Brook, ten Ph.D. students and several undergraduates hold scientific positions in CDIC.

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4. RESEARCH

CDIC Budget FY 2003
Total: \$1,298K

CDIC Projects

4.1 SciDAC: TSTT at CDIC

Scientific Discovery through Advanced Computing (SciDAC) is a five-year program to develop the Scientific Computing Software and Hardware Infrastructure to support terascale computations for DOE's research programs.

At Brookhaven we have formed an alliance with researchers at Argonne, Livermore, Oak Ridge, Pacific Northwest, Rensselaer, Sandia, and Stony Brook, to develop technologies that enable scientists to use complex mesh and discretization strategies easily, within a single simulation on terascale computers. The Terascale Simulation Tools and Technologies (TSTT) Center will provide interoperable tools to facilitate use of advanced mesh and discretization technologies. The Center will develop standardized interfaces to local mesh refinement and adaptive higher order discretization codes. Existing codes of the Center partners and new codes will be supported to create a plug and play capability, whereby an application user can experiment easily with alternative technologies. Insertion of these tools into targeted applications is part of the Center work plan.

CDIC work within TSTT currently focuses on jet breakup, spray formation, and accelerator applications, and on finite element and front tracking contributions to TSTT technology.

4.2 High Energy and Nuclear Physics

New major physics facilities are central to the vitality of the nation's HENP programs. Due to their expense and complexity, simulation codes are integral to the design process. Design errors have been a major contributor to past instances of project cancellations and missed target performance. For this reason, design teams will increasingly use high performance computing, developed in national, multi-laboratory collaborations to address simulation issues in the design, operation, and control of accelerators.

See Table 4 for a list of current CDIC projects.

TABLE 4. HIGH ENERGY AND NUCLEAR PHYSICS PROJECTS		
Project Title	Key Personnel	Comments
Muon Collider Target	R. Samulyak, Y. Prykarpatskyy, J. Glimm,	Simulation of the Muon Collider Target
SciDAC: Wake Field Effects in Accelerator Design	R. Samulyak	Parallelization of Design, Control, and Optimization Codes
Unified Accelerator Library: SIMBAD	N. D'Imperio, A. Luccio	Parallel Scaling
Targets for Spallation Neutron Source	R. Samulyak, Y. Prykarpatskyy	Thermal Impulse
MiniBooNE Detector Analysis	R. Samulyak	Shock Wave Induced PMT Failure

4.2.1 Muon Collider Target

Muon Collider Target

In order to understand the fundamental structure of matter and energy, an advance in the energy frontier of particle accelerators is required. Advances in high energy particle physics are paced by advances in accelerator facilities. The majority of contemporary high-energy physics experiments utilize colliders. The aim of the multi institutional research group Muon Collider/Neutrino Factory Collaboration is to explore the feasibility of a high energy, high luminosity muon-muon collider [1]. Such a collider offers the advantages of greatly increased particle energies over traditional electron-positron machines (linear colliders). For more information, visit the Muon Collider/Neutrino Factory Collaboration home page (<http://www.cap.bnl.gov/mumu>). Several challenging technological problems remain to be solved in the collider design. One of the most important is to create an effective target able to generate the high-flux muon beam. The need to operate high atomic number material targets in particle accelerators that will be able to withstand intense thermal shock has led to the exploration of free liquid jets as potential target candidates for the proposed muon collider. The target will be designed as a pulsed jet of mercury (high Z-liquid) interacting in a strong magnetic field with a high-energy proton beam. Global numerical studies of the mercury jet behavior under such extreme deposition is the main goal of the present research.

The proposed target for the Muon Collider is shown schematically in Figure 1. It will contain a series of mercury jet pulses of about 1 cm in diameter and 30 cm in length. Each pulse will be shot at a velocity of 30-35 m/s into a 20 Tesla magnetic field at a small angle to the axis of the magnetic field. When the jet reaches the center of the magnet it will be hit with a 2 ns proton pulse. The proton pulse will deposit about 100 J/g of energy in the mercury.

Figure 1. Schematic of the Muon Collider target.

Global numerical simulation of hydro- and magnetohydrodynamic processes in the Muon Collider target is a challenging problem of computational science. Our numerical studies have been performed using FronTier-MHD, a magnetohydrodynamic extension of the front tracking hydro code FronTier (for more details, see Section 4.5.3, Magnetohydrodynamics of Multifluid Systems).

In [2], we made some analytical estimates and studied the evolution of conducting liquid jets and the mercury target in particular as they enter a strong nonuniform magnetic field. Our numerical

simulations of the interaction of the mercury jet with a proton pulse have shown that strong waves caused by the proton energy deposition lead to surface instabilities and the breakup of the jet [3,4] (see Figure 2). They agree with recent experiments carried out at the BNL Alternating Gradient Synchrotron and CERN. We have also shown that the magnetic field tends to stabilize the Richtmyer-Meshkov type instability in the mercury jet [3,4] (see Figure 3).

Figure 2. Numerical simulation of the Muon Collider target evolution.

Figure 3. Stabilizing effect of the magnetic field on the Richtmyer-Meshkov instability in the mercury jet under the proton energy deposition. a) $B = 0$, b) $B = 2$ Tesla, c) $B = 4$ Tesla, d) $B = 6$ Tesla, e) $B = 10$ Tesla.

Our future 3D MHD studies will address the influence of the magnetic field on the cavitation phenomena and Richtmyer-Meshkov instability in the mercury target.

References

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2. Samulyak, R. Numerical simulation of hydro- and magnetohydrodynamic processes in the Muon Collider target. Lecture Notes in Comp. Sci. **2331**, 391–400 (2002).
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4.2.2 SciDAC: Wake Field Effects on Accelerator Design

Introduction. The project Advanced Computing for 21st Century Accelerator Science and Technology is a national research and development effort involving several national laboratories

and universities. The project will develop a comprehensive terascale Accelerator Simulation Environment whose components will enable accelerator physicists and engineers to address a broad range of important issues in next generation accelerators and their design. These issues, which could not be addressed without terascale resources, range from the high accuracy requirement for modeling complex accelerating structures with tight tolerances, to the high resolution requirement needed for simulation beam halos in high intensity linear and circular accelerators. Accelerator science at BNL would benefit from large-scale simulations of beam dynamics and collective beam instabilities in the BNL AGS and Booster accelerators, and simulations of devices for the electron cooling of heavy ions in the RHIC ring.

Modeling of wake fields and impedances. The CDIC/BNL research goal is to develop algorithms and parallel software libraries for modeling the interaction of particle beams with electromagnetic wake fields in high intensity accelerators, and to model the beam dynamics and beam instabilities in several accelerator facilities. The electromagnetic interaction of an intensive charged particle beam with its vacuum chamber surroundings in an accelerator plays an important role for the beam dynamics and collective beam instabilities. Wake fields, generated by a moving particle in the accelerator pipe and objects such as RF cavities, bellows, stripline monitors etc., affect the motion of all particles in the tail part of the beam. This effect is usually of the same order of magnitude as the space charge effect. While the space charge forces approach zero in the ultrarelativistic limit, the wake field effect remains finite for an ultrarelativistic beam due to resistivity of the accelerator walls and non-smoothness of the chamber (existence of RF cavities, bellows etc.). The effect of wake fields is an increasingly important issue, since operating regimes are continually moving towards higher currents and smaller bunches. To avoid collective beam instabilities that limit a machine's performance, an accurate numerical modeling of wake fields and their interaction with the beam is necessary.

Two major sources of electromagnetic wake fields in an accelerator chamber are electric currents on resistive walls and non-smooth elements of the chamber (RF cavities, bellows etc.). We have developed a parallel software module for modeling the interaction of particle beams with wake fields. The corresponding theoretical model is based on analytical approximations in terms of the multipole moment expansion of the interaction of particle beams with wake fields induced on smooth resistive walls and non-smooth superconducting elements. The module has been implemented in MaryLie, an accelerator simulation code, and used for the study of wake field effects on the beam dynamics in simple focusing-defocusing channels and circular accelerators [2,3].

Numerical implementation. In the current numerical implementation, most of the accelerator chamber elements (resistive pipe, RF cavity etc.) have associated analytical wake field models valid under certain approximations [1]. To obtain an accurate set of parameters required by a wake field model for a non-smooth element, it is desirable to perform accurate numerical calculations of wake fields induced by this element using time domain electromagnetic codes (MAFIA, Tau3P, etc.), and to fit the corresponding analytical model to numerical data. Analytical wake field models are beneficial for the study of long-range wake fields and their multi turn effects on the beam dynamics in circular accelerators. To study the beam dynamics in linear accelerators, it is also possible to use precomputed and stored accurate numerical data for wake fields induced on RF cavities and other non-smooth elements. The major routines perform the charge deposition of

macroparticle beams on a 3D grid, expansion of the corresponding charge distribution into multipole moments, computation of wake functions and wake field forces, and interpolation of the wake field forces from the grid to macroparticles. The wake field algorithm takes into account long-range wake field forces which contribute during multiple turns of the beam.

Figure 4. a) Longitudinal (solid lines) and transverse wake functions (dashed lines) for the resistive model (left image) and the resonator model (right image).

Figure 5. Numerical simulation of space charge and wake field forces in a FODO channel. The collective forces increase the emittance (right image) of the initial beam (left image).

References

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2. Ryne, R., Qiang, J., Dragt, A., Habib, S., Mottershead, T., Neri, F., Samulyak, R., and Walstrom, P. MaryLie/IMPACT: a parallel beam dynamics code with space charge. In: Proc. of the Computational Accelerator Physics Conference, Oct. 15-18, 2002.
3. Samulyak, R. and Ryne, R. Distributed modeling of wakefields in MaryLie/IMPACT. Prepared for Comp. Phys. Comm. (2003).

4.2.3 Unified Accelerator Library: SIMBAD

Working in collaboration with computational physicists at BNL's Collider Accelerator Department, we have continued development on a Particle-in-Cell (PIC) [1] code to model collective beam effects in two and three dimensions. The code was formerly known as ORBIT and is being integrated into the Unified Accelerator Libraries (UAL) [2] as the SIMBAD component for the modeling of space charge.

UAL provides a framework in which the tracking of particles takes place by pushing a “bunch” of macroparticles through a lattice using the TEAPOT code, which has also been integrated in UAL. Space charge is calculated separately using SIMBAD. Once all particles have reached a certain location, their charge density is calculated by binning to a grid. The potential Φ is found by solving the Poisson equation with the perfectly conducting wall boundary conditions:

$$\Delta\Phi = -\rho/\epsilon, \rho_{\text{wall}}(x,y,z) = 0.$$

Space Charge force components (with coefficients to account for both the electrostatic and magnetic action) are calculated as derivatives of the potential and applied to each macro particle in the transverse direction. Longitudinal Space Charge is calculated by binning the particles longitudinally and following the formalism presented in [1]. In a ring with long longitudinal bunches, the transverse motion can be uncoupled from the longitudinal, and the Poisson equation can be solved in parallel in many longitudinal beam segments.

The parallelization of SIMBAD is implemented differently in 2-d as opposed to 3-d. In 2-d, the parallelization is implemented by dividing the macro particles among the processes and collectively calculating the forces on each mesh. In 3-d, each process takes a number of longitudinal slices and calculates the space charge forces only within its own slices. This parallelization requires load balancing that considers both the number of particles and the number of slices. This is accomplished using a genetic algorithm [3]. Figure 6 shows parallel decomposition of the bunch and the resulting division of the beam.

Recently, the code was used to model high intensity beams in the Alternating Gradient Synchrotron at BNL to study its suitability as a proton driver [3]. Figure 7 shows the rms transverse emittance vs. turn number. The space charge couples the two transverse coordinates while the two emittances reach a steady state after some turns. A Montague resonance is observed.

Figure 6. Bunch decomposition and load balancing. (a) A bunch of macro particles in an RF bucket with accompanying lines to indicate the boundaries for each of 5 processes. (b) Genetic algorithm produces an optimal balance between number of particles per process and number of slices per process.

Figure 7. Emittance vs. turns for the AGS at low and high intensity. The dashed lines are low intensity, solid lines indicate high intensity. Transverse coupling is very noticeable at high intensity.

References

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4.2.4 Target for Spallation Neutron Source

The Spallation Neutron Source (SNS) is an accelerator-based neutron source being built in Oak Ridge, Tennessee, by the U.S. Department of Energy (<http://www.sns.gov>). The SNS will provide the most intense pulsed neutron beams in the world for scientific research and industrial development.

The proposed liquid mercury target design for the Spallation Neutron Source (see Figure 8) includes a main flow region inside a stainless steel structure where mercury enters from the sides, flows around a baffle into the proton beam path, and exits out the center. A cooling jacket that wraps from bottom to top around the target is used to cool the target window through which the proton beam enters. The stainless steel target structure is approximately $0.5 \times 0.4 \times 0.15 \text{ m}^3$.

One of the most important issues associated with using liquid metals as targets for pulsed proton beams is withstanding the loads caused by the rapid pressure increase resulting from the intense

heating of the liquid metal from a single pulse of protons. This heating occurs essentially instantaneously compared to acoustic time scales; therefore, the mercury undergoes a large pressure increase. In addition to a set of difficult engineering problems associated, for instance, with the design of windows able to withstand large thermal gradients and shocks, recent experiments with an SNS target prototype uncovered yet another problem critical to the target lifetime. They showed pitting of stainless steel surfaces that were in contact with mercury subject to large pressure pulses induced by the collapse of cavitation bubbles [1]. Due to the cavitation-induced erosion, it will be necessary to replace the target after two weeks of operation at frequency 60 Hz of a 1 MW proton pulse. To extend the target lifetime, future research efforts will be concentrated in two areas, each of which should lead to reduction of the erosion damage:

- Evaluation of cavitation-resistant materials and coatings.
- Investigation of mitigation techniques such as introduction of non-dissolvable bubbles into the system.

Figure 8. SNS mercury target design.

We have been working on the modeling of cavitation and bubbly fluids, and the numerical simulation of hydrodynamic processes related to cavitation-induced erosion. The main goal of the research is to explore possible ways of reducing the cavitation and extending the target lifetime. In our studies, we collaborate with the SNS targetry research group as well as scientists affiliated with the European Spallation Source Project. The areas of research include:

- Development of new equation of state models for the cavitation dynamics and flow of liquids containing non-dissolvable gas bubbles (See Section 4.3.5 for more details). The first class of models is based on the direct tracking of gas-liquid interfaces in multiphase flows (Figure 9). Such an interface tracking is a key feature of our hydrodynamic code FronTier. The second class of models uses a homogeneous description of a multiphase system as a pseudofluid. This method allows inclusion of surface tension, drag, and viscous forces.
- Global numerical simulations of the wave dynamics in the target container using the FronTier and ABAQUS codes and new EOS modules. This includes benchmarking with experimental data on the SNS target strain response to beam-induced pressure pulses,

numerical studies of the geometric effects capable of reducing reflected tensile waves, and optimization of the target container shape.

- Evaluation through numerical simulations of the efficiency of mitigation techniques which use layers of non-dissolvable gas bubbles near target windows and gas bubbles in the bulk mercury. We have been working on numerical simulations of the interaction of strong waves with bubbly flows using the homogeneous equation of state models and direct numerical simulations of the bubble dynamics based on FronTier's interface tracking capabilities.
- Numerical studies using FronTier's interface tracking technique of the hydro jet arising in a cavity collapse and its interaction with the wall.

Figure 9. Direct numerical simulation of pressure wave propagation in bubbly mercury: a) initial density; red: mercury, blue: gas bubbles, b) initial pressure; the pressure is 500 bar at the top and 1 bar at the bottom, c) pressure distribution after 100 microseconds; the pressure is 6 bar at the bottom.

Reference

1. Status Report on Mercury Target Related Issues, SNS-101060100-TR0006-R00, July 2002.

4.2.5 MiniBooNE Detector

Introduction. The Booster Neutrino Experiment (BooNE) at Fermi National Accelerator Laboratory will investigate the question of neutrino mass by searching for neutrino oscillations from muon neutrinos to electron neutrinos. This will be done by directing a muon neutrino beam into the MiniBooNE detector and looking for electron neutrinos. This experiment is motivated by the oscillation results reported by the Liquid Scintillator Neutrino Detector (LSND) experiment at Los Alamos National Laboratory. The major goal of the MiniBooNE experiment, the first phase of the BooNE project, is either to confirm or to refute startling experimental results of Los Alamos scientists. By changing the muon neutrino beam into an anti-neutrino beam, BooNE can explore oscillations from muon anti-neutrinos to electron anti-neutrinos. A comparison between neutrino and anti-neutrino results will tell us about CP- and CPT-violation.

The MiniBooNE detector is a sphere of 12 m diameter filled with mineral oil. On the interior surface of the sphere, there are attached phototubes (PMTs), with 10 cm radius and spacing 55 cm (see Figure 10). PMTs are vacuum glass containers, sensitive to impacts of pressure waves in the container. The accident on another neutrino experimental facility in Japan, the Super-Kamiokande (SuperK) detector, raised many questions about optimization of the design of such devices. About 60% of all photomultipliers used in the SuperK detector were destroyed in a few seconds due to

shock waves in the container. The shock waves were induced by an accidental implosion of one PMT. The SuperK detector is a cylindrical container filled with water and it uses 50 cm PMTs with 70 cm spacing. Because of the accident, the experiments were stopped and major repair work started.

Figure 10. Arrays of photomultipliers on the MiniBooNE detector walls.

The aim of our numerical simulation project is to evaluate the stability of the MiniBoone detector against PMT implosion induced shock waves. We will perform broad numerical simulations of the PMT implosion process and the dynamics of shock waves in both MiniBoone and SuperK geometries.

Numerical simulations. We use the FronTier code for the numerical simulation of the PMT implosion process and the dynamics of shock waves in the BooNE and SuperK containers. FronTier is a hydrodynamics code with free interface support. It is based on front tracking, a numerical method for a system of conservation laws, which allows the computation of dynamically evolving interfaces through the solution of the corresponding Riemann problem. FronTier uses high resolution hyperbolic methods for the interior domain away from free interfaces, capable of resolving shocks and rarefaction waves. The code also uses realistic equation of state (EOS) models and stiff EOS models for fluids in particular. The reader is referred to Sections 4.2.1 and 4.4.1 of this document and references therein for more information on FronTier and its further developments.

We have performed preliminary studies of the PMT collapse and the shock wave dynamics in the MiniBooNE and SuperK containers. In the shock wave numerical experiment, the wave dynamics and pressure distribution on the array of 5 PMTs were studied. Shock waves were induced by the implosion of the central PMT. The numerical simulations indicate stronger pressure rise on PMTs in the SuperK detector geometry than in the MiniBooNE. However, adding the viscosity to the fluid (mineral oil was used in MiniBooNE) does not have a significant influence on the reduction of the shock wave strength. Numerical simulations suggest that the MiniBooNE detector is much more stable than the SuperK, and the chance for a chain collapse of PMTs in the MiniBooNE is negligibly small.

Figure 11. Dynamics of shock waves in the MiniBooNE container.

Figure 12. Dynamics of shock waves in the SuperK container.

4.3 BASIC ENERGY SCIENCES

The Department of Energy's Office of Basic Energy Sciences supports research in materials and chemical sciences, geoscience, engineering, and energy biosciences. This broad-based program of fundamental research is also responsible for a number of national user facilities, including synchrotron x-ray and neutron sources and electron microscope facilities. CDIC has engaged in numerous projects in computational fluid dynamics, many body physics, and optics, which are described here. Most projects are in collaboration with BES scientists and support the BES missions. See Table 5.

TABLE 5. CDIC BASIC ENERGY SCIENCES PROJECTS		
Project Title	Key Personnel	Comments
Magnetic Nanowires	J. Davenport	Density Functional Theory
Superconductivity	J. Davenport	Density Functional Theory
Scalable Localizable Density Functional Theory	J. Davenport, D. Volja, J. Zheng	Up to 5000 Atoms
Surface Magnetism of Uranium	J. Davenport, N. Stojic	Density Functional Theory and Classical Monte Carlo

Cavitating and Bubbly Fluids	R. Samulyak, Y. Prykarpatskyy	Spallation Target Model
Laser Ablation Plasma Plumes	R. Samulyak, Y. Prykarpatskyy	Carbon Nanotubes
Photonic Devices	J. Glimm, N. D’Imperio	FDTD Maxwell Solver

4.3.1 Magnetic Nanowires

Magnetism in One-dimensional Nanowires

Nanotechnology allows structures of a limited number of atoms that may play an important role in future applications, such as spintronics, magneto-optical devices, and quantum computers. The experimental efforts require extensive theoretical support because the results of recent measurements open many questions that remain to be answered. Magnetism in low-dimensional systems such as monatomic nanowires, namely linear chains of magnetic atoms, grown on non-magnetic substrates is particularly interesting. Cobalt chains adsorbed on platinum surfaces display magnetic order which has been studied by *ab-initio* calculations and experimentally by x-ray magnetic circular dichroism (XMCD) using synchrotron radiation. These systems display the largest orbital magnetic moment ever found in a 3d transition element.

A numerical simulation within the framework of the density functional theory is of great importance in order to interpret these experiments correctly. We apply the super-cell technique, where the nanowires are modeled as a repeat structure, shown in Figure 13. Such a structure with a stepped-substrate surface mimics the real material fairly well. The chosen inter-chain distance is large enough to avoid interactions between different wires. The calculations are performed using the full-potential linearized-augmented-plane-wave (FLAPW) method [2]. The wave functions are calculated in the scalar-relativistic approximation, while the spin-orbit coupling, essential for the XMCD effects, is included as a perturbation with the second-variational method. In the same manner, we optionally include an orbital-polarization (OP) term [3, 4], which takes partial account of the correlation effects associated with Hund’s rule. The local-spin-density approximation (LSDA) is used for the exchange-correlation potential. Figure 14 shows the spin density, calculated as the difference in the charge density for the electrons with up and down spins. Besides the large peaks at the sites of the Co atoms, there are also lower peaks in the spin density at the sites of the Pt atoms. The magnetization is obviously induced in the substrate, which partly explains the existence of ferromagnetism in the quasi one-dimensional wires.

Figure 13. Periodic structure of the cobalt chains (red spheres) on the platinum surface.

Figure 14. Calculated spin density of the cobalt nanowires on platinum.

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4.3.2 Superconductivity: Charge Distribution in the Superconductor Magnesium Diboride

MgB₂ has recently been found to display superconductivity at the surprisingly high temperature of 39K [1]. This fact has stimulated a large research effort to determine the cause of the high transition temperature, as well as other properties of this otherwise unremarkable material. We have utilized first principles density functional theory to calculate the charge density in MgB₂ and compare it with transmission electron microscope and synchrotron x-ray measurements carried out at Brookhaven. We used the full potential linear augmented plane wave (FLAPW) method to solve the density functional equations [2]. The calculated lattice constants are in good agreement with previous calculations and with experiments. The same technique had been used earlier to study the distribution in energy of the occupied and empty states [3].

MgB₂ forms in a hexagonal crystal structure, with the boron atoms arranged in a honeycomb fashion in planes that are structurally the same as graphite. The magnesium atoms are located in the hollow positions in parallel planes above and below.

Figure 15 shows a contour plot of the difference charge density in the boron plane [4]. The difference density is obtained by subtracting the density of isolated atoms from that of the compound. The red areas between the atoms show clearly the build up of the bond charge.

Figure 15. Charge density contours in the hexagonal compound MgB_2 calculated from first principles density functional theory.

Experiments measure the structure factors of the charge distribution, which are related to the Fourier transform of the density. The calculations described here agree with the experiments to within 3%. Calculations using only the atomic density, which are typically used in diffraction experiments, disagree with the data by up to 28%, clearly showing the importance of quantum mechanical calculations of x-ray diffraction. We have also studied the details of the x-ray absorptive edge, finding excellent agreement with experiments [5,6].

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4.3.3 Scalable Localizable Density Functional Theory

Nanoscale science and technology and biology are driving a search for new ways to calculate the electronic properties of clusters containing many thousands of atoms. Density Functional Theory (DFT) has been shown to yield accurate total energies, charge, and spin densities in molecules and crystalline solids but has been limited in the size system that can be treated.

The density functional equations consist of coupled Schrodinger and Poisson equations, which must be solved self consistently. Usually one chooses a basis set (for example Gaussian type orbitals or plane waves) thereby converting the Schrodinger equation into an eigenvalue problem. The number of such basis functions will scale linearly with N , the number of atoms in the system. Solving the eigenvalue problem will then scale as N^3 . Hence for large systems, there is a premium on efficiency, or reducing the number of basis functions required per atom. Gaussian type orbitals (GTOs) have the advantage of being highly localized in space, decaying like $\exp(-ar^2)$. However, they are not maximally efficient, in the sense that many Gaussians are required to accurately represent the wave functions. Plane waves have the disadvantage that they are not localized at all, but rather extend over the whole system. In addition their use generally requires a “supercell” in which the system is repeated periodically in space, leading to inaccurate treatment of surface and edge effects in some cases.

We solve these problems by using a mixed numerical and localized analytical basis set. We partition the space into nonoverlapping spheres surrounding each atom and an extra-atomic region outside the spheres. Inside the spheres the basis consists of numerical solutions of the Schrodinger (or Dirac) equation for the spherical part of the potential. Outside the spheres, the basis is given by Slater type orbitals, which have the form

$$\phi_{nlm}(\vec{r}) = r^{n-1} \exp(-\zeta r) Y_{lm}(\vec{r})$$

where the Y s are spherical harmonics. These functions are not as localized as GTOs but achieve the same accuracy more efficiently.

At each sphere boundary these functions are matched onto the numerical solutions inside the sphere. Such a scheme has already been implemented for periodic systems and is known as LASTO, the Linear Augmented Slater Type Orbital method [1]. It is a local orbital version of the Linear Augmented Plane Wave (LAPW) method, considered the most accurate method for solving the DFT equations.

The Poisson equation is solved on a numerical grid using sparse matrix techniques and the hypre library [2]. Hypre is a set of highly parallel preconditioners and solvers suitable for large sparse systems. The eigenvalue problem is solved using SLEPc [3], a set of codes for the solution of large eigenproblems. SLEPc uses the PETSc [4] interface that provides a large library of structures and routines for partial differential equations.

For the largest systems we use a technique known as “divide and conquer” [5]. In this method, a large cluster is partitioned into subsystems, and the charge density is calculated for each. The computational effort scales like SN_s^3 , where S is the number of subsystems and N_s is the number of atoms in the subsystem. This scheme is possible because the charge density (more generally, the density matrix) is localized in space even when the eigenfunctions are not [6].

Using divide and conquer, along with the localized basis set provided by STOs, we expect to be able to calculate the charge and spin density of clusters containing up to 5000 atoms.

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4.3.4 Prediction of Surface Magnetism in Uranium Metal

Uranium, the heaviest naturally occurring element, has been studied for many years. Metallic uranium has an interesting complex crystal structure, as is shown in Figure 16. It is the only nonmagnetic element known to form an incommensurate charge density wave state at low temperatures. At room temperature it crystallizes in an orthorhombic structure (shown in Figure 16), and on heating passes through tetragonal and body centered cubic (bcc) phases before melting at 1408K. As one of the actinides, it has partially filled $5f$ states, yet unlike the $4f$ (rare earth) elements and the heavier actinides, the $5f$ electrons are believed to be relatively delocalized and contribute to the metallic bond. Many uranium alloys display heavy fermion behavior, indicating some form of incipient localization.

In this work we have used first principles density functional theory, including the spin orbit interaction, to calculate the magnetic properties of thin films [1]. We find, surprisingly, that the surfaces of the films are magnetic, even though the bulk material is not. We predict that this magnetic surface layer is also present at the crystalline surface. We have also calculated the structural properties and bulk moduli of the competing phases. We find that the bcc phase is mechanically unstable, meaning that the energy as a function of tetragonal distortion has negative curvature. Describing the mechanical stability of nonequilibrium phases is important for phase diagram construction, the structure of grain boundaries, and epitaxial thin films.

The calculations were performed with the full potential linearized augmented plane wave method as embodied in the WIEN2k code [2]. This is widely recognized as the most accurate method for solving the density functional equations (a set of single particle equations obtained by reduction from many body problems applying the density functional theory). The WIEN2k code includes

Figure 16. Alpha uranium crystal structure. $a = 2.836\text{\AA}$, $b = 5.866\text{\AA}$, $c = 4.935\text{\AA}$, $y = 0.1017$.

Figure 17. Calculated spin density on outermost plane of uranium. The units are Bohr magnetons.

local orbitals to better describe semi core states. We also used the generalized gradient approximation (GGA) for exchange and correlation as described by Perdew et al. in [3]. Use of the GGA leads to a significant improvement in the calculated volume compared with experiment [4]. Structures studied included the simple, face centered, and body centered cubic, body centered tetragonal, orthorhombic, and hexagonal close packed. We determined the cohesive energy, equilibrium volume, and bulk modulus for each structure. Structural energy differences and vacancy formation energy for the BCC lattice were also found. To study surfaces, films of 1 – 7 layers were constructed in supercell geometry.

All of the films displayed large magnetic moments of approximately 0.65 Bohr magnetons per atom, concentrated in the surface plane (1 Bohr magneton is the magnetic moment of a single electron--it is noninteger in metals because of chemical bonding effects). The spin density in the outermost plane is shown in Figure 17. The multilobed angular dependence shows clearly that the moment is primarily due to the 5f electrons. We also calculated the surface and spin projected density of states and predict that the magnetic effects should be easily observable in experiments such as spin polarized photoemission or circular dichroism.

If verified, this would be only the second example found of a nonmagnetic element that possesses a surface magnetic moment and illustrates the possibility of designing completely new magnetic materials.

The mechanical instability of the bcc phase is illustrated in Figure 18, which shows the energy as a function of volume and c/a ratio for tetragonal distortions. The total energy of the bcc phase is 0.22 eV / atom above the ground state (orthorhombic) phase.

Figure 18. Mechanical instability of the BCC structure, located along the $c/a=$ ridge above. The energy is displayed as a function of unit cell volume and ratio of lattice axes c/a . We changed the c/a ratio, thus deforming the BCC structure ($c/a = 1$) into a body-centered tetragonal lattice structure, which has an energy minimum at $c/a = 0.8123$ and $V = 20.653 \text{ \AA}^3$ (139.370 bohr^3).

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4.3.5 Cavitating and Bubbly Fluids

An accurate description of cavitation and wave propagation in cavitating and bubbly fluids is a key problem in modeling and simulation of hydrodynamic processes in a variety of applications ranging from marine engineering to high energy physics. We are interested in the study of cavitation and bubbly fluids occurring in liquid mercury targets that interact with high intensity proton pulses. Such targets are key components of advanced accelerators such as the Spallation Neutron Source (<http://www.sns.gov>) and Muon Collider/Neutrino Factory (www.cap.bnl.gov/mumu).

We have been working on two different approaches to this problem. The first one (the **direct method**) is based on unique interface tracking capabilities of our hydro code FronTier. The second approach (the **homogeneous method**) is based on a continuous description of the liquid-vapor or liquid-non-dissolvable gas mixtures by means of homogeneous equation of state models.

Direct method. We have been studying a liquid-vapor or liquid-non-dissolvable gas mixture as a system of one-phase domains separated by free interfaces. The FronTier code is capable of tracking simultaneously a large number of interfaces and resolving their topological changes (the breakup and merger of droplets) in two- and three-dimensional spaces. Different equation of state models are used for gas/vapor bubbles and the ambient liquid. Though computationally intensive, such an approach is very accurate in treating important effects in bubbly flows, including bubble oscillations, heat transfer, drag, viscosity, and surface tension. To account for the phase transition induced mass transfer across free interfaces, we have been developing a nonlocal Riemann solver governing the evolution of interfaces.

The current computational capabilities of our hardware allow the use of this approach for the study of wave dynamics in thin layers of bubbles in two and three dimensions. We have performed numerical simulations of classical shock-tube experiments in bubbly fluids and obtained a good agreement with experimental data. It is prohibitively expensive, however, to study large bubbly volumes by direct numerical simulations. The homogeneous approach described below is used for such systems.

Homogeneous method. The advantage of the homogeneous method compared to the direct one is its computational simplicity and, as a result, low computational requirements for the simulation of large systems. The homogeneous flow approximation provides a simple technique for analyzing two-phase (or multiple phase) flows. It is accurate enough to handle a variety of practically important processes. Suitable average properties are determined and the mixture is treated as a pseudofluid that obeys an equation of single-component flow [1].

We have developed a simple isentropic homogeneous equation of state for two-phase liquids and implemented the corresponding software library in the FronTier code. The code was applied to study the interaction of mercury with an intensive proton pulse in the geometry typical for mercury thimble neutrino factory experiments carried out at the BNL AGS and CERN ISOLDE, and good agreement with experimental data was achieved [2] (see Figure 19). An accurate treatment of cavitation is critical for the quantitative description of the behavior of mercury under such extreme thermodynamic conditions.

This simple EOS model has a limited range of applicability. The isentropic approximation, which is defined by the length and time scales, and the value of thermal conductivity, does not apply for many bubbly flow regimes. The EOS does not include the drag, viscous, and surface tension forces, etc. To improve the EOS modeling, we have been developing a homogeneous full thermodynamics model for bubbly fluids using a Rayleigh-Plesset type equation [1] for the evolution of a scalar quantity representing the space distribution of an average gas bubble size. This approach will allow us to implicitly include the drag, surface tension, and viscous forces. To study the cavitation problem, we will also include a term accounting for the mass transfer due to the phase transition. To the best of our knowledge, the latter is an open problem in cavitation

studies. The EOS models will be implemented as software modules and used in the FronTier and ABAQUS codes. The two approaches described in this section are being used to study cavitation processes in mercury, and mitigation techniques capable of reducing the rarefaction wave strength and cavitation-induced erosion in high power mercury targets (see Sections 4.2.1 and 4.2.4).

Figure 19. Experimental data and numerical simulation of the evolution of the mercury splash due to the interaction with a proton beam (beam parameters: 24 GeV, $3.7 \cdot 10^{12}$ protons). Top: images of the mercury splash at 0.88 ms, 1.25 ms, and 7 ms. Bottom: numerical simulations using the FronTier code and analytical, isentropic, two-phase equation of state.

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4.3.6 Laser Ablation Plasma Plumes

Introduction

The interaction of laser light with solid targets and the properties of the laser-produced plasma have been investigated for many years [2]. Nevertheless, laser ablation of solid material is still a growing field in basic science, engineering, and material processing technologies. The experiments with the expansion of a laser-induced plasma plume into a non-reactive background gas offer an easy and versatile technique for the growth of high-quality thin films of a wide range of materials, including metals, semiconductors etc. Laser ablation also has applications in the production of carbon nanotubes. In addition to these applications, laser ablation plasma studies are very important for the modeling of various processes in space physics and plasma chemistry.

In the majority of cases, laser ablation occurs under a residual background pressure, when a pulsed laser with pulse length of tens of nanoseconds and energy of a few J/cm^2 ablates the target material.

The resulting plasma plume expands in vacuum or in background gas. Despite a number of experimental and theoretical works and applications of laser ablation processes, the laser-solid (film)-plasma interaction mechanism is not yet completely understood.

Laser ablation experiments. In a typical laser ablation experiment for nanoparticle production, a target (aluminum or silicon) in non-reactive background gas (argon) at a low or atmospheric pressure is ablated with a laser, creating a thin melted Knudsen layer and a rapidly expanding vapor plume (Figure 20).

Figure 20. Schematic of a laser ablation plasma experiment.

The vapor (plasma) ejected by laser radiation supercools because of its expansion and interaction with the cold ambient gas. The supercooled vapor condenses partially on the target surface and partially in the gas phase, in the form of nanosize particles. At high laser flux density or low ambient gas pressure, a supersonic vapor flow is formed where adiabatic expansion is the predominant cooling mechanism. At lower laser flux densities, a subsonic vapor jet is created where the heat conduction and diffusion mixing with the ambient gas are the predominant mixing mechanisms. The formation of nanoparticles and nanotubes depends on metal catalyst particles in the vapor.

Numerical simulations. Several approaches with different applicability ranges have been applied to the simulation of laser ablation experiments. In particular, the laser plume expansion has been studied using the particle-in-cell technique, continuum gas dynamics, and scattering models [3,4]. The continuum gas dynamics approach is suitable for modeling the plume expansion into background gas at pressures higher than hundreds of mTorr. Previous studies have employed high resolution TVD methods. These methods have numerical difficulties at early stages of the plume dynamics due to high pressure and density gradients. To avoid this problem, we have modeled the edge of the expanding laser plume as a sharp interface discontinuity using front tracking capabilities of our code FronTier.

We have been simulating numerically experiments by S. Harilal, M. Tillack et al. [1] which showed a very interesting qualitative change in the behavior of plasma plumes as the background gas pressure increases. Our numerical model includes the effect of the light absorption in the vapor plume and other physical phenomena. In the future, we will also improve the equation of state modeling. It will contain the ionization potential for weakly ionized plasmas obtained by solving

simultaneously the Saha equation for the ionization potential together with an equation of state. Our future goal is to demonstrate the controllability of the plume expansion dynamics by a magnetic field.

Figure 21. Numerical simulation of the expansion of a laser ablation plume into background gas.

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4.3.7 Numerical Simulation of Photonic Devices

Photonic structures have numerous applications: light emitting diodes, low loss optical devices with increased extracting capability (high Q, low volume and thin cavities, surface grating couplers), lasers, waveguides, low-loss waveguide bends, junctions, couplers and many more. Photonic crystals are a novel class of optical materials fabricated with at least two different dielectric permittivities in a periodic arrangement. They have the ability to suppress, enhance, or otherwise control the emission of light in a selected frequency range by altering the density of states. A complete photonic band gap (PBG), i.e., a range of frequencies for which light cannot propagate through the crystal in any direction, is a spectral region where the density of states in an infinite crystal vanishes.

We have developed a parallel, scalable, finite-difference time-domain (FDTD) [1] code capable of simulating various electrodynamics problems of interest, including photonic crystals. The code can handle complex geometry, realistic initial and boundary conditions, finite size effects including absorbing boundary conditions using the Perfectly Matched Layer (PML) [2], dispersive and nonlinear media, and surface waves. Our primary focus is on the simulation of realistic experimental structures, such as waveguides, laser cavities, and frequency doublers.

To validate the code, we calculated the TE modes for a two-dimensional, triangular-lattice photonic crystal [3]. The sample consisted of an array of circular gallium arsenide cylinders embedded in air

with a defect applied via the removal of the central rod. The structure was modeled in 3-D and placed in the FDTD computational domain that was surrounded by a PML. An oscillating electric dipole oriented perpendicular to the photonic crystal plane was introduced at the center of the defect. A frequency response curve was plotted to determine the resonant frequency and the distribution of the electric field radiated by the oscillating dipole after 200 cycles was visualized (Figure 22). The results compare very favorably to experimental results [4] and numerical results obtained using a different method [5].

Currently, we are applying our results on defect modes and localization effects to laser structures that are laterally confined by a photonic crystal and capped with Bragg reflectors longitudinally.

(a)

(b)

Figure 22. (a) The frequency response curve for a photonic crystal with $a=1.27$ cm and $R=0.48$ cm. (b) The spatial distribution of the electric field radiated by an oscillating dipole moment after 200 cycles.

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4.4 BIOLOGICAL AND ENVIRONMENTAL RESEARCH

See Table 6 for a list of projects.

Novel algorithms and hardware allow fine-scaled parallelism for structural biology. We project long simulated times (1-10 μ sec for all atom simulations). This result will allow exploration of new time scales in structural biology. We are emphasizing conformational changes in proteins with known structures, in collaboration with BNL biologists.

Brookhaven has strong experimental programs in atmospheric chemistry and brain physiology. Both programs are data intensive. The data challenge is not only data quantity, but especially data understanding. We have developed new tools for interactive visual and statistical data analysis. We are actively using these tools in diverse applications. See also Section 4.5.4.

TABLE 6. BIOLOGICAL AND ENVIRONMENTAL RESEARCH PROJECTS		
Project Title	Key Personnel	Comments
Molecular Dynamics on the QCDOC	J. Davenport, Y. Deng, J. Glimm, A. Shah	Molecular Dynamics on the QCDOC
Cancer Detection	W. Zhu, J. Kovach	Ovarian Cancer
Atmospheric Aerosols	W. Zhu, K. Mueller, D. Imre	Pattern Detection Software
Human Brain Function	W. Zhu, N. Volkow, J. Fowler	Spatial Correlations in Brain PET, MRI Data
Cardiac Electrophysiology	S. Evans, F. Fenton, J. Glimm, H. Hastings, W. Oh	Fibrillation, Sudden Cardiac Death

4.4.1 Molecular Dynamics on the QCDOC

Molecular dynamics simulations [1, 2] are ideal for massively parallel computing because the time spent on communication can be a small fraction of the time spent on computation. However, most molecular dynamics (MD) simulations have been performed on machines where this potential has not been realized because of slow communication limiting the effective use of large numbers of processors.

We have explored [3,4] the use of a new machine designed for quantum chromodynamics (QCD) by a team of elementary particle physicists [5] mainly at Columbia University, The Riken BNL Research Center and IBM. This machine consists of approximately 10,000 IBM PowerPC processors with extremely fast nearest neighbor communication and 4 megabytes of memory located on the same chip. For this reason, it has been named QCDOC for quantum chromodynamics on a chip. It is expected to achieve of order 5 teraflops (or 5×10^{12} floating point operations per second) at a cost of roughly \$500 per processor.

We project a dramatic level of fine scale parallelism for molecular dynamics simulations based on novel architectural and algorithmic principles, for this machine and its successor, Blue Gene / Light.

The architectural principle is the 6D mesh communication topology, supported by 24 wires per processor (bidirectional send/receive for each mesh dimension). This mesh can be thought of as a

programmable distributed switch, and at the level of 10K processors or more, it vastly outperforms technologically feasible switches in terms of effective bandwidth and latency.

The algorithmic principle is fine-scaled parallelism enabled by the rapid communication, i.e. small problem sizes per processor. We plan to compute entirely within L2 cache, and completely avoid the bottleneck of communication delays to main memory. With fine-scaled parallelism, we assign about 10 particles per processor.

We project an ability to simulate 1-10 μ sec of real time for all atom MD simulations of 10K to 100K atoms using this machine. We have developed algorithmic and hardware performance models to support this prediction.

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4.4.2 Detection of Early Stage Ovarian Cancer

Diagnosis of cancer and other ailments from a drop of blood in your doctor's office? With no invasive or surgical testing? A recent breakthrough has moved this dream closer to reality. Professor Wei Zhu, CDIC staff member and member of the Department of Applied Mathematics and Statistics, John Kovach, MD, Director of the Long Island Cancer Center and a team of graduate students studied detection of ovarian cancer [1]. At an early stage, ovarian cancer has a high (90%) cure rate, but cannot be readily detected. At late stages, when detection usually occurs, the cure rate is 35%. Annually, 14,500 women die from this disease in the U.S.

The breakthrough in early stage ovarian cancer detection allowed a 100% specific diagnosis (no false positives; no false negatives) in test samples. The idea has two steps, and builds on earlier work of Petricoin et al., reported in *Lancet* [2]. The hardware, or physical measurement step, is by a mass spectrometer. This machine looks at blood fractions and trace proteins, and records mass (in relation to charge). Of course there are many hundreds of thousands of these signals ("markers"). The second step, addressed by Zhu and Kovach, is to find the needle in the haystack. Which markers distinguish a normal patient from one with ovarian cancer? This is a problem in statistics and its solution enables the diagnostic procedure.

The statistical problem is solved using diagnostic data, that is, blood samples from patients with known diagnosis, having ovarian cancer or normal. The data is divided in half, one half to train the statistics and the other half to test the conclusions. All markers are assessed for their ability to

distinguish between normal and afflicted patients in the training set. About 150 markers show a statistically unusual pattern of difference between these populations. This number depends on the resolution power of the mass spectrum equipment. Selection of six or so of the markers from the 150 identified defines the test. A subject with a positive reading on these six markers is diagnosed with ovarian cancer. When the test is applied to the testing set, 100% accuracy results.

Where does this breakthrough lead? The immediate answer, if confirmed in further testing, is to eliminate most of the 14,500 annual US deaths from ovarian cancer. But the methods are not specific to this disease. Many disease conditions will be signaled by trace proteins in the blood. It is not hard to imagine a revolution in medical diagnosis resulting from extensions of this discovery.

The trail leads further. Mass spectrum machines can preserve specified marker samples, and on further analysis, fractionate them, leading to identification of the proteins and genes active in (for example) ovarian cancer. The metabolic understanding of cancer will benefit greatly from such studies. Moreover, some distinguishing markers are under expressed in the cancer patients. These represent proteins missing in the cancer patients. Some might be involved in the body's defense against cancer. A short list of candidate cancer defense proteins will also be a far-reaching medical advance.

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4.4.3 Atmospheric Aerosols

The purpose of this project is to develop data processing tools for the classification and time series analysis of atmospheric aerosol particles. Atmospheric aerosols play an important role in both climate and public health. Current research is focused on determining the chemical composition of aerosols, and thus the composition of air and its evolution over time. Massive mass spectra data, on the scale of terabytes per week, have been collected continuously over time by researchers in the Atmospheric Sciences Division at Brookhaven, using their cutting-edge, field deployable high precision mass spectrometer. The first task is to determine the chemical composition of each aerosol based on its mass spectrum. To achieve this, we classify aerosols by their chemical compositions and thus determine the air composition at each time point. Finally, we study the time series evolution of atmospheric compositions identifying normal as well as abnormal patterns in real time.

To convey the analysis results to the scientists in an intuitive way and to incorporate their expert knowledge into the data analysis phase, an interactive graphical user interface utilizing modern scientific visualization techniques becomes a necessity. Large-scale BNL data collections have reached sizes for which straightforward visualization techniques are starting to fail. In this spirit, our proposed approach couples a powerful Bayesian classification and multivariate time series analysis engine with an intuitive and responsive graphical user interface to fine-tune the underlying models. We call this application *SpectrumMiner*, a significant component of a more general visual

data mining framework and application, called ViStA, which we are currently developing at BNL (for more detail see Section 4.5.4).

The statistics engine. We first classify aerosols based on their mass spectra through an iteration of expert-machine interaction using a Bayesian classifier. The Bayesian classifier can incorporate not only explicit classification rules but also prior knowledge in terms of a partial training data set. We have also been implementing automatic procedures to elucidate the structure of the compounds. To study the evolution of aerosols and the changes in atmospheric composition versus time, both the univariate and the multivariate time series analyses are employed to unravel trends and patterns.

The traditional statistical classifier would take only explicit classification rules. Machine learning techniques such as the neural network would take only a training set. However, the semi-supervised clustering approach we are taking requires the classifier to learn from both the explicit rules and the implicit rules embedded in a partial training set established by the experts as they survey the current clustering results and make adjustments to the clusters. For this we have implemented an interactive Bayesian classification framework that could absorb the up-to-date prior information in both the explicit and implicit formats, and produce the updated posterior classification results.

For efficient classification and automatic structure elucidation, we have been constructing a molecule library where the signature profile and class membership of each molecule is established. The molecules are classified along a natural chemical classification tree with two categories--organic and inorganic--at the initial node. Subsequently, the organics are further divided into classes of carboxylic acids, aldehydes, ketones, alkenes, alkanes, aromatics, etc. We begin with the spectra of known molecules (NIST library or lab-generated).

Visualization. The statistical analysis engine is combined with a highly visual interface to facilitate interactive exploration, mining, classification and survey of these large, high-dimensional data collections. In order to empower scientists to control and fine-tune the mining and classification process in an intuitive and interactive way, SpectrumMiner’s hierarchical classification algorithm is user-steerable via a novel multi-modal visual interface. An important component of this interface is the *interactive dendrogram* [1], where hierarchy nodes are placed on concentric circles whose radii are determined by the dissimilarity of the node’s sub-tree. We chose a circular layout of the dendrogram since it makes better use of space than its linear counterpart. It inherently dedicates less drawing space to the higher-level, less numerous nodes, and distributes more space to the many leaf nodes along the circumference of the circle. See Figure 23, where we show a screen capture of SpectrumMiner, with the interactive dendrogram located on the bottom right. Edges are colored using a rainbow colormap to indicate the number of data items they carry. To the left of the dendrogram is the node viewer. Selecting a particular node will display the average spectrum of all data items classified into the node (window with white background), as well as the node’s data composition (window with blue background just below). We are currently incorporating the classification steering capabilities into our system. By inspecting the present classification in the node viewer and the dendrogram, scientists may decide that some particles, or the entire node, have been misclassified. To correct this error, they then simply drag the concerned particles or node into the proper location within the hierarchy, which subsequently triggers a refinement of the classification rules.

Figure 23. SpectrumMiner's interactive dendrogram interface.

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4.4.4 Analysis and Visualization of Human Brain Function

A major goal of statistical analysis in brain research is to extract from a vast amount of brain image data (PET and fMRI) the essential features that characterize brain functions. We are developing two novel approaches for such analysis [3, 4, 6, 7]: (1) Correlational and Path Analysis to uncover brain functional networks, and (2) coefficient of variation (CV) -- a measure of brain regional variability or heterogeneity. These analyses are being implemented in BrainMiner, an interactive brain functional analysis and visualization tool [1-7].

Correlational and path analysis. The correlations in brain activity are calculated on the basis of predefined anatomical regions-of-interest (ROIs). The correlation coefficient is then employed to quantify similarity in response, for various regions during an experimental setting. To account for anatomical variability, each test subject's volumetric brain data is first transformed into a common

anatomical coordinate system (the Talairach-Tournoux space). Statistical analyses of brain functional relationships include:

1. The correlational analyses, including the Pearson product-moment correlations, the partial correlations and the canonical correlations.
2. Cluster analysis.
3. Principal component analysis (PCA) and the factor analysis (FA).
4. Path analysis (Figure 24) and time series analysis.

Figure 24. Path analysis of the visual attention pathway based on fMR data. The initial path model with 16 paths (solid arrows) and the fitted model with 3 added paths (dotted arrows) and 2 latent variables (K and L). Significant pathways are labeled in red (positive path coefficients) and blue (negative path coefficients). The table lists the 95% Confidence Intervals (CI) for the estimated path coefficients in the 3-ball tracking paradigm. Again, significant path coefficients are labeled in red (positive) and blue (negative).

Measuring brain functional variability. It is well known that the two most essential statistics are mean and variance. In ROI-based brain functional studies, the analysis of the regional mean is a fully developed practice; however, the same is not true for the variability. We have developed the analysis for brain functional homogeneity/heterogeneity based on the coefficient of variation (CV). The CV is the ratio of the standard deviation to the mean. It is a measure of regional variability independent of the underlying measurement unit. We have applied such analysis to the comparison of brains affected by Alzheimer's disease (AD) with normal brains [1]. Our results indicate that such analysis is providing new insight into disease etiology and additional information on diagnosis.

The amount of statistical data can be enormous, and effective tools are essential if the brain researcher is to grasp and discover functional relationships quickly from the statistical data. For this purpose, the statistical routines of BrainMiner are paired with a powerful visualization tool that facilitates this task [1-2]. This visualization tool, as well as the statistical routines, is also part of

the ViStA visual data mining application that we are currently developing at BNL. More detail on ViStA is provided in Section 4.5.4.

Results. We are continuing our effort towards the discovery of brain functional networks. Intriguing results on brain functional homogeneity/heterogeneity have already been obtained. In analyzing the PET images of 35 subjects with AD and 35 age and gender matched healthy controls, we found that AD subjects showed a significantly larger CV for the whole cortex but had a significantly greater number of regions with increased homogeneity (decreased CV) than the controls. At the regional level the reductions in CV in the AD subjects were associated with reductions in metabolism that were most accentuated in the parieto-temporal cortex, except for the precuneus, which had a marked reduction in metabolism but increased CV. Discriminant analyses showed that the combination of variables that best discriminated between AD and controls were metabolism and CV in left parietal, CV in right precuneus and global CV (94% sensitivity and 100% specificity) [3]. BrainMiner allows many types of interactive explorations of brain functional image data. It is currently used by a number of brain researchers and is being refined continuously.

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4.4.5 Cardiac Electrophysiology

Sudden cardiac failure is a major cause of death. The causes and conditions leading to sudden cardiac death are complex and varied, and have been the subject of extensive studies. In collaboration with researchers from Hofstra University and Beth Israel Medical Center, we have been studying the dynamics of ventricular fibrillation, an irregular and chaotic heart rhythm that almost always results in sudden cardiac death.

We have been modeling cardiac electrophysiology through computer simulation. For this purpose it is common to use the monodomain equation that limits the electrical activity within cells. In reality, the ion-mediated current travels into and out of cells, requiring a bidomain model to more accurately simulate complex cardiac electrophysiology, using the equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{1}{\chi C_m} \nabla \cdot \sigma_e \nabla u_e + \frac{f(u)}{R_m C_m} \\ \nabla \cdot \sigma_i \nabla u + \nabla \cdot (\sigma_i + \sigma_e) \nabla u_e &= 0 \end{aligned} \quad (1)$$

Here u_i and u_e are the intra and extra cellular potentials and $u = u_i - u_e$ is the transmembrane potential, F_i and F_e are conductivity tensors, and C_m , R_m , and χ are the membrane capacitance, membrane resistance and surface-to-volume ratio. The reaction term $f(u)$ represents the ionic current.

We developed a code to solve the bidomain equations. With this code, we will be able to study the onset and the dynamics of ventricular fibrillation.

In Figure 25, we present a 2D simulation using the bidomain code. The transmembrane potential is plotted at 50 msec intervals. An initial stimulus in the first frame at the center of the domain has propagated radially. Since we used anisotropic conductance, the wave propagates with different speeds in the x and y directions. At $t=194$ msec (before the fourth frame), we stimulated the center again and observed spiral waves.

Figure 25. Successive time frames showing the propagation of the transmembrane potential and development of spiral waves, based on the bidomain equation.

The simulations will be validated by comparison with experimental data, and the code will be used in a large-scale study of wave stability and scroll wave dynamics in realistic 3D anatomy. Large-scale simulations will provide critical insights into basic cardiac physics and dynamics. Moreover, the use of these models will allow experiments that cannot be performed with animal models because variability among individuals within a species makes it difficult to isolate causal factors.

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4.5 ADVANCED SCIENTIFIC COMPUTING

See Table 7 for a list of projects.

TABLE 7. CDIC ADVANCED SCIENTIFIC COMPUTING PROJECTS		
Project Title	Key Personnel	Comments
TSTT: Atomization and Spray	J. Glimm, M.N. Kim, A. Marchese, C. Tzanos, R. Samulyak, X. Li	Diesel Engine Design
TSTT : Frontier-Lite	X. Li, Z. Xu	Tech Transfer
Magnetohydrodynamics of Multifluid Systems	R. Samulyak, W. Oh, J. Glimm, J. Davenport	Multiple Applications
ViStA: Visual Statistical Analyzer	K. Mueller, W. Zhu	Clustering, Spatial Correlations, Pattern Detection
Uncertainty Quantification	J. Glimm	Decision Making
Visualization	K. Mueller, A. Peskin, M. McGuigan	Viz Theater
Cluster Computing	N. D'Imperio, E. McFadden	Cost Effective

4.5.1 TSTT: Atomization and Spray

Jet Breakup and Spray Formation in a Diesel Engine

The design of a fuel efficient, nonpolluting diesel engine is the subject of intensive international research efforts. The breakup of the injected jet of diesel fuel into spray is of key interest to such investigations because much of the pollution comes from unburned fuel deposited on the walls of the engine chamber, and because control of the spray droplet size can mitigate this effect. Spray formation is sensitive to many details of the injection system design, including the driving pressure in the nozzle, the nozzle shape, and the flow turbulence and phase transitions in the nozzle.

For the above reasons, a simulation study of the breakup of the diesel jet into spray is of considerable interest. Factors complicating such a study include:

1. the stiff equation of state (EOS) for the liquid diesel fuel;
2. presence of shock waves or near shock waves and phase transitions in the flow field;
3. the multiscale nature of the flow field, especially regarding turbulence in the nozzle and the multiscale breakup of the jet into droplets and spray; and

4. sharp boundaries for the liquid diesel fuel – ambient chamber gas interface for the duration of the breakup period.

We report preliminary progress on the numerical modeling of the jet breakup, based on the front tracking code FronTier. The work has been carried out by a team from BNL, ANL, and Stony Brook University. We modeled the diesel fuel as isentropic, with an analytic EOS. The EOS is given by a gamma law gas in the vapor region, by a stiffened gamma law gas in the liquid region, and by the homogeneous equilibrium model [5] along an isentrope in the mixed region (where vapor and liquid co-exist). P vs. V is graphed in Fig. 26.

Figure 26. P vs. V isentrope for diesel fuel.

Figure 27. Geometry of injection reservoir and nozzle leading to combustion chamber.

Figure 27 displays a detail in the experimental setup at ANL [1]. A finite pulse of diesel fuel is injected at a pressure of 500 bar into a chamber of SF₆ (a heavy, inert gas chosen to simulate the compressed air in a diesel engine).

Using synchrotron x-ray imaging, ANL scientists have measured the mass on line segments passing through the jet in both axial and radial directions. From this data they also note the velocities of the tip and the tail of the fuel jet as it enters the combustion chamber [1, 2, 3, 4]. We have installed into our code diagnostics to record similar data in our simulations.

Figure 28 shows the density of the diesel fuel in preliminary simulation studies of the jet breakup [6]. As expected, the simulation shows the fuel cavitation at the nozzle inlet and continued phase transitions throughout the body of the jet.

Figure 28. Top: AMR grids used in simulation. Bottom: Density of diesel fuel as computed by *FronTier*.

Figure 29. Tip velocity and experiment.

Our present agreement with experiment is semi-quantitative. Some parameters not measured experimentally but important for simulation have been discovered. Parameter and mesh refinement studies are planned for future efforts. Our studies will include the following four aspects:

1. the initial pressure build-up of the fuel container (wave reflections and transmissions);
2. the response of the jet velocity to the applied pressure in the fuel container;
3. cavitation, one factor in formation of the spray;
4. entrainment, another factor for the formation of the spray.

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4.5.2 TSTT: Frontier-Lite

The Front tracking code FronTier has achieved, in several cases, the first, and in some cases the only simulations to show agreement with laboratory experiment for acceleration-driven fluid mixing flows [1].

In Figure 30 we compare tracked and untracked mixing rates. We compare using original scales. In the left frame, we observe the factor of two difference in the mixing rates, attributed to numerical mass diffusion effects in the TVD simulation. In the right frame, we compensate for the observed numerical mass diffusion, and obtain approximate agreement for 3D Rayleigh-Taylor mixing.

We have given a simple theoretical calculation based on the renormalization group and self similar scaling [2], which also gives mixing growth rates in agreement with experiment. Thereby we achieve agreement of experiment, theory, and *all* simulations, suitable reinterpreted.

There is a growing interest in the transfer of the Front Tracking technology to other codes. We have merged FronTier with the AMR code Overture from LLNL. In Figure 31 we show the AMR refined patches and the tracked interface separating two fluids in distinct colors, for this combined code.

Figure 30. Left: The mixing penetration of the light fluid into the ambient heavy fluid is plotted versus the acceleration light scale Agt^2 . Right: We used observed numerical mass diffusion to define a renormalized Atwood number $A(s)$ and an acceleration length scale $2\int A(s)ds$.

Figure 31. A spherical implosion studied with the Front Tracking/AMR code.

We are exploring the possibility of merging FronTier with the LANL code SAGE.

To respond to the growing interest in the use of FronTier, we are developing a simplified version of the Front Tracking software, called FronTier-Lite, in the form of libraries which can be linked to other codes, and provide front tracking enhancements to them. We will combine FronTier-Lite with PNNL codes to model the dynamics of cells for biological studies.

We have also improved the basic tracking algorithm. In a still experimental development [3, 4, 5], we have developed a new tracking algorithm, based on the tracking of an interface in both space and time. This method simplifies the differencing associated with tracking and transfers most of

the difficulty to the computational geometry of a description of the moving interface. The result is now fully conservative, even at the tracked front, and it gains one order of accuracy in its rate of convergence. For these two reasons, the new algorithm is a very promising development.

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4.5.3 Magnetohydrodynamics of Multifluid Systems

Introduction. The purpose of this project is to study numerically fundamental and applied problems of free surface magnetohydrodynamic (MHD) flows. Using our recently developed methods and software tools, we have been studying hydro and MHD processes in the target for the Muon Collider/Neutrino Factory, liquid metal flows in magnetic confinement fusion devices, and laser ablation plasmas. Our primary goal is to improve through mathematical modeling and numerical simulations the understanding of MHD processes, and the design of experiments and devices critical for targeted applications.

Development of models, algorithms, and computational software. Numerical simulation of free surface magnetohydrodynamic (MHD) flows is a challenging problem that requires effective methods for solving coupled hyperbolic and elliptic (or parabolic) systems of equations in complex and moving geometries. The method of front tracking for resolving discontinuities and their topological changes in hyperbolic systems has been implemented in the FronTier code. We have recently developed the corresponding methods for elliptic systems based on finite element discretization on grids dynamically conforming to the moving interface. Scalable parallelism uses direct methods to solve the elliptic or parabolic term on each processor and an iterative technique for ensuring matching conditions across processor domain boundaries. We have also been developing an elliptic solver for FronTier-MHD based on the embedded boundary methods, which is expected to be advantageous for highly complex interfaces. The development of these numerical tools is combined with modeling of the equation of state for cavitating and bubbly fluids since the simulation of fluids under extreme thermodynamic conditions is needed for most of the targeted applications. See Section 4.3.5 for more details.

Our numerical simulations of MHD processes in liquid metals have used approximations typical for the low magnetic Reynolds number flows. We have also been developing methods and software components for free surface highly conducting materials (plasmas) with high magnetic

Reynolds number. The FronTier-MHD code has been used to study several fundamental and applied problems described below.

Figure 32. Numerical simulation of shock waves in plasmas. Comparison of the wave propagation in non-conducting gas (left) and in plasma (right).

Targets for advanced accelerators. The design of liquid mercury targets able to generate high-flux beams is among the most important problems of the design of advanced accelerators such as the Muon Collider / Neutrino Factory, and the Spallation Neutron Source. Large-scale numerical simulations of hydro and MHD processes in mercury are critical for improving the target design and reducing the number of costly experiments. The Muon Collider target has been proposed as a pulsed jet of mercury interacting with strong proton beams in a 20 Tesla magnetic field. Using the FronTier-MHD code, we have been studying the Richtmyer-Meshkov instability in the mercury jet in the presence of cavitation and the influence of the magnetic field on the surface instability and cavitation (see Sections 4.2.1 for details).

Plasma facing components. Liquid metals can be used as plasma facing components in magnetic confinement fusion devices. We have been studying numerically the behavior of liquid lithium and mercury jets in transverse and longitudinal magnetic fields. Such lithium jets will be used in the divertor region of the new National Spherical Torus Experiment at the Princeton Plasma Physics Laboratory.

Figure 33. a) Liquid lithium jets in the tokamak divertor. b) Aspect ratio of a liquid metal jet in a transverse field as a function of the longitudinal coordinate.

Laser ablation plasma plumes. Plasma plumes created by pulsed intensive laser beams can be used in a variety of technological processes, including the growth of carbon nanotubes and high-temperature superconducting thin films. We have performed numerical simulations of the plasma plume evolution (see Section 4.3.6). Our future goal is to demonstrate the controllability of the plasma plume evolution by means of magnetic fields.

Future plans. We will continue the development of models, numerical methods, and software components, and numerical simulations of complex regimes of free surface magnetohydrodynamic flows. Our primary goal is to improve through mathematical modeling and numerical simulations the understanding of MHD processes in fluids and plasmas, and to optimize the design of experiments and devices critical for targeted applications.

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4.5.4 ViStA: Visual Statistical Analyzer

It is well known that once the data become too large in size and/or dimensionality, automated data mining approaches begin to fail. To address these shortcomings, our current efforts target a classify-refine mechanism that inserts the scientist into a tight loop in the data mining process. Interaction with the system is very natural and intuitive, since the user may reorganize, restructure, or fine-tune certain components of the model or portions of the data directly within the visual display. The changes in the data organization or model are promptly recognized by the statistics engine, which then performs the necessary parameter adjustment/tuning to reflect the changes made by the user. Subsequently, a new data organization or model is computed and presented visually to the user, who may then opt to begin a new iteration cycle. Both our SpectrumMiner (Sections 4.4.3) and our BrainMiner applications (Section 4.4.4) use this paradigm with great success. Future work will also use this paradigm in our proteomics analysis (Section 4.4.2). In essence, ViStA is the general framework within which all of the different mining tools are unified. In the following we shall give a few examples of the visual tools that are currently available.

Viewing in the native domain. We have developed a 3D visualization interface that displays correlational data in the native domain. This tool is currently mostly used within the BrainMiner project, where the data and the functional relationships implied by the data are displayed within the brain anatomy. The correlation matrix is a 6-D object and a workable tool for its visualization is a challenge. With user selection of a single row or column, the problem reduces to three-dimensional visualization. For the brain function correlation matrix, these data are presented, along with an MRI volume and a digitized version of the Talairach brain atlas. Both can be sliced in three orthogonal directions and can be overlaid on each other. A basic view with a few regions of interest (ROIs) is shown in Figure 34, which shows the Graphical User Interface (GUI) of our newly developed 3D brain visualization software, along with a basic view of a small number of ROIs embedded into a cut-out area of a normalized/standardized MRI brain. Similar to the 2D viewer, the colors of the ROIs denote the strength of the correlational relationship, on a rainbow scale. The root ROI is colored in yellow. The GUI allows the user to slide the cutting planes up and down and back and forth, to rotate the volume, and to select certain brain surfaces, such as

white matter, gray matter, and skull, to be semi-transparently superimposed. The correlation thresholds can also be selected, and many more features are available. The number of ROIs to be displayed, however, can become quite large (about 120-140), which poses challenging problems in the visualization task: in a space too crowded with statistically significant ROIs it becomes very hard, if not impossible, for the user to tell the 3D positions of the individual ROIs. To overcome these difficulties, a number of techniques [1-2] were devised, some of which are illustrated and described in Figure 34.

Viewing in an abstracted feature domain. An alternative way to view and edit causal and hierarchical relationships is in a complementary abstracted feature-centric display. We illustrated this type of display in Section 4.4.3 by way of our SpectrumMiner domain application, but similar strategies will also be available to edit causal models for our BrainMiner domain applications. A particular challenge is imposed by time-varying data. Our interactive dendrogram viewer provides the following two mechanisms to cope with this kind of data: (i) the 4D time-slice selector and (ii) the 3D ThemeRiver. We shall describe these two displays in turn.

Figure 34. (*Left*) The present 3D visual interface of BrainMiner, along with a basic view of a small number of ROIs embedded into a cut-out area of a normalized/standardized MRI brain. The colors of the ROIs denote the strength of the correlational relationship, on a rainbow scale. The root ROI is colored in yellow. A legend is shown on the left to illustrate the color mapping. The two pointers in the legend can be used to select the range of statistical significance. Only ROIs within that range are displayed. The GUI also allows the user to slide the cutting planes up and down and back and forth, to rotate the volume, and to select certain brain surfaces, such as white matter, grey matter, and skull, to be semi-transparently superimposed. The correlation thresholds can be selected by moving the pointers in the color bar in the upper left corner of the display. When the sliders are moved, the application adjusts the color range such that the entire range of rainbow colors is always utilized. Two studies (baseline and drug) can be loaded simultaneously. The display can then be switched between three correlation matrices: those of the two loaded studies as well as the difference correlation matrix. The latter display shows the ROIs that have changed, under the influence of the drug, their statistical relationship with respect to the selected root ROI; (*center column top:*) superimposing a Talairach atlas slice (or an MRI slice) that can be slid up and down the volume; (*right column top:*) enhancing the ROIs by colored halos or coasters, where the colors code their height and depth on a rainbow color scheme, to aid the perception of 3D depth relations; (*center column bottom:*) near cortex ROI-correlations projected onto the cortex surface; (*right column bottom:*) depth cues provided drop lines.

The 4D time-slice selector. The interactive dendrogram represents time-varying data as a cylindrical shape composed of a stack of circular time-slice dendrograms. The time-slice selector shown above the dendrogram in Figure 35 shows the unwrapped outer surface of this cylinder, with each horizontal slice capturing the leaf nodes of one time-slice dendrogram. Patterns in the data distribution over time are clearly visible. Stepping across the time slices will animate the data-related coloring of the dendrogram’s arcs.

The 3D ThemeRiver. To show the fluctuations of different variables (i.e., nodes in the time-varying dendrogram) over time, we use the ThemeRiver paradigm [3] that visually illustrates multiple variables as parallel streams in which the width of the stream maps to node magnitude. A limitation of the existing ThemeRiver scheme is that only one attribute can be displayed per theme. We therefore have devised a 3D extension, which enables us to display two attributes of each variable in the data stream. The new 3D ThemeRiver [4] can display any ternary relationships within the data, and not just as a function of time. The surface itself is modeled as a smooth 3D Bezier mesh, where constraints have been added to prevent overshoot at extreme points of the dependent variables. Users can draw any free-hand curve into the dendrogram, which maps the nodes above the intersected edges as streams into the 3D ThemeRiver window (see Figure 35).

Figure 35. Left: The dendrogram with a user-drawn closed freeform line specifying the time axis-centric surface to be visualized with 3D ThemeRiver. Right: A 3D ThemeRiver visualization of 17 clusters of organic aerosols. Width encodes overall cluster distribution and the height encodes incidence of zinc. The horizontal axis represents the increasing concentrations of ozone in the atmosphere.

Focussed viewing while preserving visual context. In the dendrogram, a number of features are available to enable focus with context, including collapsible sub-trees and node coalescing, search by label and feature, node-content browsers, and non-linear rubber-sheet distortion using an interactive, graphics-hardware-accelerated technique (see Figure 36) [4].

Figure 36. Rubbersheet zooming. Left: unwarped dendrogram; Right: a user-specified arc segment (shown as a black-framed area) is angularly expanded and radially shrunk. Notice the radial distortion of the dendrogram's polar rings.

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4.5.5 Uncertainty Quantification

Quantification of Uncertainty and Computer Assisted Decision Making

The need for computer assisted decision making is driven by two related factors. The first is the importance of complex scientific/technical decisions, such as those related to global warming, for which controlled experiments are not feasible. The second is the need for rapid or timely decisions,

using incomplete information, such as in shortening the time to market duration of a product design cycle, mandating a reduction of the role of the human in the loop.

A key issue, and the central one considered here, is an accurate assessment of errors in numerical simulations [1,2]. Errors are assessed statistically, based on a formula

$$\text{error} = \text{exact solution} - \text{approximate solution}$$

The essential difficulty is that an "exact" or sufficiently improved solution requires more resources, as does the ensemble needed to characterize the error statistically. Similarly, the dependence of the error statistics on the problem parameters adds to the resource requirements.

Fortunately, we have developed several approaches to mitigate this UQ-explosion of resource requirements.

We have shown that linear models may be sufficient to describe errors even for deeply nonlinear problems [4]. We have shown that complex problems can be decomposed, and models for the total error can be expressed as a composition of error models for each of the components [5].

We have shown that the dependence of errors on parameters can be expressed in linear regression models [2] and that total prediction errors can be attributed quantitatively to prediction errors ascribed to various sources (data insufficiency, inverse problem error, forward simulation error, ...) [5]. Dependence of the solution error on the numerical algorithm is studied in [3].

In general, we have used simple Gaussian models to express solution error, characterized by the mean and covariance. Because the solution is a field quantity (depending on time, space variables) this error is a field quantity also. With limited data on the solution error, it is desirable to reduce the dimension of the error mean and covariance. The reduction is problem dependent, but an interesting outgrowth, in our shock physics applications, has been a wave filter post processing algorithm to identify, locate, and label shock and contact waves in a shock wave interaction problem [4].

We have also used these tools to compare different algorithms. For example, we find that use of Front Tracking reduces the error in a simple spherical implosion or explosion problem by an amount equal to mesh refinement to a factor of 4 to 8 per linear dimension [3].

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4.5.6 Visualization

Klaus Mueller, a faculty member of the Stony Brook University Visualization Laboratory, is developing efficient volume rendering algorithms for interactive visualization of large datasets occurring in science, medicine, engineering, and entertainment (<http://www.cs.sunysb.edu/~mueller>).

One current area of interest is point-based volume and surface rendering. Here, we are seeking to exploit state-of-the-art commodity graphics hardware, in conjunction with rendering optimizations, such as smart volume encoding and occlusion culling, to render large 3D and 4D datasets at high quality and speed. 4D datasets, such as time-varying datasets, usually come on 4D Cartesian Cubic (CC) grids. In recent research, we explore the use of 4D Body Centered Cubic (BCC) grids to provide a more efficient sampling lattice. We use this lattice in conjunction with a point-based renderer that further reduces the data into an RLE-encoded list of relevant points. We achieve compression ranging from 50-80% in our experiments. Our 4D visualization approach follows the hyperslice paradigm: the user first specifies a 4D slice to extract a 3D volume, which is then viewed using a regular point-based full volume renderer. The slicing of a 4D BCC volume yields a 3D BCC volume, which theoretically has 70% of the datapoints of an equivalent CC volume. We reach compressions close to this in practice. The visual quality of the rendered BCC volume is virtually identical with that obtained from the equivalent CC volume, at 70-80% of the CC grid rendering time. The images below show a 4D turbulent jet dataset, hyper-sliced along various axes and volume rendered in 3D.

In another line of research on point-based representations, we explore methods for converting an image or volume sampled on a regular grid into an irregular point hierarchy. The conversion process retains the original frequency characteristics of the dataset while providing a reduced number of points. First, we determine the local frequency characteristics of the source dataset at different scales. Then, we analyze this scale-space representation of the object to construct a hierarchy of points of different extents and coefficients. Finally, this hierarchy is traversed during image synthesis to identify the reduced set of points that still can represent local object detail, or satisfy some user-controlled threshold. Using an implementation of our approach, we were able to obtain a point reduction of up to an order of magnitude for images and up to one fourth for volumes. We have found that the images reconstructed even from a greatly reduced point set still maintain a high level of quality. The fundamental approach is particularly attractive for splat-based volume renderers, as their rendering complexity is directly related to the number of points in the dataset. To prove the concept, we have modified an existing splatting algorithm to render variable-sized points, and we were able to generate high-quality renderings, even for greatly reduced point sets.

Figure 37. 4D turbulent jet dataset. Top left : 4D CC grid ; bottom left : 4D BCC grid; top right: hyperslice at $z=62$; bottom right: hyperslice at $x=35$.

Figure 38. Left: A time instance of a time-varying jet shockwave dataset rendered with points; Right: A time instance of a turbulent flow dataset rendered with point-primitives.

4.5.7 Cluster Computing

Linux clusters have become important providers of computing cycles in the scientific world. (<http://www.ccd.bnl.gov/bcf/cluster/>). The CDIC cluster, named Galaxy, consists of 256 Intel P3 and P4 processors running at speeds up to 2.4 GHz. Arranged in dual processor nodes, most have 1 Gbyte of memory per node. A RAID storage facility with 1.4 terabytes of disk is attached to this machine. Parallel computations are performed using the message passing interface, MPI (www-unix.mcs.anl.gov/mpi) and through threads using Open MP.

Our goal is to continue to explore the frontier of the commodity component world, as processor, motherboard bus, and memory speeds increase, as fiber cable decreases in price, and as switch speeds increase in performance and decrease in price. We will determine optimal configurations and architectures, within the overall framework of our design. Results from this research will be published and posted on the network, to benefit others seeking a similar price/performance advantage.

The Galaxy computer provides computing cycles to CDIC affiliates and projects. Convenient and assured access to local parallel computing is an essential requirement for the development of parallel simulation codes, and it is thus a key component of the CDIC strategy to make state-of-the-art computing technology available to benefit BNL scientific programs.