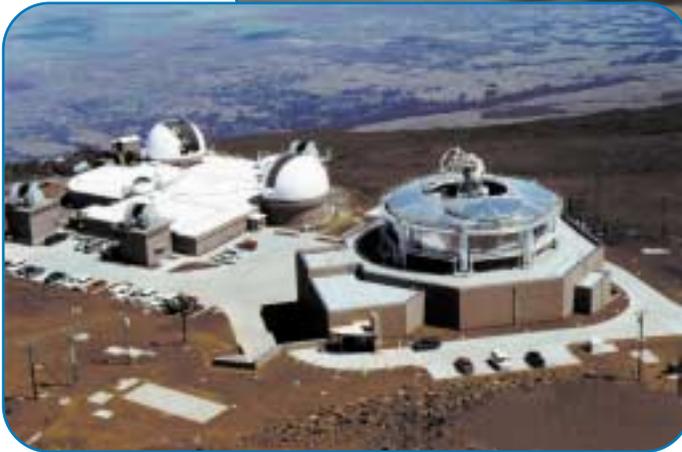




APPLICATION BRIEFS 2001



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MAUI HIGH PERFORMANCE
COMPUTING CENTER

550 Lipoa Parkway, Kihei, Maui, HI 96753
(808) 879-5077 • Fax: (808) 879-5018
E-mail: info@mhpc.edu
URL: www.mhpc.edu

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WE L C O M E

This is the seventh annual edition of Maui High Performance Computing Center's (MHPCC) *Application Briefs*—which highlights some of the successes our customers have achieved this year.

MHPCC is a national supercomputing Center established in September 1993 and is an Air Force Research Laboratory Center managed by the University of Hawaii. A leader in scalable parallel computing technologies, MHPCC is primarily chartered to support the Department of Defense (DoD), and other government organizations.

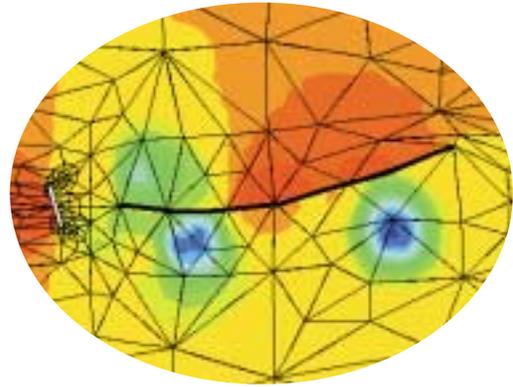
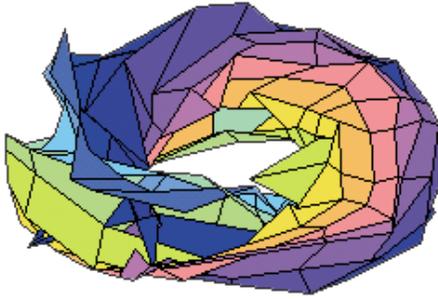
MHPCC offers an innovative environment for High Performance Computing (HPC) applications. This includes:

- **Computational Resources:** A stable and secure parallel computing platform for prototyping, benchmarking, and testing applications. MHPCC is ranked as one of the top computing Centers in the world in terms of computational capabilities.
- **Performance Storage:** MHPCC users have access to more than eight terabytes (TB) of disk storage and nearly twenty four TB of on-line tape storage.
- **High-Speed Communications Infrastructure:** OC3 connections, offering 155 megabit per second (Mbps) capacity, provide direct access to MHPCC resources—over the Defense Research and Engineering Network (DREN) and the Hawaii Wide Area Network
- **Support Services:** An expert staff provides MHPCC users with systems, network, and applications support and assistance in code porting and application development.

MHPCC is a well-established member of the High Performance Computing community, participating in collaborations and partnerships that extend its basic capabilities. MHPCC is a:

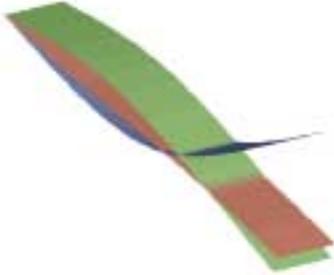
- Center of the Air Force Research Laboratory. MHPCC works closely with DoD and other government researchers to support Research and Development (R&D) and Testing and Evaluation (T&E) efforts.
- Distributed Center of the DoD High Performance Computing Modernization Program (HPCMP). MHPCC provides resources to the DoD research community, as well as Pacific Region DoD organizations, including the Air Force's Maui Space Surveillance Complex.
- Air Force Research Laboratory resource for the Maui Space Surveillance System.
- Member of Hawaii's growing science and technology community.



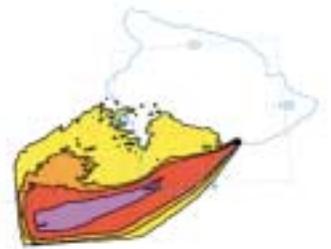


APPLICATION BRIEFS

The user application briefs in this publication represent selected research efforts that have taken place at MHPCC during 2001. Each application brief was written by an individual researcher or research team, and reflects their first-hand experiences using MHPCC resources. These articles reflect the diverse nature of our users and projects.



The application briefs in this document result from the efforts of more than 60 authors. We acknowledge the contributions of each of these individuals and are grateful for their work. We especially welcome back those authors who have become regular and frequent contributors. One author, Joel T. Johnson, is recognized for his seventh consecutive year of contributions to this publication. Many others are repeat contributors and we thank them. We especially welcome those making their MHPCC Application Brief debut this year. We thank them all for their hard work and dedication.



The shaded box at the top of each brief's first page is a short summary of the article. Author and/or organizational contact information can be found in the shaded box at the end of each brief. The notation at the bottom of each page indicates each project's primary functional area (DoD, government, academic, or commercial).



And finally, feedback regarding this publication is solicited. Please direct any communications to: editor@mhpcc.edu. Mahalo.

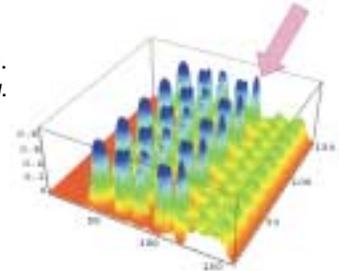
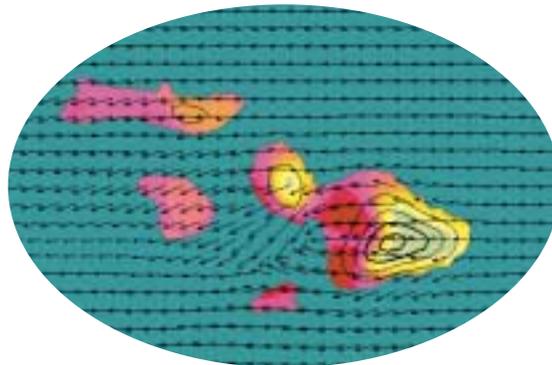


TABLE OF CONTENTS

Designing an Energy-Harvesting Eel Through Parallel Simulations	1
G. E. Karniadakis and R. M. Kirby	
Improving Jet Engine Turbine Thermal Barrier Coatings via Reactive Element Addition to the Bond Coat Alloy	2
Emily A. Jarvis and Emily A. Carter	
Advanced Space Surveillance Data Management and Processing	4
Kathy Schulze, Bruce Duncan, Maria Murphy, Michele Hershey, Steve Gima, Flo Cid, Bob Brem, David Tyler	
High Performance Computing Support for Analysis of Entity-Based Simulations of Land Combat	6
Alfred Brandstein, Gary Horne, Brian Widdowson, Ted Meyer, Mary McDonald, John Kresho, Steve Upton, Bruce Duncan, Brent Swartz, Bob Swanson, Maria Murphy, Ron Vilorio, DJ Fabozzi	
Numerical Study of Inner Magnetospheric Particle Drift Paths in AMIE Electric Field During Magnetic Storms	8
Margaret W. Chen	
Solvated Electron States in 12 Molecule Water Cluster	10
Apostol Gramada, Eric J. Bylaska, John H. Weare	
Numerical Computation of Scattering from a Penetrable Target above a Rough Interface	12
Joel T. Johnson	
Advanced Distributed Systems Technology for Pacific Naval Assets	14
D. J. Fabozzi, Carl Holmberg, Bob Swanson, Bruce Duncan	
Ensemble VOG Forecasts for Kilauea	16
Steve Businger, Roland Draxler, John Porter	
Modeling Dislocation-Grain Boundary Interactions in Polycrystal Copper Plasticity	17
Farid F. Abraham	
High-Resolution Weather Modeling for Improved Fire Management	18
Kevin Roe, Duane Stevens, Carol McCord	
Routine High-Resolution Forecasts/Analyses for the Pacific Disaster Center	20
John Roads, Jongil Han, Duane Stevens, Derek Funayama, Carol McCord, Kevin Roe, Francis Fujioaka	
The Role of Initial and Boundary Conditions for Dynamical Seasonal Forecasting	22
Thomas Reichler and John Roads	
General Earthquake Models: Self-Organizing Patterns of Earthquakes Observed in Numerical Simulations and Data	24
John B. Rundle, Kristy Tiampo, Andrea Donnellan	
Ab Initio Calculations Characterizing an Effective Hamiltonian for Polymeric Photonic “Muscles”	26
James Newhouse, Debi Evans, Joe Ritter	
Isomerizations and Relative Kinetic Stability of LJ_n Clusters in a Carrier Gas	28
Curotto Emanuele	

TABLE OF CONTENTS CONTINUED

MHPCC Assists Project EAST Students in Mapping Ground Features at Kealia Pond National Wildlife Refuge, Maui, Hawaii	29
Scott Splean	
Novel Ultra-Lightweight Space Telescopes Using Optically Active Polymer Membrane Mirror Shape Control	30
Joe Ritter, James Newhouse, Debi Evans, Jim Brozik	
Imagining of Nuclear Motion Using Ultra-Short Intense Laser Pulses	32
André Bandrauk and Szczepan Chelkowski	
Spatially Adaptive Neural Nets with Exotic Topology	34
Frank L. Gilfeather and John A. Holbrook	
Performance Modeling of Data Parallel Applications	36
Daniele Tessera and Anshu Dubey	
Assessing the Utility of Patient Simulation Using Immersive Virtual Reality to Enhance Distance Learning in a Medical Education Curriculum: Project T.O.U.C.H.	38
Joshua Jacobs M.D., Stanley Saiki M.D., Dale Alverson M.D.	
Electron-Impact Ionization of Helium	40
Igor Bray	
Density Functional Study of the Retrocyclization of Norbornadiene and Norbornene Catalyzed by Fe⁺	41
Michael L. McKee	
INDEX OF AUTHORS	Index-1
INDEX OF ORGANIZATIONS	Index-2

Designing an Energy-Harvesting Eel Through Parallel Simulations

G. E. Karniadakis and R. M. Kirby

This work addresses the problem of coupled flow/structure interaction for the purpose of designing an energy-harvesting eel for underwater power extraction. This work is being conducted in concert with experimental efforts at Princeton University and by Ocean Power Technologies, and was showcased in a documentary segment on the Discovery Channel Canada. This project studies flow past a pitching bluff body with a rigid and a flexible splitter plate placed downstream of the object. The study was accomplished using direct numerical simulation (DNS) based on spectral/hp element methods. The pressure distribution on the splitter plate was examined, with the particular goal of using this pressure difference for driving a fully coupled fluid-structure interaction problem between the plate and the flow. Examination of time series data for different points along the plate shows the effect of both primary and secondary vorticity on the coupled system. Variations in the pitching of the bluff body to attain maximum extractable power through large membrane deformation was sought.

Methodology: The parallel simulations were performed using spectral/hp element methods implemented in the incompressible Navier-Stokes solver Nektar. The computation was performed on a hybrid mesh composed of unstructured triangular and quadrilateral elements, filled with a Jacobi polynomial of variable order P . The flexible splitter plates are modeled by the coupling of incompressible Navier-Stokes equations with the membrane-beam equation. The fluid/structure coupling is achieved by an Arbitrary Lagrangian Eulerian (ALE) formulation, which allows "arbitrary" motion of the fluid/plate interface. The interaction is accomplished by incorporating the instantaneous pressure distribution on the flexible plate with the resultant deformation, velocity, and acceleration of the fluid/plate interface. Nektar has been written in C++/C using MPI for parallel portability.

Results: Analysis of history point information for the rigid plate configuration provided us with the natural shedding frequency of the bluff body. We then used this information to determine the frequency at which to vary the bluff body. Preliminary results indicate enhanced amplitude excitation, even when small pitching is introduced. These computational results are being incorporated into the design of the energy-harvesting eel.

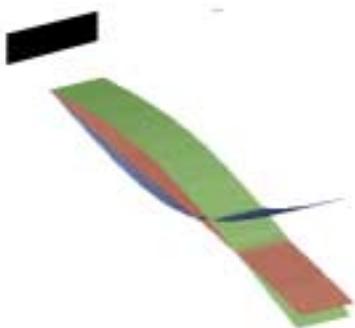


Figure 2. *Extracted flexible splitter plate displacement (flow features removed for visualization purposes) at three different instances of time. The three different instances are denoted by the three different colors.*

Research Objectives: The goal of this project is to understand the lock-in mechanism of a flexible splitter plate placed in the wake of a pitching bluff body. The purpose of this study is to design a better "energy-harvesting eel", a piezo-electric membrane from which power can be extracted due to the material deformation. Maximum amplitude vibration of the structure, and therefore maximum power extraction, was sought. To this end, we varied the amplitude of the pitching bluff body with values ranging from zero pitch to 30 degrees in an attempt to isolate the conditions for sustainable maximal amplitude response.

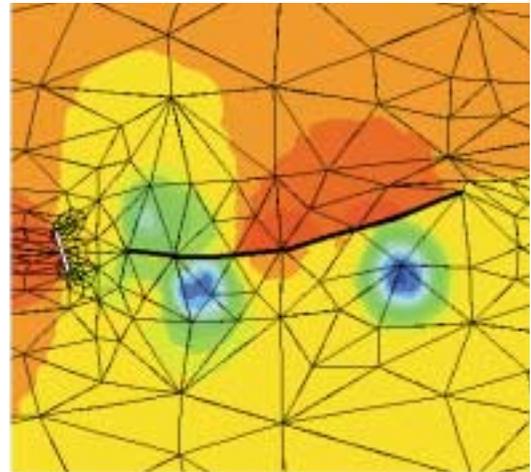


Figure 1. *Pitching bluff body with a flexible splitter plate at $Re = 1000$. The bluff body is pitching a maximum of 10 degrees at the shedding frequency of the bluff body. Instantaneous pressure contours around the bluff-body/flexible plate system are shown. The flexible plate is modeled using the linear membrane-beam equation.*

Author and Contact: George E. Karniadakis

Author: R. M. Kirby

Organization: Brown University, Division of Applied Mathematics, Providence, RI, 02912

URL: www.cfm.brown.edu/crunch

Resources: IBM SP at MHPCC

Sponsorship: Office of Naval Research and DARPA

Improving Jet Engine Turbine Thermal Barrier Coatings via Reactive Element Addition to the Bond Coat Alloy

Emily A. Jarvis and Emily A. Carter

Thin ceramic coatings on jet engine turbine blades can shield the temperature to which the underlying superalloy is exposed by hundreds of degrees Celsius. The higher temperature operation afforded by the ceramic top coat of the thermal barrier coating allows the engine to operate with greater power and fuel efficiency. After repeated thermal cycling, the ceramic film spalls, exposing the superalloy to the harsh temperature and the oxidative/corrosive gases of the combustion chamber. Previously, we characterized ideal interfaces within the thermal barrier coating. Improved understanding of the atomic-level interactions at heterogeneous interfaces^{1,2}, gained in these studies allowed us to extend our research into largely uncharted territory over this past year. Specifically, we are attempting to serve in a predictive role by suggesting chemical modifications that should inhibit the failure of these jet engine turbine thermal barrier coatings.

Research Objective: Our research aim is twofold. First, we characterized ideal interfaces in a typical thermal barrier coating to investigate fundamental interactions at heterogeneous interfaces and atomic-level culprits in materials failure. In particular, we explored the interactions occurring at ceramic/Ni interfaces, since nickel is the primary component of the turbine blade metal alloys. Armed with understanding gained through our ceramic/Ni studies, the second phase of our research is to search for means of limiting or eliminating thermal barrier coating failure. Our focus thus far has been on suggesting chemical means by which interface adhesion could be enhanced by forming stronger covalent and ionic bonding interactions across the metal-ceramic interface.

Methodology: We perform planewave, pseudopotential density functional calculations, employing the generalized gradient approximation (PW91) to the exchange-correlation

potential, using the Vienna *Ab Initio* Simulation Package³. The 3-D periodic boundary conditions allow effective simulation of bulk crystals, surfaces, and interfaces, neglecting long-range relaxation effects. Interface adhesion energies are calculated by subtracting the total energy of the combined interface or coated substrate from the sum of the energies of isolated substrate and coating slab calculations, normalizing this value by the area of the interface periodic cell. For several metal/ceramic interfaces, we also performed high temperature annealing and quenching to simulate the harsh temperature environment of the jet engine and to ascertain that the relaxed ionic coordinates were not trapped in an unfavorable local minimum energy configuration.

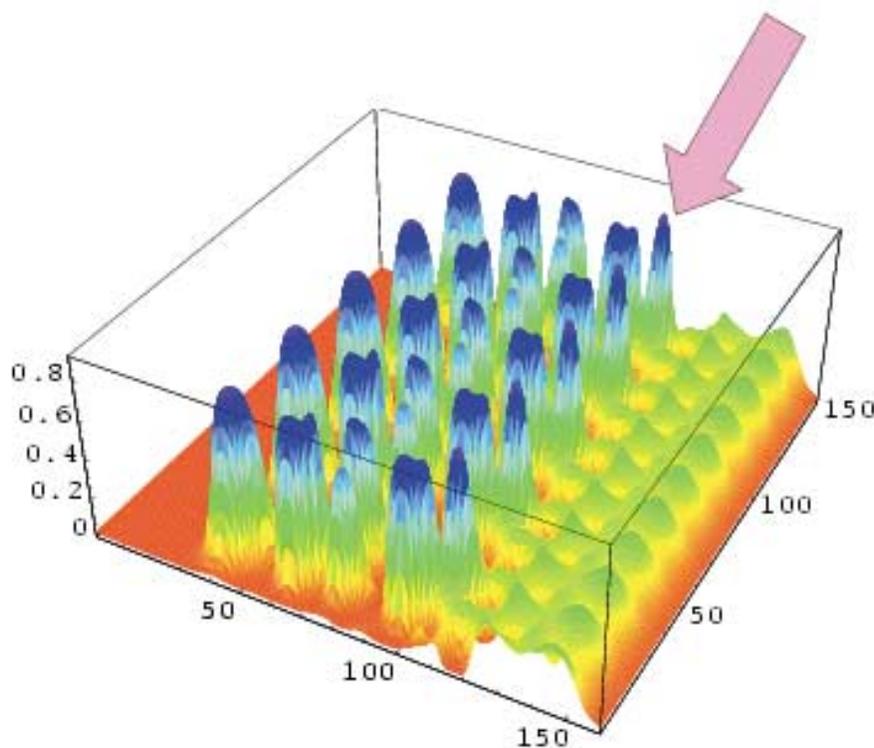


Figure 1. Valence electron density localization of a cross-sectional view of the SiO₂/Ni interface. Red is zero and purple indicates the highest localization. The violet arrow indicates the region of localized bonding between the SiO₂ and the nickel substrate. The other blue peaks correspond to the oxygen ions, and the nickel ions are located at the rows of lime colored bumps.

Results/Significance: A significant source of thermal barrier coating failure is related to the Al_2O_3 scale that grows via bond coat alloy oxidation during thermal cycling of the jet engine. Our calculations of the clean $\text{Al}_2\text{O}_3/\text{Ni}$ interface showed that the interfacial bonding is very weak for thick Al_2O_3 films. By contrast, we find that introducing certain early transition metals to the bond coat alloy results in significantly increased interface adhesion at these metal-ceramic interfaces. These elements have open d-shells; thus, they are able to form stronger bonds to the closed-shell ions of the highly ionic Al_2O_3 coating than can the late transition metals, which have a mostly filled valency leading to closed-shell repulsions. Furthermore, our investigation of the interface bonding behavior of nickel with SiO_2 , an oxide with a strong covalent component to its bonding, displays that this interface does not suffer from the unfavorable adhesion properties exhibited by $\text{Al}_2\text{O}_3/\text{Ni}$. It is hoped that modifying the composition of the bond coat alloy to include certain early transition metals will provide a straightforward means to improve operational lifetimes of thermal barrier coatings. Likewise, our calculations of the SiO_2/Ni interface imply that ultimately it may be preferable to alter the bond coat composition such that its oxidation product has a stronger covalent character than Al_2O_3 .

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- 3) G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993) and 49, 14251 (1994); G. Kresse and J. Furthmuller, Comput. Mat. Sci. 6, 15 (1996).

Author and Contact: Emily A. Carter

Author: Emily A. Jarvis

Organization: University of California, Los Angeles, Department of Chemistry and Biochemistry, Box 951569, Los Angeles, CA, 90095

URL: www.chem.ucla.edu/carter/

Resources: IBM SP3 at MHPCC and DEC Alpha ES40s at the University of California

Sponsorship: Air Force Office of Scientific Research, HPCMP Challenge Project C54

Advanced Space Surveillance Data Management and Processing

Kathy Schulze, Bruce Duncan, David Tyler, Maria Murphy, Michele Hershey, Steve Gima, Flo Cid, Bob Brem

The Air Force Research Laboratory (AFRL) operating location on Maui, Hawaii has a two-fold mission. First, it conducts research and development (R&D) and operations on the Maui Space Surveillance System (MSSS) at the Maui Space Surveillance Complex (MSSC). Second, it oversees operation of the Maui High Performance Computing Center (MHPCC). AFRL is integrating world class Air Force assets to enhance space surveillance with the primary objective of detecting, tracking, and identifying, all tasked space objects within its area of coverage. MSSS is a national resource that provides support to various government agencies, the scientific community, and the United States Space Command's space surveillance mission. MSSS acquires gigabytes of information per day from its various sensors and instruments. Developers at MHPCC have developed a data reduction environment known as the Maui Image Manager and Online Systems Archive (MIMOSA). MIMOSA is a key step in a multi-faceted plan to more closely integrate MSSS telescopes and the High Performance Computing (HPC) infrastructure and tools of MHPCC. MIMOSA provides a web-browser environment that encompasses all aspects of telescope imagery data reduction including, file transfer for image reconstruction, processing for calibration data and object imagery, file format conversion, data viewing, and storage. The current MIMOSA environment provides all required functionality for data reduction. A significant amount of relational database management system work has also been accomplished.

Background: Images of earth-orbiting satellites acquired by ground-based telescopes are blurred by atmospheric turbulence, telescope jitter, and background noise. These effects can be mostly overcome by adaptive optics and image processing. High performance, massively parallel supercomputing is needed to handle the data sets to perform the image processing in the rapid turn-around times required. MHPCC is supporting the MSSS mission by capitalizing on the HPC abilities of its supercomputers, and developing the MIMOSA Web-based "data pipeline" to effectively manage, reduce, view and store MSSS data. The web-based nature of MIMOSA utilizes the MHPCC supercomputer parallel architecture, but requires no knowledge of the Unix operating system. After collecting the data using various imaging sensors at the MSSS, the operators can open a Netscape browser window and transfer the data from the MSSS computer systems to the MHPCC computer systems for storage and data reduction. Data reduction is completed via an integrated job submit web page allowing parameter and input file selection and job submission to the parallel batch queue. Job status pages keep the operators updated on data reduction progress. After data reduction is completed, the MIMOSA data

viewing capabilities allow the operators to review the data reduction and create the specific output file format required for the MSSS customers. All of these functions are performed using a simple web browser

Research: The MSSS Visible Imager sensor on the 3.6 meter (m) Advanced Electro Optical System (AEOS) and the Generalized Multiwavelength Infrared Instrument (GEMINI) sensor on the 1.6 m telescope collect volumes of data each day. As an example, a single observation of an orbiting satellite by GEMINI can easily yield 3 GB of data, and GEMINI observations occur around the clock. MIMOSA is being designed, developed, and tested to provide easy access, processing, and interpretation of all these data so that users can more easily and efficiently gain useful information and perform their duties better and faster. MIMOSA combines functions and data products to provide the means to display and extract as much information as possible. The MIMOSA environment is providing the capability to turn data into information as described further below.

Methodology: MSSS telescope sensor information is furnished to MHPCC via a fiber optic OC3 link rated at 155 Mbps. The MIMOSA environment is served from an SGI Origin 200 workstation called "Crux", located at MHPCC. For image reconstruction, MIMOSA is currently using IBM P3 Winterhawk2 parallel HPC system hardware in the MHPCC main computer room called "Corona", employing 8 nodes rated at 48 GFLOPS. Any validated user can access MIMOSA from a client machine on the internal MHPCC network and complete MSSS data reduction. In the future, fully-functional versions of MIMOSA may be served from machines at MHPCC and MSSS for remote access by DoD users, allowing log-ins by authorized individuals using proper security procedures and networks. This means MIMOSA users could search for, view, process, archive, and download data collected by MSSS staff from virtually anywhere on the planet.

Before MIMOSA, all MSSS data reduction was completed on computer systems located at the observatory. A requirement while designing the MIMOSA environment was for the operators to be able to reduce the telescope data using the MHPCC computers, then place the reduced data products back onto the MSSS computers for final processing before sending the imagery to the customer. The design for MIMOSA included transferring the data from and to the MSSS, file format conversion utilities, data reduction capabilities, and data viewing with some image enhancements. All of these capabilities were required to be integrated into an easy to use and maintain environment which could also offer on-line help for all functionality. Using a myriad of Hyper-Text Markup Language (HTML), Common Gateway Interface (CGI) ModPerl scripts, Java, C and Fortran 90 code, the MIMOSA environment has been developed. The MIMOSA Home Page is shown in Figure 1. Each of the tabs across the top of the web page forms are selectable, offering a top-down division of the MIMOSA functions.

Other tabs and functions include Data Transport, Data Conversion, Data Reduction, View Data, Research & Development, and Help. Using MIMOSA, multiple short exposure frames collected from the MSSS telescopes can be combined together to produce one reconstructed image. Many reconstructed images can be combined to form a movie of a satellite pass. The current MIMOSA environment allows users to view and process telescope data in a "point-and-click" Graphical User Interface (GUI), web-browser environment. CGI's are initiated from web pages and create command files for all data reduction jobs. Shown in Figure 2 is the MIMOSA web page for bispectrum speckle imaging data reduction batch job submission. When the operator clicks the submit button on the batch job submit page, a perl script generates the LoadLeveler job submission and input files from the entries on the form and submits the job to the MHPCC batch queue. Future operational concepts call for an immediate execution ("do now") button that will allow priority bypassing of the queue. The data reduction page is complete with on-line help. All raw, calibration, and recovered image data can be viewed using MIMOSA's image viewers. Large files can be paged through quickly using a "movie" viewer and selected frames can be viewed in more detail using a single frame viewer.



Figure 1. MIMOSA Home Page



Figure 2. Bispectrum Data Reduction Job Submit Page

Significance: Use of MHPCC computing platforms and MIMOSA for data processing frees up MSSS computational resources to be used for other purposes, such as tracking and data acquisition. This means much greater flexibility in MSSS tasked and R&D and operations. As an example, MSSS processing of GEMINI data is currently controlled only from the GEMINI control workstation. However, a consequence of this is that use of the workstation for data reduction means that objects of interest may go unobserved. Additionally, using the workstation to control GEMINI's cameras and optics for an observation means that time-critical data cannot be processed.

The MIMOSA environment tool set allows for integrated data reduction, data storage, and visualization for the purpose of producing high quality data products for Space Command. Further MIMOSA work is planned for FY02. The environment is in the final stages of development, currently undergoing operator beta testing. At the completion of beta testing, a complete operational test and evaluation (OTE) cycle is planned. Successful completion of OTE and the beginning of the operational use of MIMOSA will mark the first joint effort between the MSSS and MHPCC giving the Air Force MSSS mission full use of the MHPCC supercomputing assets. MIMOSA allows users to do their jobs faster and more efficiently, and has no limit to the number of algorithms and system performance enhancements that can be integrated. MIMOSA provides an overall "umbrella" environment in which many other applications can work, and provides the basis for anticipated continued and expanding key research and operations activities in support of the Air Force's MSSS space surveillance mission.

Author and Contact: Kathy J. Schulze
 Organization: KJS Consulting, P.O. Box 591, Georgetown, DE, 19947
 Author and Contact: Bruce Duncan
 Authors: Maria Murphy, Michele Hershey, Steve Gima
 Organization: Maui High Performance Computing Center (MHPCC), 550 Lipoa Parkway, Kihei, HI, 96753
 Authors: Flo Cid and Bob Brem
 Organization: Boeing LTS, 535 Lipoa Parkway, Kihei, HI 96753
 Author: David Tyler
 Organization: Albuquerque High Performance Computing Center, 1601 Central Avenue N.E., Albuquerque, NM, 87131
 Resources: IBM P3 HPC "Corona" and SGI Origin 200 Server "Crux" at MHPCC

High Performance Computing Support for Analysis of Entity-Based Simulations of Land Combat

Alfred Brandstein, Gary Horne, Brian Widdowson, Ted Meyer, Mary McDonald, John Kresho, Steve Upton, Bruce Duncan, Brent Swartz, Bob Swanson, Maria Murphy, Ron Vilorio, D. J. Fabozzi

The Marine Corps Combat Development Command's (MCCDC) Albert Program involves research to assess the general applicability of the "New Sciences" to land warfare. While simulations based on these New Sciences (or complexity theory, which models behavior and interaction at the entity level) are considered part of an infant science, they do provide insight into evolving patterns of macroscopic behavior that result from collective interactions of individual agents. Simulations based on entity-level interactions represent a significantly different approach from the traditional attrition estimation techniques based on Lanchester equations, which assert that the loss rate of forces on one side of a battle is proportional to the number of forces on the other side. The MCCDC Albert Program is an effort to investigate how complexity theory may be applied to land combat in a manner to augment and, perhaps in some cases, replace Lanchester modeling in the future.

Research Objectives: Continuing the development of a complex systems analyst's toolbox for exploiting emergent, collective patterns of behavior on the battlefield, MCCDC is using several multiagent-based simulations of notional combat, including Irreducible Semi-Autonomous Adaptive Combat (ISAAC) and Socrates. These models simulate the interaction between two or more variable size forces of agents. The action of each agent is determined by parameters, such as the agent's ability to sense its surroundings and to communicate with other agents. In addition to the common physical parameters measured by the model (such as range of fire and probability of kill), more abstract concepts are also modeled. Such concepts can include an agent's attraction to friendly and opposing forces and the influence of behaviors based on determinable thresholds, such as the tendency of

an agent to follow orders. The magnitude and granularity of these independent variables provide the analyst with great flexibility in simulating various hypotheses. This same flexibility, coupled with the stochastic nature of the simulations, requires a significant computational capability to determine likely outcomes with any statistical significance for each single hypothesis. This requirement becomes even greater for the analyst wishing to study hypotheses over multiple varying independent parameters, a requirement that easily overtaxes the capability of a single personal computer.

Methodology: The Maui High Performance Computing Center (MHPCC) has worked in concert with military analysts from MCCDC, and other supporting contractors, to develop methodologies and tools needed for the large-scale analysis of agent-based distillation models. This development includes the processing and data reduction required for statistical analysis of such simulations, as well as tools for analysts to visualize and comprehend the phenomenology of the simulations. Specifically, in support of MCCDC's data farming methodology, MHPCC has ported the core engine of the ISAAC and Socrates models to the IBM SP parallel supercomputer, a cluster of Windows workstations, and the new Linux Supercluster. The resultant codes can execute and statistically reduce multiple combat hypotheses. The output of the multiple simulation runs is a set of statistically calculated fitness values that are used as measures of battlefield effectiveness. The Generalized Visualization Toolkit provides analysts the ability to assess the combined results of the model outputs, as well as the ability to simultaneously conduct a comparative analysis of multiple playbacks (time/space representations of battlefield agents). The information generated from this exhaustive execution of model simulations, along with the associated mechanisms for visualization, will provide analysts with the tools required to investigate multiple hypotheses with statistical significance.

Results: This year's activities have continued to refine the current system and have provided more tools to aid the analytical process. MHPCC has developed a Web-based submission system (www.projectalbert.org) that allows analysts to submit large scenario runs over the Web, thereby allowing analysts to easily explore a given scenario in many ways. MHPCC also designed and implemented the Parallel Execution System (PES), a set of portable Java programs which allow multiple models (currently ISAAC and Socrates) to be executed in parallel on the many platforms available at MHPCC. These platforms include the IBM SP (via the Maui Scheduler), the Windows cluster (via the Condor scheduler), and the Linux Supercluster (via the MauiME scheduler). The PES is designed to improve the overall portability, performance, scalability, and turn-around time in producing model output files. It is also designed to more easily integrate future models into the PES. This will allow these models to be run in parallel on the various MHPCC platforms, while simultaneously allowing the Visualization Tool Kit to be used on the resulting output. SMP parallelism is achieved by simultaneously executing as many model runs as will fit the number of CPUs available on a computational node. MHPCC also implemented the Generalized Visualization Toolkit, which allows analysts to view the results of any model incorporated into the PES. An XML file is used to completely describe each user-defined scenario. This file is created by user interaction with the Web-based submission system, then passed to the PES for model execution, and finally used in the Visualization Toolkit for the display of the results. MCCDC has successfully applied these tools to reinforce intuitive conclusions. Comparison of these results with several historical battles has further validated the various models' applicability. MCCDC has also used the Albert program and associated products as a springboard for other collaborative activities. Such activities include the participation of analysts from a variety of nations at international conferences, where the participants research analytical methods and a new generation of modeling tools.

Significance: This initiative has led to a continuing evolution and refinement of what may prove to be the new generation of analytical models. MHPCC will continue to collaborate with MCCDC to further develop simulation, visualization, and statistical methodologies that may eventually improve MCCDC's ability to evaluate the applicability of these simulations to actual combat doctrine. Future efforts will expand to cover new technologies, including one (Pythagoras) which will explore the applicability of soft logic to help find solutions in future generations of simulations and models.

Several visualization tools have been developed at MHPCC as part of Project Albert. These tools provide MCCDC analysts with a variety of ways to explore the output of multiple simulations. One of the more widely used means of analyzing model output is the 3-D landscape plotting tool provided by the Albert Visualization Toolkit application. The once ISAAC-specific interface has been generalized to facilitate immediate use by the different models being investigated by Project Albert. The ISAAC implementation was limited to five input parameters and a specific set of measures of effectiveness (MOEs). The new generalized landscape tool accepts any number of inputs and MOE output parameters (however, a minimum of two input parameters other than the random number input is required). In addition to plotting statistically reduced MOEs, the landscape plot can display raw or unreduced data, functionality not available for the ISAAC landscape plots. In addition to selecting the statistical function, users can also select the color, title, and combination of MOEs (including weighting and linearity) to characterize each output. Statistics are now also generated "on-the-fly" within the Visualization Toolkit, eliminating one step in processing of data before it reaches the analyst.

Figure 1 shows the generalized landscape tool displaying three out of five available outputs created by the user. The color of each plot corresponds to an output listed on the bottom left corner of the dialog. This study has six input parameters, two of which are on each of the X and Y axis; the remainder are represented by S which controls the values of the other four input parameters based on the settings chosen by the user via the slider bar. The blue output plot shows the mean function of the MOE of Force 1 Maximizing the Enemy Center-of-Mass Distance to the Friendly Flag (i.e., how well did Force1 keep the majority of the enemy away from its flag?). Similarly, the blue output plot shows the same MOE, but from Force2's perspective. Finally, the green plot displays the standard deviation for Force1 maximizing enemy casualties. By stacking the three outputs, conclusions or questions regarding relationships between the MOEs relative to input parameters and their values can be developed.

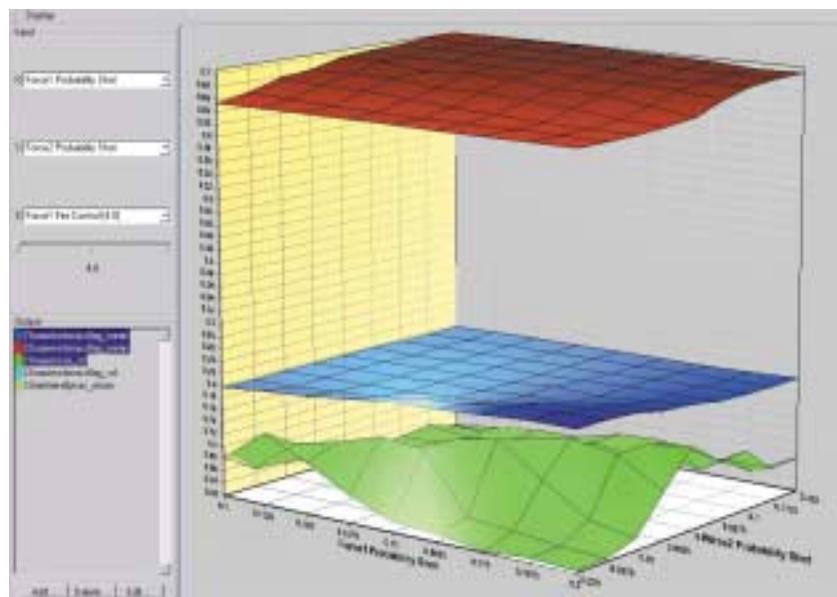


Figure 1. *Project Albert's Landscape Tool*

Author and Contact: Brent Swartz

Authors: Bob Swanson, Maria Murphy, Bruce Duncan, Ron Vioria, D. J. Fabozzi

Organization: Maui High Performance Computing Center (MHPCC), 550 Lipoa Parkway, Kihei, HI, 96753

Authors: Alfred Brandstein, Brian Widdowson, Mary McDonald

Organization: Marine Corps Combat Development Command (MCCDC)

Authors: Gary Horne, Ted Meyer, Steve Upton, John Kresho

Organization: Mitre Corporation

URL: www.projectalbert.org

Resources: IBM P3, IBM Linux Supercluster, and Windows workstations at MHPCC

Sponsorship: Marine Corps Combat Development Command

Numerical Study of Inner Magnetospheric Particle Drift Paths in AMIE Electric Field During Magnetic Storms

Margaret W. Chen

This is a numerical study of the drift of inner magnetospheric ions and electrons with the Assimilative Model of Ionospheric Electrodynamics (AMIE)¹ mapped into a model magnetic field. We compute quasi-steady-state AMIE drift paths and drift times of particles for times during several magnetic storm events. We compare the drift paths from the realistic AMIE electric field with those that correspond to a simplified semi-empirical analytical electric field model that we had used in the past. Knowledge of realistic charged particle drift trajectories in the inner magnetosphere is relevant to Air Force and other satellite systems because during magnetic substorms energetic (1-10 keV) electrons may be injected into the plasma sheet. These energetic electrons may possibly cause surface charging on spacecraft that are orbiting at geosynchronous altitude. In addition, enhanced fluxes of relativistic electrons (with energies on the order of MeV) that may follow magnetic storms may cause deep dielectric charging on spacecraft that orbit in the inner magnetosphere.

Research Objectives: We compute drift paths and drift times of ions and electrons under the realistic AMIE electric field in a model magnetic field so as to understand the drift characteristics of ions and electrons in the inner magnetosphere. Our eventual goal is to incorporate the AMIE electric field in our simulations of the Earth's ring-current and diffuse aurora.

Methodology: The AMIE potentials are an analytic expansion of basic functions that depend on magnetic latitude and magnetic local time. These potentials are fit to electric field data that is inferred from ground-based magnetometers and, if available, satellite and radar data. We model the magnetospheric magnetic field as a

superposition of a dipolar magnetic field and a uniform southward field parallel to the dipole axis. In this field model, the field line equation simply relates the magnetic latitude to the field line label L at the altitude of 110 km in the ionosphere in which AMIE potentials are specified. Thus, we can describe AMIE potentials analytically everywhere in the model magnetic field, given the AMIE coefficients for a particular time period. We construct a Hamiltonian of the particle motion, assuming that particles conserve their first two adiabatic invariants. Particle drift shells are just contours of the constant Hamiltonian that we calculate. We compute the particle drift time by computing derivatives of the Hamiltonian with respect to the spatial coordinates.

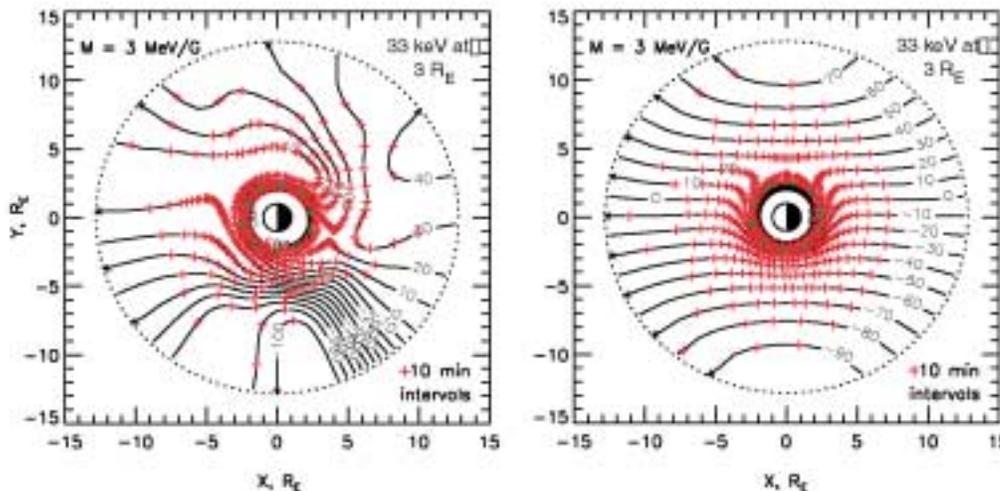


Figure 1. The black curves correspond to drift paths for ions having the first invariant of 3 MeV/G. The red plus signs mark 10-minute intervals of the drift time as the ions drift from the nightside boundary. Drift trajectories under the AMIE electric field at 0800 UT on 19 October 1998 are shown in the left panel and drift trajectories in the simplified analytical electric field model for the same total AMIE cross-polar-cap potential are shown in the right panel.

Results: We calculated quasi-steady-state drift paths using the AMIE electric field for selected times of the 19 October 1998 magnetic storm. We found that the AMIE electric field is stronger in inner than outer magnetosphere during main phase. Particle drift paths in AMIE are skewed because the AMIE potentials are skewed. During the early main phase of the 19 October 1998 storm, the electric field in the evening sector of the AMIE model is stronger than in any sector of the simplified model. Thus, we find rapid (about 20 to 30 minutes) inward transport of ring-current ions and electrons to the region where the partial ring-current is observed to form on time scales of about 20 to 30 minutes after the interplanetary magnetic field goes southward. We calculated quasi-steady-state AMIE drift paths during the early main phase of the very large 15 July 2000 "Bastille Day" magnetic storm. We found that the ions from the plasma sheet can be transported to very low L ($=2$) values. This deep penetration of ring-current ions is consistent with a very strong ring-current that was observed during this storm.

Significance: The incorporation of realistic electric field models in numerical models of inner magnetospheric dynamics is very important, as recent electric field observations² show that the storm time electric field at low L values may be much stronger than what is predicted in simplified electric field models that are commonly used. From the drift characteristics of representative ring-current particles, this study shows that the drift times and locations for a couple of real magnetic storms are consistent with ring-current observations. Knowledge of realistic charged particle drift trajectories in the inner magnetosphere is relevant to Air Force and other satellite systems, because during magnetic substorms, energetic (1-10 keV) electrons may be injected into the plasma sheet. These energetic electrons may cause surface charging on spacecraft that are orbiting at geosynchronous altitude.

References:

- 1) Richmond, A. D., and Y. Kamide, Mapping Electrodynamic Features of the High-Latitude Ionosphere from Localized Observations: Technique, J. Geophys. Res., 92, 5471-5759, 1988.
- 2) Rowland, D. E., and J. R. Wygant, Dependence of the Large-Scale, Inner Magnetospheric Electric Field on Geomagnetic Activity, J. Geophys. Res., 103, 14, 9, 59-14, 964, 1998.

Author and Contact: Margaret W. Chen
Organization: The Aerospace Corporation, P.O. Box 92957, M2-260, Los Angeles, CA, 90009-2957
URLs: www.aero.org
Resources: IBM SP at MHPCC and Sun Enterprise 3000 at the Aerospace Corporation
Sponsorship: Department of Defense

Solvated Electron States in a 12 Molecule Water Cluster

Apostol Gramada, Eric J. Bylaska, John H. Weare

A quantum mechanical approach was used to study the solvated states of an electron attached to a 12 water molecule cluster with emphasis on the stability of the surface and interior states. The analysis of the calculations showed the existence of both interior-like and surface states in a cluster of this size. We also calculated the Vertical Detachment Energy (VDE) for both states and found that its variation with temperature and relative values for the two states qualitatively confirm the predictions.

Research Objective: We use a quantum mechanical approach to study the solvated states of an electron attached to a 12 water molecule cluster. Our main interest is focused on the investigation of the stability of surface and interior states, a topic that has been the subject of a continuous debate in the literature, due in part to existent disagreements between experimental and theoretical results. In particular, the minimum size of the cluster that can contain a stable interior state is still a controversial topic.

Methodology: A parallel program based on Density Functional Theory, and the Car-Parrinello molecular dynamics approach, has been used to do the geometrical optimization of the 12 molecule water cluster. The exchange-correlation energy is based on a local spin-density scheme with gradient correction included, and a plane wave decomposition is used for the representation of the Kohn-Sham orbitals. The interaction with the core electrons is described through generalized norm-conserving Hammann pseudopotentials. The initial ionic configuration was generated by classically annealing a cluster in which the excess electron was mimicked by a chlorine ion. A steepest descent and/or conjugate gradient calculation was used to obtain the electronic state on the initial ionic configuration and for reequilibrating the electron states at different stages of the simulations.

Results: We performed quantum molecular dynamics simulations on 12 molecule water clusters using IBM SP parallel machines at the Maui High Performance Computing Center. The analysis of the calculations completed thus far shows the existence of both interior-like (hybrid) and surface states in clusters of this size. Both states are stable on a time scale of 1 picosecond and within a temperature range of 300 K. The difference in their energy, however, is small and therefore further annealing is needed for a definite conclusion regarding their relative stability. We calculated the Vertical Detachment Energy (VDE) for both states and found that its variation with temperature and relative value for the two states confirm qualitatively the predictions, based on previous pseudopotential-based calculations. However, the absolute value of the VDE is systematically higher in our calculations for both the hybrid and the surface states.

Significance: Accurate quantum mechanical calculations of the solvated electron state in big water clusters represent a very challenging problem. So far, systematic calculations have been performed only in rather small systems with a special interest for 6 water molecule clusters. The onset of relevant features related to the transition to bulk behavior, however, is predicted to happen beyond 10 water molecules according to calculations based on pseudopotential models. Our work aims at addressing these range of cluster sizes through accurate calculations.

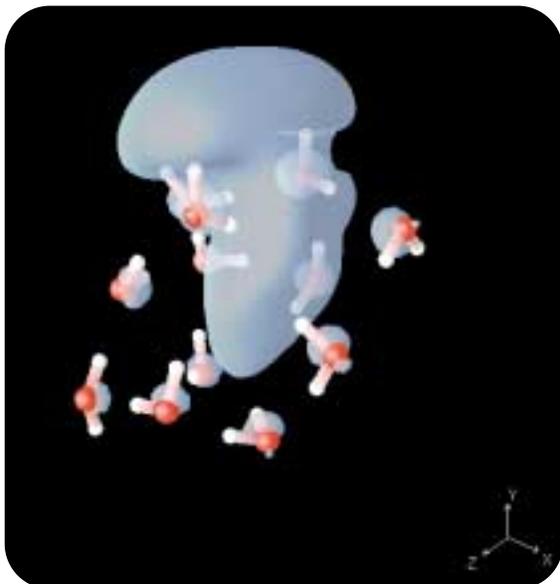


Figure 1. A hybrid state of a solvated electron in a 12 water molecule cluster. Red: Oxygen atoms, White: Deuterium atoms.

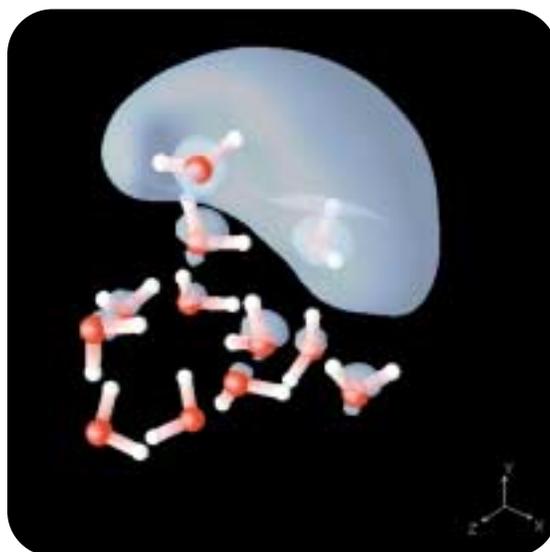


Figure 2. *A surface state of a solvated electron in a 12 water molecule cluster. The color code is the same as in Figure 1.*

Author and Contact: Apostol Gramada

Organization: San Diego Supercomputer Center, University of California, 9500 Gilman Drive, La Jolla, CA, 92093

Author: Eric J. Bylaska

Organization: Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA, 99352

Author: John H. Weare

Organization: University of California San Diego, Dept. of Chemistry and Biochemistry, 9500 Gilman Drive, La Jolla, CA, 92093

URL: www.ucsd.edu

Resources: IBM SP at MHPCC and IBM SP at Pacific Northwest National Laboratory

Acknowledgments: We would like to thank the Office of Naval Research for providing the computer time through Grant No. N00014-97-1-0751 and MHPCC for additional computer time through a university account.

Numerical Computation of Scattering From a Penetrable Target Above a Rough Interface

Joel T. Johnson

Radar systems operate by measuring scattered electromagnetic fields from an object under view. Since in many cases targets may be located near ground or sea surfaces, scattering from rough surfaces can influence target returns and cause problems in detection and identification algorithms. Simple models can be made to describe these effects analytically, but in many cases the inherent approximations break down. Use of efficient algorithms and parallel computing resources now makes numerical solution of coupled 3-D target/surface geometries possible so that the scattering physics can be studied without approximation.

Methodology: The studies of this project involve predicting scattered fields from a target above a statistically described rough surface. A Monte Carlo simulation is used to capture scattered field statistics, and a standard numerical method, the method of moments, is used for scattering calculations. To improve computational efficiency, an iterative rather than direct matrix solver is used. In addition, the “canonical grid” and “discrete dipole” methods are used to compute surface-to-surface and target-to-target point couplings, respectively, in order ($N \log N$). The studies of interest involve frequency

swept calculations; since single frequency results are obtained from the algorithm, parallel computing resources are applied by running separate frequency calculations on individual nodes. Time domain responses can then be synthesized from multiple frequency data in a post-processing step. Because surface roughness effects are stochastic, a parallel Monte Carlo simulation is also used to capture scattered field statistics.

Results: A Monte Carlo simulation has been completed for a simple penetrable (plastic-like) object above a moderately rough soil surface, intended to model a target above rough ground. The Monte Carlo simulation used twenty surfaces which were realizations of a Gaussian random process with an isotropic Gaussian correlation function described by rms height 1 cm and correlation length 3.58 cm. Figure 1 illustrates the geometry considered, while Figure 2 plots time domain backscattered field statistics at normal incidence (direct surface backscattering is removed) obtained from 2 to 5 GHz data. Results show that average (coherent) fields in the presence of surface roughness can be significantly different from those with a flat surface, and that the standard deviation of time domain fields (incoherent) can also be significant.

Significance: The results of this project can be applied to assess and to extend radar signal processing algorithms for the detection and identification of targets in the presence of clutter. Detailed studies of numerical results can also suggest means for developing improved analytical models of the surface-target scattering process.

Backscattering computed at 16 frequencies from 2–5 GHz for normal or 45 degree incidence

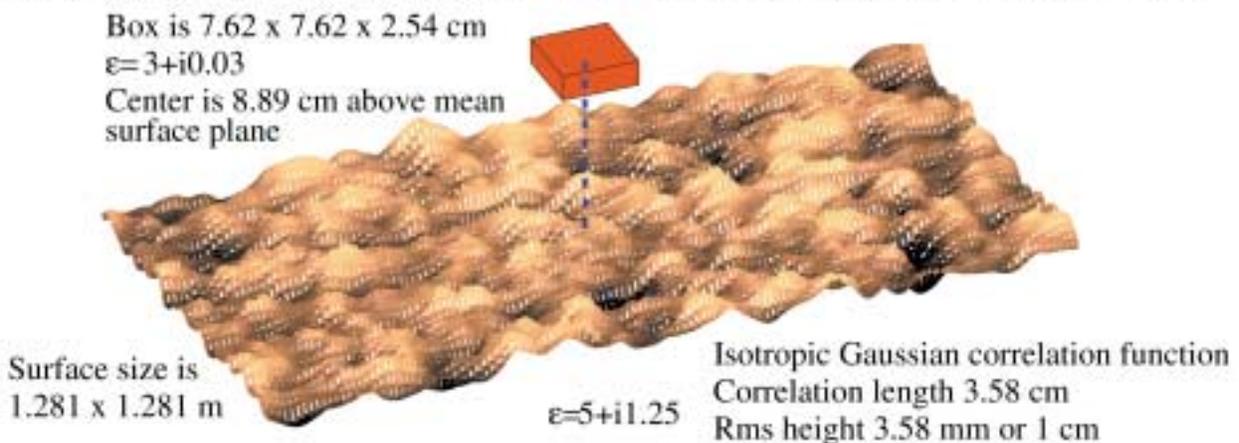


Figure 1. Geometry of target-above-surface problem considered

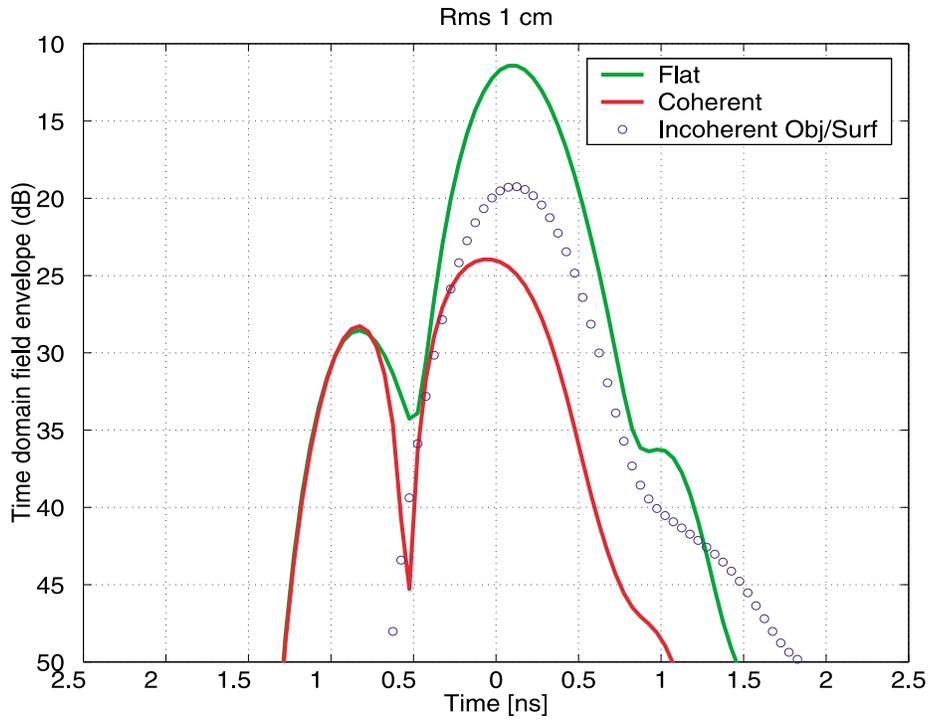


Figure 2. Time domain backscattered field statistics for normal incidence. Average (coherent) fields in the presence of surface roughness are significantly different from those with a flat surface, and field standard deviations (incoherent) are also significant.

Author and Contact: Joel T. Johnson
 Organization: The Ohio State University, 205 Drees Laboratories, 2015 Neil Avenue, Columbus, OH, 43210
 URL: <http://eewww.eng.ohio-state.edu>
 Resources: 64 IBM SP nodes at MHPCC
 Sponsorship: Department of Defense

Advanced Distributed Systems Technology for Pacific Naval Assets

D. J. Fabozzi, Carl Holmberg, Bob Swanson, Bruce Duncan

The Maui High Performance Computing Center (MHPCC) developed proof-of-concept control and distribution utilities for the Office of Naval Research to manage Pacific Missile Range Facility's (PMRF) sensor data. The suite of utilities, entitled the Naval Asset Look Up (NALU) System, manage data streams from the PMRF Instrumentation Network (iNet) in anticipation of the Ultra-high-frequency Electronically Scanned Array (UESA) radar system. The current implementation manages simulated distributed services between the PMRF on Kauai, MHPCC on Maui, and remote clients throughout the United States. Based on Sun Microsystems® Jini(TM) technology, NALU identifies data sources on a demonstration PMRF iNet and then transports and displays the simulated data stream to the Naval Research Laboratory (NRL) "client application" Simulation Display (SIMDIS).

Research Objective: As one of the Navy's major test ranges, the Pacific Missile Range Facility (PMRF) supports a wide variety of training exercises, developmental tests, and tracking of space, air, surface, and sub-surface units within its 42,000 square mile test range. Historically, data is multicast to the internal iNet and visualized locally. With the NALU system, the potential exists to provide range traffic information to remote test managers located anywhere on the Internet (or on other wide-area networks). The NALU system also provides the basis for establishing other spontaneous wide-area network connections supporting additional

distributed computing, remote visualization, and command and control applications.

Results: The current demonstration test bed was developed by MHPCC and Sun Microsystems Professional Consulting Services. It "wraps" the legacy utilities Gen25 (which simulates iNet traffic), ReadNet (which transforms and filters the raw PMRF data), and SIMDIS (final visualization) within Jini services. The iNet multicast streams are then "tunnelled" through unicast streams to allow remote access and display utilizing wide-area connectivity.

The Java/Jini entities used in implementing the NALU system are shown in the block diagram Figure 1. They include the NALU Data Manager (NDM), the NALU Service Manager (NSM), the NALU Service Objects (NSO), the tunnel objects, and the NALU Client Objects (NCO).

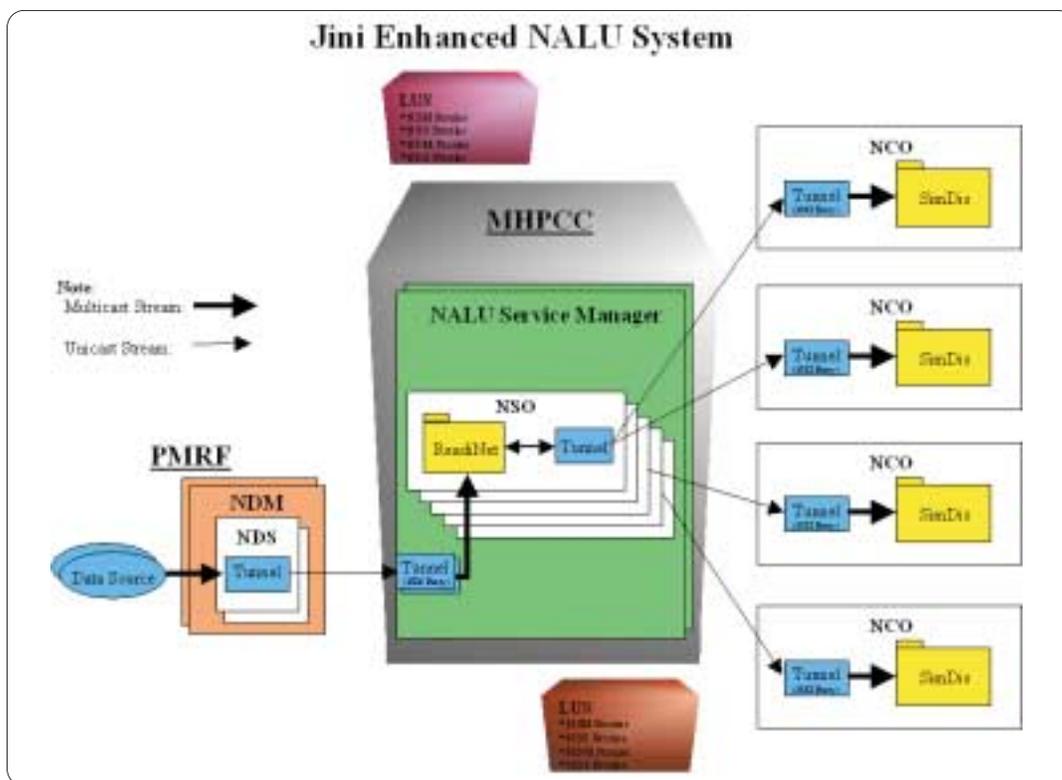


Figure 1. Block diagram of the NALU system. The yellow blocks are "legacy" software. "Tunnels" connect the legacy software to allow wide-area network connections.

Significance: The UESA project for the E-2C Airborne Early Warning radar system and advanced dynamically-managed, enterprise-wide, common integrated information networking systems are among the cornerstones for tomorrow's Navy. The NALU proof-of-concept development and demonstrations have been successful in supporting the Office of Naval Research (ONR) Future Naval Capabilities (FNC) thrusts in the areas of platform protection, missile defense, and command & control technologies. Under this activity MHPCC demonstrated the ability to provide a multi-source data server (NALU) for remote users to request and filter data collected at PMRF, provide spontaneous wide area network (WAN) sockets between instrumentation networks and remote applications, and simulated sensor feeds and job submits to IBM SP supercomputers. Figure 2 below shows a NALU client program that allows a remote user to select a data stream for viewing. Figure 3 shows a screen image of the SIMDIS visualization tool for remote situation awareness. This advanced distributed systems technology development and demonstration showed the ability to utilize "legacy" applications and applications program interfaces, and combine existing network client/server programs into a higher-scaled, more flexible, robust network environment. The NALU concept provides for location-independent data sources, services, and clients that are configurable at start-up or dynamically. It also enables streaming, high bandwidth applications over WAN's and is supportive of the Navy's network centric warfare objectives.



Figure 2. Java client program for NALU: This tool allows the user to select a data stream for SIMDIS viewing.



Figure 3. Typical screen image of the SIMDIS visualization tool showing four platforms, including an aircraft carrier, a cargo ship, a submarine, and a helicopter.

Author and Contact: D. J. Fabozzi

Authors: Carl Holmberg, Bob Swanson, Bruce Duncan

Organization: Maui High Performance Computing Center (MHPCC), 550 Lipoa Parkway, Kihei, HI, 96753

URL: www.mhpcc.edu

Resources: Sun Ultra 80 and IBM RS 6000 SP at MHPCC and a Sun Ultra 10 at PMRF

Acknowledgements: MHPCC graciously acknowledges Keith Lee of Sun Microsystems and Dr. John Binford of the Naval Research Laboratory for their contributions to the NALU project.

Ensemble VOG Forecasts for Kilauea

Steve Businger, Roland Draxler, John Porter

The transport and dispersion of emissions of SO₂ and SO₄ from Kilauea are modeled in a probabilistic rather than deterministic approach using ensemble methods. These pollutants can form volcanic fog (VOG) which, depending upon meteorological conditions, may have health or visibility consequences. The probability results permit local air quality planners to account for model errors in their decision process.

Research Objective: Increasingly faster computational platforms can now complete multiple simulations quickly enough to permit enhancing deterministic model predictions with additional measures of prediction uncertainty. Errors in air quality model results can occur because of inadequate spatial or temporal data resolution, sampling errors, unrepresentative observations, and excessive simplification in the model's representation of physical processes. The dispersion model uses an ensemble

trajectory approach, in that the starting pollutant particle position is varied to account for uncertainties in the source height and model, versus actual terrain heights. These initially small errors may grow quickly in divergent flows.

Methodology: The forecast system is comprised of two components: (1) the meteorological prediction, and (2) the ensemble plume dispersion forecast. The meteorological data are taken from the 10 km and 4 km output fields from the mesoscale version of the Regional Spectral Model (RSM). The dispersion calculations use the HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model. The dispersion model was modified to run in a multi-processor computational environment as an "embarrassingly parallel problem". The dispersion ensemble is composed of 32 members (27 spatial variations and 5 emission variations). The dispersion is calculated through a 3-dimensional Monte Carlo approach. A fixed number of particles (2500) are released, at a constant rate, over each 48 hour meteorological forecast period.

Results: A "probability exceed" plot, the probability of NOT exceeding a specific concentration, is shown in Figure 1. In this example, the contours represent the probability that the air concentration will be less than the user-selected level of 1 µg/m³ (C+0 = 10⁰). The innermost contour indicates that only 50% of the ensemble members had higher concentrations within the contoured region. Air concentrations decrease with distance from the source; hence, a greater probability of not exceeding the selected level.

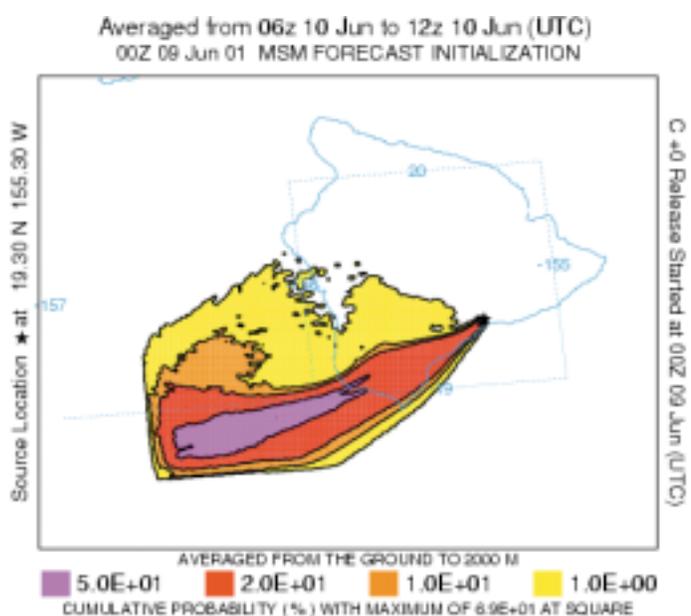


Figure 1. "Probability Exceed" Plot

Significance: Deterministic model predictions provide a sense of confidence that is not always supported by the underlying model assumptions. These issues are well known among the model developers and other experts, but are frequently overlooked when the model results are transmitted to the consumer of these products. Model pollutant-prediction-uncertainty information can be critical for economic decisions, regulatory applications, and human health issues, especially for the atmospheric release of hazardous materials.

Author and Contact: Roland Draxler

Organization: NOAA Air Resources Laboratory, 1315 East West Hwy., Silver Spring, MD, 20910

URL: www.mhpc.edu/projects/contrib/ensemble or www.arl.noaa.gov/data/ensemble

Authors: Steve Businger and John Porter

Organization: University of Hawaii, Dept. of Meteorology, 2525 Correa Road, Honolulu, HI, 96734

URL: www.eos.hawaii.edu/bkgnd_aer/aerosol_page.html

Resources: IBM SP at MHPCC

Modeling Dislocation-Grain Boundary Interactions in Polycrystal Copper Plasticity

Farid F. Abraham

We have focused on one of the key issues in polycrystalline plasticity, the unit mechanisms involving the interactions between dislocations and grain boundaries (GB). Using a combination of large-scale molecular dynamics simulations based on an embedded atom potential and an analysis in terms of the line-tension model, we have identified and characterized the geometrical parameters that govern the occurrence of slip transmission, absorption, and blockage in dislocation-GB interactions. The results provide a guideline for the development of quantitative micro-constitutive equations for dislocation-GB interactions to be used in meso-scale simulations of polycrystal plasticity.

Research Objectives: Quantitative modeling of polycrystal plasticity requires a computational approach that couples the physics of individual dislocations to the evolution of large collections of dislocations, and ultimately, to the aggregate behavior of grain microstructures under stress. As a step in the construction of such a model, one must understand the unit defect mechanisms that govern the behavior of the system at the atomistic level and provide the basis for a description on higher scales. One of the fundamental issues in this context concerns the elementary interactions between dislocations and grain boundaries.

Methodology: Characterization and quantification of such interactions is a very challenging task, given the complex nature of the involved unit mechanisms. Figure 1 gives an illustration of the complexity involved in characterizing and

quantifying dislocation-GB interactions. It shows an atomistic configuration obtained from large-scale Molecular Dynamics (MD) simulations of dislocation-GB collisions in Cu modeled. In these simulations, dislocations were emitted from a crack tip in one of two grains separated by a symmetric tilt boundary. Under the influence of the crack-tip stress, dislocation loops are nucleated on two planes oblique to the crack front. As the dislocations continue to expand under stress, their interaction with the boundary is seen as the dislocations penetrate the grain boundary.

Results: The results obtained from such atomistic simulations can be cast in the form of a database characterizing the outcome of dislocation-GB encounters as a function of the relevant collision parameters. The main obstacle here is a possibly large number of parameters required to fully characterize such collisions. The purpose of this work is to investigate which of the possible parameters are most relevant in characterizing and quantifying dislocation-GB collisions. In order to do so, we exploit dislocation-GB collisions within the framework of a simple "line-tension" model.

Significance: While crude, our model provides qualitative indications suggesting relatively simple functional relationships between GB/slip geometry and slip transmission conditions. The obtained results are verified by comparison with large-scale MD simulations and experimental data. This information serves as a guideline for specifically targeted atomistic and dislocation dynamics studies aimed at providing quantitatively accurate material-specific slip transmission rules in the dynamics of polycrystalline plasticity.

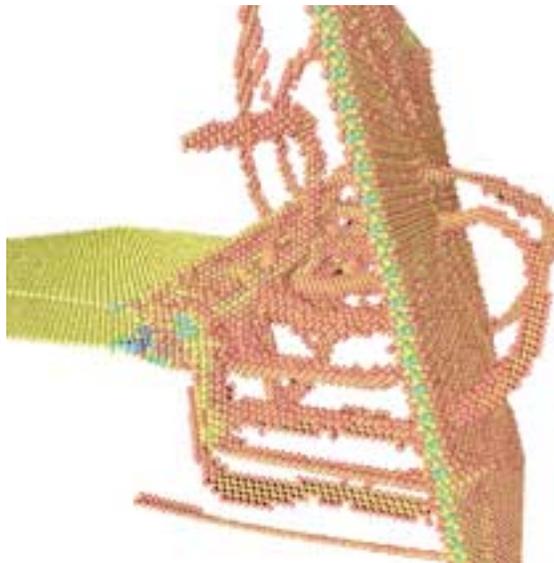


Figure 1. Atomistic configuration obtained from large-scale Molecular Dynamics (MD) simulations of dislocation-GB collisions in Cu modeled.

Author and Contact: Farid F. Abraham

Organization: IBM Research Division, Almaden Research Center, K18/D1, 650 Harry Road, San Jose, CA, 95120

Resources: IBM SP at MHPCC

Acknowledgement: In collaboration with R. Miller (University of Saskatchewan, Saskatoon, Saskatchewan, S7N 5A9 Canada), and M. de Koning and V. V. Bulatove (Lawrence Livermore National Laboratory, University of California, CA, 94550)

High-Resolution Weather Modeling for Improved Fire Management

Kevin Roe, Duane Stevens, Carol McCord

Several weather variables, such as wind, temperature, humidity and precipitation, make direct impacts on the practice of managing controlled burns and fighting wild fires. State-of-the-art Numerical Weather Prediction (NWP) enables the short-term forecasting of near-surface weather. This project integrates three complementary model types to aid federal agencies in real-time management of fire¹. A highly complex, full-physics mesoscale weather prediction model, MM5, is applied in order to estimate the weather fields up to 72 hours in advance. A nested grid technique is used to incorporate terrain down to a one-kilometer grid scale². A diagnostic fire behavior model, FARSITE, takes the near-surface weather fields and computes the expected expansion of wind, humidity, and fuel driven fire³. A tracer, transport and diffusion model is applied in order to provide estimates of smoke and haze.

Research Objectives: Fires are highly dependent on wind and terrain, which require the forecasts to be done at a high-resolution. Currently the National Weather Service produces forecasts on the order of 30-50 km resolution and has publicly stated that they do not intend to go below 10 km. Since fires can travel rapidly (especially uphill) and their spread rates are strongly dependent on winds, it is important to have wind forecasts and terrain information at a much finer resolution than 10 km. If the terrain data given to the NWP models is not at a fine level, they will miss details such as ridges and valleys, as well as make the model "think" the mountains are smaller because it is only an average terrain height. An example of how this can be a problem is the Idaho/Montana fires of 2000 (Figure 1) where fire spread rapidly through mountainous regions. The fire fighters/incident managers were relying on

coarse forecasts to predict how the weather would behave; this caused problems because the forecasts were generated using data that prevented the model from accurately seeing the terrain details. A resulting problem was higher wind speeds than what was predicted. Finer resolution (i.e., 1 km resolution) simulations may still not be completely accurate, as there may be deficiencies in the physics behind the model, unpredicted events, and sub-kilometer information that could be relevant for wind channel effects. Despite this, these simulations would be a significant improvement over what is currently available.

Methodology: The procedure for enabling incident managers to utilize fine resolution weather forecasts consists of many segments^{1,2}, which occur as follows:

- (1) Prescribed burn or wildfire is identified
- (2) Required resolution is requested (i.e., 3 km, 1 km, etc.)
- (3) Forecast length and interval output requirement is inputted into the model
- (4) Nested domains are created to cover fire
- (5) MM5³ collects global analysis data (and possibly observational data) and does pre-processing to put the data in a format usable by the model
- (6) Simulation is run
- (7) Data is converted to a format suitable for FARSITE⁴⁻⁷ and made ready for download
- (8) Incident managers in the field download the data
- (9) Incident managers do fire behavior simulations using this data

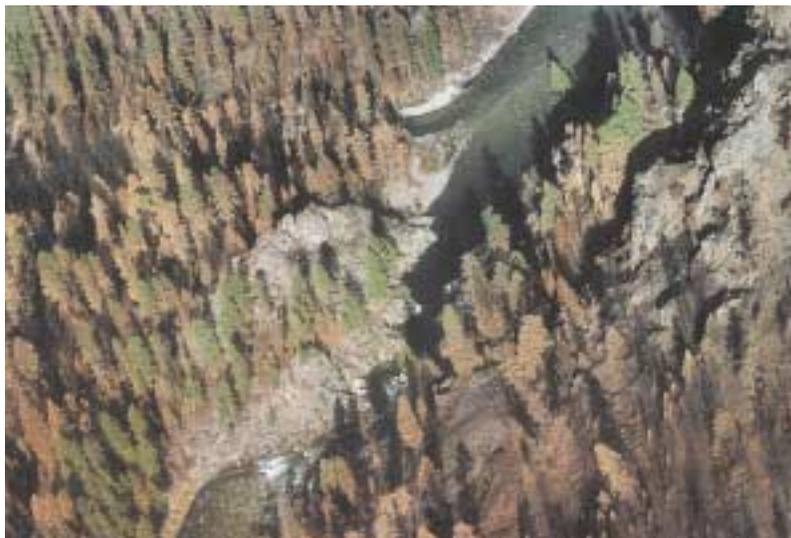


Figure 1. *The Pistol Creek fire swept down the canyon, crossed the middle fork, and blasted the hillside.*

Results: Timing is crucial to make the above methodology work. In order for the incident managers to get the data they need when it is still a prediction, it is crucial to streamline the process. Below is an example of the time required given the current state of the project:

- (a) 2-3 hours to create domains that will accurately handle the required area to be covered.
- (b) MM5 collection of global analysis data from NCEP takes about a $1\frac{1}{2}$ hour to download. Observational data is harder to determine as it is dependent on the sources, but, since the data files are usually very small, it rarely takes more than a few minutes. Pre-processing usually takes about 5 minutes for a 24 hour forecast (10 minutes for a 48 hour forecast).
- (c) 3 hours for a 24 hour forecast. This is a rough number, as the required area coverage and resolution determine run size but 3 hours were required for a 1 km resolution, 24 hour MM5 simulation over the Little Pistol Creek fire of 2000 in Idaho. Run time would be linear if the forecast time is changed to a 48 hour forecast, under the same conditions, it would take approximately 6 hours.
- (d) Approximately fit to 1 hour to produce the required data for the fire behavior simulation (again depending on the length of the forecast).
- (e) Since the simulations that the incident managers do in the field (to determine the appropriate course of action) is beyond the scope of this paper, these simulations will not be included in the time estimation; although the simulations are generally done on laptops in a few minutes.

In short, an initial 24 hour forecast would require approximately 7 hours to complete (an initial 48 hour forecast would require 10 hours). Subsequent 24 hour forecasts in the same area would require 4 hours (7 hours for a 48 hour forecast).

Conclusions: We have created a methodology that will produce fine-resolution weather forecasts. These forecasts can provide useful information for the management of prescribed burns and wildfires. This methodology is focused on providing the required forecasts in a timely manner in order to be useful to the incident managers who will do simulations based on these forecasts and to more effectively manage their available resources.

Future work would entail increasing the resolution of the model (i.e., sub-kilometer resolution simulations), decreasing the response time of the entire operation, and expanding the coverage area. Other areas of potential work include: improving the land-cover and vegetation data, working with other fire fighting organizations, and providing feedback to weather models from the actual fire's behavior (e.g., using a dispersion model).

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Author and Contact: Kevin Roe

Organization: Maui High Performance Computing Center (MHPCC), 550 Lipoa Parkway, Kihei, Maui, HI, 96753

Authors: Duane Stevens and Carol McCord

Organization: University of Hawaii at Manoa, Dept. of Meteorology, HIG 350, 2525 Correa Road, Honolulu, HI, 96734

URL: www.mhpcc.edu/projects/wswx/mm5

Resources: IBM SP3 at MHPCC

Sponsorship: USDA Forest Service

Routine High-Resolution Forecasts/Analyses for the Pacific Disaster Center

John Roads, Jongil Han, Duane Stevens, Derek Funayama,
Carol McCord, Kevin Roe, Francis Fujioka

One of the key aspects of disaster forecasting, response, and mitigation planning is readily available—accurate and timely local-scale weather and climate information. In Hawaii, where weather and climate variations are affected by the steep island topography, there is a clear and acknowledged need for improved weather and climate forecasts at a variety of time and space scales. In that regard, nested mesoscale models could provide a valuable tool to resolve weather patterns for the entire state, as part of a Pacific Disaster Center (PDC) contract. The Hawaii Weather/Climate Modeling Ohana (HWCMO) has implemented quasi-operational mesoscale weather forecasts. Near real-time, high-resolution weather forecasts are made available to the general public on our MHPCC web site (<http://www.mhpcc.edu/~wswx>) and we are also analyzing climatological characteristics of these forecasts. It should be noted that weather forecasts have not previously been systematically applied to the individual islands on scales less than ten kilometers, and MHPCC is the testing ground for future high-resolution operational forecasts.

Research Objective: As part of our support to the Pacific Disaster Center (PDC), the Hawaii Weather/Climate Modeling Ohana (HWCMO) developed a dynamical/physical modeling capability to make short-term (out to 48 hours and even 72 hours upon demand) weather predictions for the individual island counties of the State of Hawaii. We initially used a version of the Mesoscale Spectral Model (MSM), which was developed by the National Centers for Atmospheric Prediction (NCAP). The MSM is able to resolve weather parameters (such as temperature, humidity, winds, rainfall) on horizontal scales down to approximately two kilometers for Hawaii. Since the MSM is nested within the operational global model, the local forecast domain can be relocated anywhere in the world. These predictions can therefore provide local-scale weather information (down to horizontal scales of two kilometers) for environmental disaster managers. Since March

1998, when we ported and implemented the National Centers for Environmental Prediction (NCEP) MSM on a single node of the MHPCC IBM SP2, we have made routine predictions possible. For example, we now routinely run the atmospheric model for individual counties with grid point resolutions of: 2 km for Oahu and Kauai, 3 km for Maui County, 4 km for Hawaii County, and 10 km for the entire Hawaiian Archipelago. Near-surface meteorological variables, including temperature, relative humidity, rainfall, and wind, as well as a derived fire weather index and drought index (soil moisture), are computed by the model.

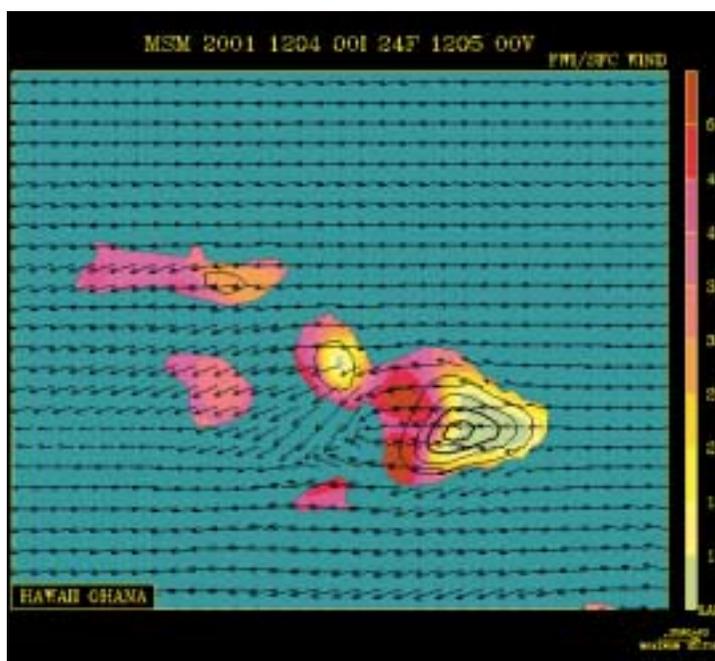


Figure 1. 24 hour Fire Weather Index (FWI) and surface wind forecast for Maui and surrounding islands at 3 km resolution. The forecast was initialized on December 6, 2001, at 00 UTC and validates December 6, 2001 at 00 UTC. This is a typical FWI forecast provided regularly on <http://www.mhpcc.edu/~wswx> for Maui and other Hawaiian islands. Red colors indicate regions of increased fire danger.

Results: During 2001, a number of significant improvements to the previous HWC MO forecasting system were made, including the following:

- (1) Switching the input NCEP files to come directly to NCEP, which significantly increased the forecast start time and increased the reliability of our quasi-operational system;
- (2) Increasing the number of vertical levels to 42 to make the MSM more consistent with the operational global analysis and 3-day aviation forecast;
- (3) Adapting the MSM to the new open-MP SP processors, which means that each county can use at least four processors for numerical computations and additional processors for graphics computations;
- (4) Experimenting with making 72 hour forecasts, but have since cut back to 48 hour forecasts to conserve resources while waiting for demand to build for these extended range forecasts;
- (5) Augmenting current fire weather forecasts with fire danger and drought forecasts that are more compatible with standard USFS fire danger ratings;
- (6) Experimenting with an alternate Mesoscale Model 5th generation (MM5) to see whether it provided any significant advantages over our present mesoscale modeling system (MM5 is more well known and utilized by more agencies, like the USAF, than our MSM); and
- (7) Developing a user manual to describe our system and system output (this user manual will be posted on our web site, upon completion) as part of our work for PDC.

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Author and Contact: John Roads

Author: Jongil Han

Organization: Scripps Institution of Oceanography, UCSD, 0224, La Jolla, CA, 92093

Authors: Duane Stevens and Derek Funayama

Organization: University of Hawaii at Manoa, Dept. of Meteorology, HIG 350, 2525 Correa Road, Honolulu, HI, 96734

Authors: Carol McCord and Kevin Roe

Organization: Maui High Performance Computing Center, 550 Lipoa Parkway, Maui, HI, 96753

Author: Francis Fujioka

Organization: Riverside Fire Laboratory, US Forest Service, Riverside, CA

Resources: IBM SP2 at MHPCC and DEC Alphas at Scripps Institution of Oceanography

Sponsorship: US Department of Agriculture, Forest Service, NOAA Office of Global Programs, NOAA CDEP Program, NASA PDC Program.

The Role of Initial and Boundary Conditions for Dynamical Seasonal Forecasting

Thomas Reichler and John Roads

Changes in climate are often associated with extreme variations that pose serious threats for society. The anticipation of such events a few months ahead can greatly diminish their negative impacts. In recent years there has been considerable improvement in computer-based dynamical climate forecasts, and research centers around the world have started to make seasonal forecasts with numerical weather prediction models on a routine basis. Our research is aimed at developing better seasonal climate predictions with Atmospheric General Circulation Models (AGCMs). The proper specification of sea surface temperatures (SST) as the lower boundary condition for the model are known to be key in producing skill on such long time scales, but still there remain many unknowns in how the information from persistent initial and boundary conditions can be utilized. A related question is how sensitive a seasonal forecast is to uncertainties in the SST forecast, and what time scale this error propagates into the atmospheric forecast. Our strategy for answering these questions is a series of experiments, with a state-of-the-art dynamical climate model, which has been forced with different combinations of initial and boundary conditions.

Research Objectives: This study uses the global spectral model developed at the National Center for Environmental Predictions with a horizontal resolution of approximately 300 km and 28 vertical layers. In each experiment, we simulated the evolution of the atmosphere from mid-December through the end of March of the following year, over a 22-year period (1978-2000). Since the chaotic nature of the atmosphere requires a probabilistic approach, we repeated each experiment ten times by starting from slightly perturbed initial conditions but forcing with identical boundary conditions.

Methodology: Our measure of forecast skill uses the pattern similarity of the 500 hPa height (mid-atmosphere) surface between

observations and model data. When forcing the model with observed sea temperatures and sea ice, we find instantaneous skill on all time scales from day 1 out to day 107 (Reichler, et. al., 2001c). There exist considerable differences in skill from year to year, which can be explained to a large extent by anomalous forcing from unusually warm or cool waters over the tropical Pacific during ENSO (El Niño Southern Oscillation) events. Years with large anomalous tropical SSTs are more predictable than years with weak tropical SST forcing. By taking monthly or seasonal time averages, the skill increases dramatically since the noisy components are effectively filtered.

Results: An important question is how much the proper specification of initial conditions contributes to seasonal forecast skill. Our analysis shows that even though the atmospheric circulation is highly chaotic, the effect of initial conditions lasts surprisingly long. We find that the influence of the initial conditions, without forcing from the boundaries, lasts for approximately 40 to 60 days (Reichler, et. al., 2001a). When starting the model from random initial conditions with no boundary forcing, it takes the atmosphere roughly 40 to 50 days to fully adjust to the new boundary conditions. When started from observed initial conditions, anomalous boundary forcing from the oceans affects the overlying atmosphere after roughly 14 days. Even for seasonal means, we find that proper initial conditions are important for a good skill. This is particularly true for years with only weak boundary forcing.

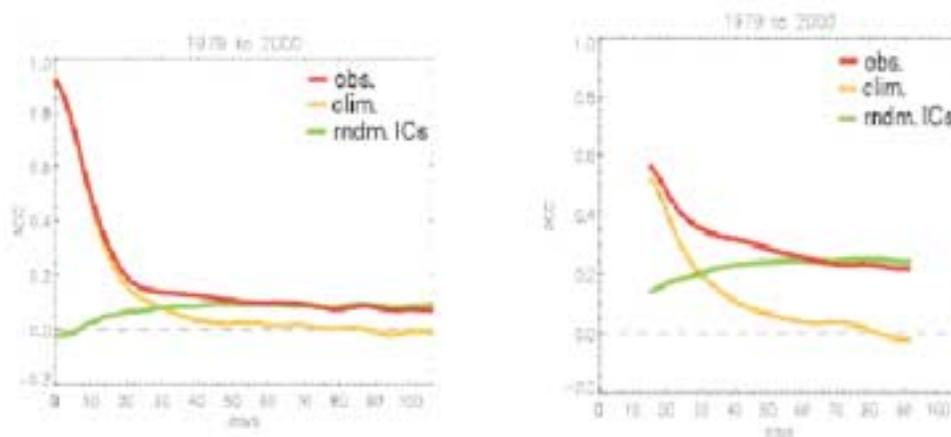


Figure 1. Time evolution of instantaneous (left) and 30 day time averaged (right) skill for forcing with observed SSTs (red), no forcing (yellow), and forcing with observed SSTs but initializing with random ICs (green).

Significance: We also looked at the effects of using persistent SST instead of real SST forecasts (Reichler, et. al., 2001a). The seasonal mean skill (January-March) drops by only 10% when using persistent SSTs, compared to using observed SSTs. This result shows that the error associated with persistent SST forecasts is tolerable on seasonal time scales. At longer lead times of 6 months, the difference in seasonal mean skill (April, May, June) between observed and persistent SST increases to 30%. At these time scales, the use of more sophisticated SST forecasting techniques may be critical.

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Author and Contact: John Roads
Author: Thomas Reichler
Organization: Scripps Institution of Oceanography, UCSD, 0224, La Jolla, CA, 92093
URL: <http://ecpc.ucsd.edu>
Resources: IBM SP2 at MHPCC and DEC Alphas at Scripps Institute of Technology
Sponsorship: NOAA Office of Global Programs.

General Earthquake Models: Self-Organizing Patterns of Earthquakes Observed In Numerical Simulations and Data

John B. Rundle, Kristy Tiampo, Andrea Donnellan

Self-organization processes in complex earthquake fault systems occur at all scales, from the microscopic scale (10^{-8} to 10^{-4} m) to the laboratory scale (10^{-4} to 10^1 m) to the field scale (10^1 to 10^6 m). The strong space-time correlations that are responsible for the cooperative behavior of these systems arise both from the threshold dynamics, as well as from the mean field (long range) nature of the interactions. As we have described elsewhere, driven threshold systems can be considered to be examples of phase dynamical systems when the rate of driving is constant. In earthquake faults, the stress is typically supplied at a steady rate, but is dissipated episodically by means of the earthquakes. Due to the mean field nature of both the simulated and real threshold systems, it is found from simulations that as the size of the system is increased, the amplitude of the "small fluctuations" decreases roughly as $1/\sqrt{N}$.

Research Objective: Earthquakes in seismically active regions have long been known to demonstrate self-organizing spatial and temporal patterns of behavior that are difficult to interpret, or to use in forecasting future activity. The patterns arise out of the fundamentally nonlinear nature of the underlying dynamics. One of the major problems has been that large events responsible for the greatest damage repeat at irregular intervals of hundreds to thousands of years, a limited historical record that has frustrated phenomenological studies. An alternative approach, which is the primary goal of the General Earthquake Model (GEM) project, is to develop a "numerical laboratory" in which the physics of earthquakes can be investigated from a systems viewpoint. One of the first goals of our

team's work has been to quantitatively define the major space-time patterns observed in active regions, so that changes in the observed patterns can be correctly interpreted in terms of future hazards. The impact of this new simulation technology on earthquake science will be to allow hypothesis testing and data integration on a scale not here-to-fore possible.

Methodology: Using both simulations and observed earthquake data, it can be shown that the space-time patterns of earthquakes can be represented by a time-dependent system state vector in a Hilbert space. The length of the state vector represents the temporal frequency of events throughout the region, and is closely related to the rate at which stress is dissipated. Since the information about the system state is represented solely by the phase angle of the state vector, these systems are called "phase dynamical" systems. The analysis of such systems proceeds by using mathematical procedures similar to those used to described quantum mechanical systems. Changes in the norm of the state vector observed in a real system, such as the southern California earthquake fault system, represent only random fluctuations, and can essentially be removed by requiring the system state vector to have a constant norm.

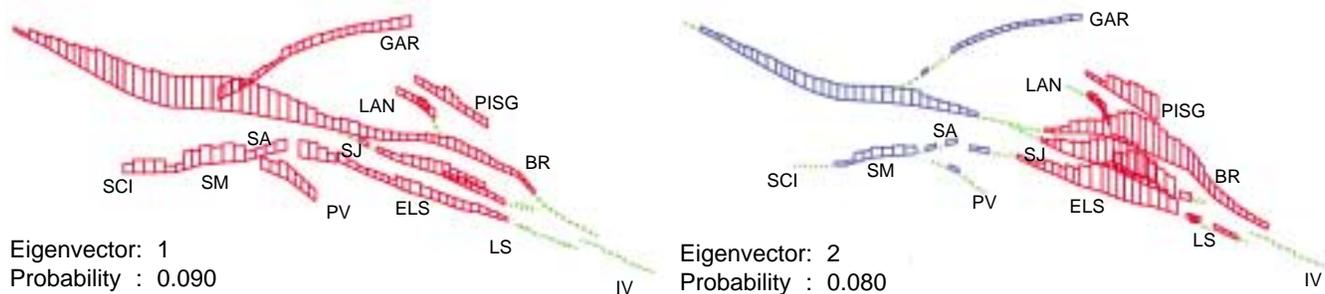


Figure 1. First two eigenpatterns $\phi_n(x_i)$ of $N = 215$ total eigenpatterns from a numerical simulation of earthquakes on the major faults of southern California. Activity at red (blue) areas are positively correlated with other red (blue) areas, and activity at red and blue areas are negatively correlated. For example in eigenpattern 2, red areas tend to be active on average when other red areas are active, and blue areas are active when other blue areas are active. However, red areas tend to be active when blue areas are inactive, and vice versa. The data set used was 5000 time steps of simulated earthquakes on the fault system shown. Faults shown are San Andreas (SA); Garlock (GAR); Landers (LAN); Pisgah (PISG); San Jacinto (SJ); Elsinore Fault (ELS); Laguna Salada (LS); Palos Verdes (PV); Santa Monica (SM); and Santa Cruz Island (SCI).

Results: The idea of analyzing space-time earthquake patterns arising from pure phase dynamics has led us to modify a method frequently used in atmospheric science, "Principal Component" or "Karhunen-Loeve" analysis. In this method, we spatially coarse-grain either the faults or the geometric region under study to produce either N fault segments or N spatial boxes. For such a lattice of boxes, a set of orthonormal basis vectors $\varphi_n(\mathbf{x}_i)$ can be constructed, where \mathbf{x}_i denotes the spatial location of the i^{th} segment or box ($i = 1, \dots, N$). Physically, the $\varphi_n(\mathbf{x}_i)$ represent spatial patterns ("eigenpatterns") of earthquake activity defined on the N segments or boxes. In the examples below, we show the first two eigenvectors produced both by a simulation, and from actual data in southern California.

Significance: Earthquakes in urban centers are capable of causing enormous damage, with costs in the hundreds of billions of dollars, and with many thousands of lives lost. The difficult problem of forecasting damaging earthquakes depends on understanding the physical significance of patterns of these events in space and time, and how changes in the patterns of small earthquakes are related to the occurrence of future great and catastrophic events. Our work allows understanding and interpretation of these patterns, and may point the way toward the development of the first practical earthquake forecast technologies.

KLE1 for Southern California Seismicity, 1932-1998

KLE2 for Southern California Seismicity, 1932-1998

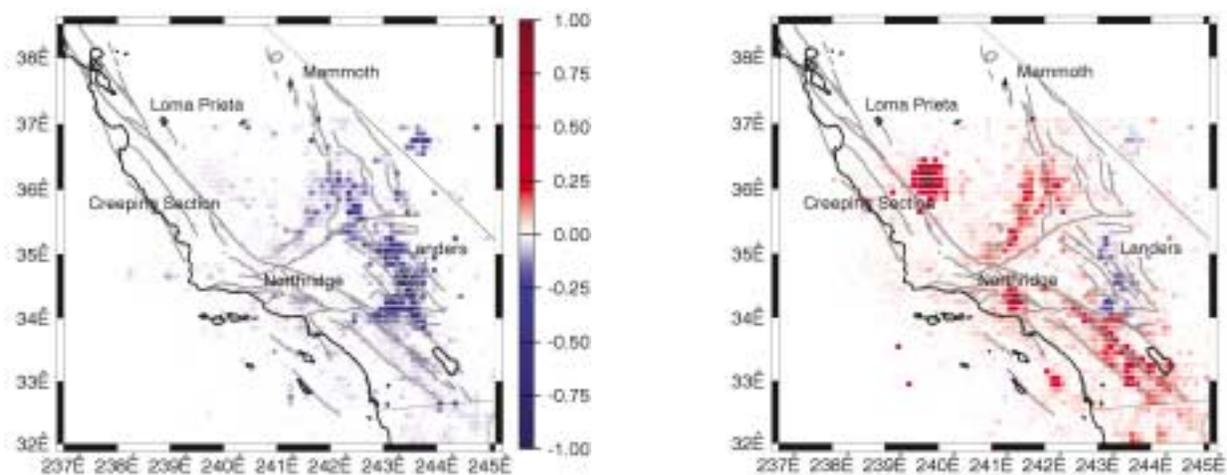


Figure 2. *First two eigenpatterns from earthquakes in southern California. The data set used is all the instrumentally recorded earthquakes larger than magnitude = 3 that have occurred in southern California since 1932.*

Author and Contact: John B. Rundle
 Author: Kristy Tiampo
 Organization: University of Colorado, Campus Box 216, University of Colorado, Boulder, CO, 80309
 Author: Andrea Donnellan
 Organization: Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, California, 91109
 URL: <http://geodynamics.jpl.nasa.gov/gem/>
 Resources: IBM SP at MHPCC
 Sponsorship: NASA, NSF, DOE

Ab Initio Calculations Characterizing an Effective Hamiltonian for Polymeric Photonic "Muscles"

James Newhouse, Debi Evans, Joe Ritter

Nanoscale "photonic muscles" are studied by a research group associated with Prof. Debi Evans at the University of New Mexico (UNM). The photonic molecular muscles act as nano-scale actuators to correct the less-than-ideal original figure of the space-based optics proposed by Dr. Joe Ritter. Dr. James Newhouse is using parallel machines at MHPCC to calculate parameters for the Effective Hamiltonian of the polymer/pyrene excimer/excimer system (one of several proposed) via *ab initio* calculations using Gaussian 98 A.11, and Q-Chem 2.0.1/1.2. The Effective Hamiltonian is used by Prof. Debi Evans in molecular dynamics simulations to simulate the force and throw of different variants of the molecular muscles, and the behavior of energy transport along the polymer/pyrene system to the site of excimer formation by means of Frenkel excitons. The excited states of the molecules are obtained using the Time-Dependent Density Functional Theory method in Q-Chem.

Research Objectives: The research group proposes to design, construct, and characterize a new class of molecular motors called polymeric muscles, which are polymer molecules that have the ability to contract and generate forces. Because they are the simplest to design and build, but still very versatile, they will focus on photon-powered polymeric muscles, or "photonic muscles". Structurally, photonic muscles are composed of two major parts: a parent polymer molecule (e.g., polystyrene) and a chromophore that forms tightly-bonded excimer pairs when excited by light (e.g., pyrene). The chromophores are attached to the parent polymer by linker arms at regularly spaced intervals so that when the photonic muscle is exposed to light excimer pairs form and the polymer contracts.

Significance and Vision: The overall goal of the "photonic muscles" project is to develop a new kind of molecular machine, the polymeric muscle, and use it to build useful nano-devices. A polymeric muscle is a polymer molecule with the ability to contract and generate forces. The simplest photonic muscle is a polymer molecule with pendant groups spaced along its length (see Figure 1). The pendant groups form tightly bonded excimer pairs when excited by a photon, so that the polymer molecule contracts when exposed to light and thus converts radiant energy into mechanical work. A simple example of such a photonic polymer has been synthesized, and the first experiments (which demonstrate its ability to contract when illuminated) have been carried out. The photonic muscle should be both strong (piconewtons at the single molecule level) and fast (tens of microseconds).

Methodology: The exciton model requires calculation of the adiabatic surfaces and the coupling between them. Given that an *ab initio* electronic structure calculation for the entire polymer is not feasible, a small fragment of the polymer [most likely a chromophore dimer] will be used to generate this data on the assumption that these dimer units are essentially uncoupled. As a starting assumption, distortion of only one mode will be considered. If more than one mode is strongly coupled to the dynamics, subsequent wavepacket propagation will be done using the time-dependent Hartree approximation, which scales favorably with the nuclear degrees of freedom.

Exciton properties in the absence of coupling to the polymer backbone will be accessed from electronic structure calculations. For localized excitations, the Frenkel-exciton model is directly applicable, and can be used to generate the necessary Hamiltonian for the dynamical processes. The Frenkel model describes a general aggregate made out of L interacting two-level chromophores. To describe its electronic states we introduce the exciton creation (annihilation) operators (B_n^\dagger / B_n) which add (eliminate) an excitation on the nth chromophore that satisfy the fermion commutation relations. Using these operators, the Frenkel Hamiltonian reads:

$$\hat{H} = \sum_{kn} A_{kn} B_k^\dagger B_n + \sum_j H_{loc}(x_j) + \sum_{j,k} x_j \Delta_{jk}^\dagger B_j^\dagger B_k$$

The first term represents the purely excitonic system:

$$A_{kn} = \omega_k \delta_{kn} + J_{kn}$$

where ω_k are the on-site exciton energies, and J_{kn} are the site-to-site exciton transfer matrix elements. Diagonalization of A_{kn} would give the one-exciton eigenstates and energies of the system in the absence of coupling to the polymer vibrational modes. *Ab initio* simulations of chromophore dimers and trimers will be used to obtain the above matrix elements for the exciton states in the absence of nuclear interactions.

The polymer vibrational modes are taken to be harmonic [the second term in the Hamiltonian], and the coupling to the exciton motion is taken to be a bilinear coupling [the third term in the Hamiltonian]. The dissipative effects of the polymer distortion are more difficult to obtain.

Results: *Ab initio* calculations by Dr. James Newhouse have focused on the excited states of pyrene and characterization of the pyrene dimer by means of the CIS method in Gaussian (Configuration Interaction Singles) and the XCIS method in Q-Chem (extended Configuration Interaction Singles).

Significance: Fundamental understanding of the behavior of exciton energy transfer in the polymer/pyrene excimer/exciton system and the nature of the forces generated and the distance over which the photonic muscles would act (throw) will result. The effective design of such nanoscale systems will be learned, making them useful in many different applications as outlined in the UNM proposal. Application to correcting space-based optics is a challenging example.

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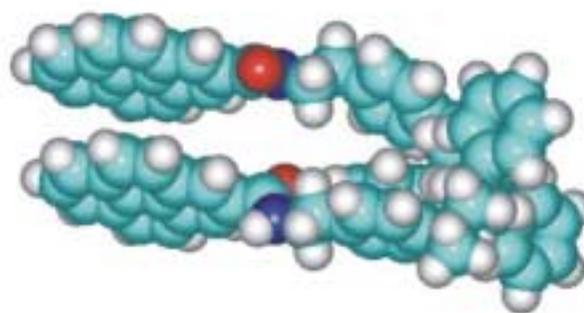
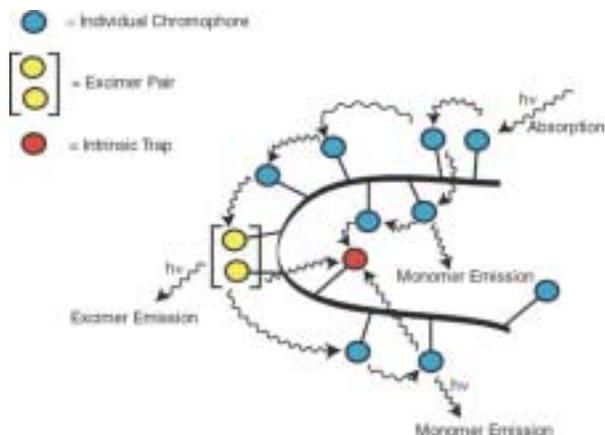


Figure 1. Paths of energy migration and deactivation from the "Nanoscale Photonic Muscles: Fundamentals and New Techniques" by Brozik, Evans, Hampton, Keller, and Lopez (University of New Mexico)

Figure 2. Four polystyrene repeating units with attached pyrenes in approximate excimer orientation. HyperChem Model.

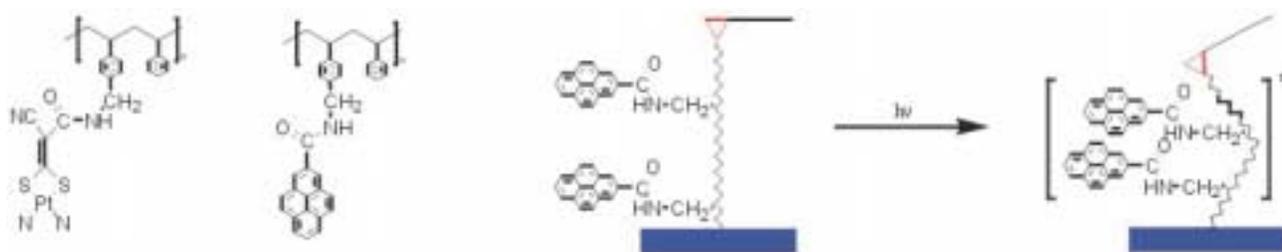


Figure 3. Conceptual model of "photomuscles". Average conformation will be greatly contracted in the excited state because excimer will hold the contracted geometry longer than a single randomly occurring fluctuation. From the "Nanoscale Photonic Muscles: Fundamentals and New Techniques" by Brozik, Evans, Hampton, Keller, and Lopez (University of New Mexico).

Author and Contact: James S. Newhouse
 Organization: Maui High Performance Computing Center, 550 Lipoa Parkway, Kihei, Maui, HI, 96753
 Author: Debi Evans
 Organization: University of New Mexico, Department of Chemistry, Albuquerque, NM, 87131
 Author: Joe Ritter
 Organization: SAIC, Technology Research Group, 590 Lipoa Parkway, Building B, Kihei, HI, 96753
 Resources: IBM SP3 and SGI Octane dual R12000 at MHPCC
 Sponsorship: Defense University Research Initiatives on NanoTechnology

Isomerizations and Relative Kinetic Stability of LJ_n Clusters in a Carrier Gas

Curotto Emanuele

We have investigated the kinetic stability of Lennard-Jones clusters at relatively elevated temperatures inside carrier gases. Heat capacity and isomerization data demonstrate that Lennard-Jones clusters become kinetically more stable as the carrier gas density increases.

Research Objectives: The anomalous melting of weakly bound complexes has been the subject of numerous theoretical investigations¹⁻⁵. These exotic molecules melt at a temperature that is significantly lower than the freezing temperature as a result of their finite size. Studying the phenomenon experimentally is very challenging for two main reasons: a) The temperatures involved are very low (20 to 60 K) requiring specialized

techniques such as jet expansions, and b) at temperatures above melting, the cluster may not "melt" at all, but "evaporate" instead, depending on the experimental conditions. Our group has explored the possibility of using a chromophore inside a cluster to follow the melting spectroscopically, but the issue of stability at these relatively elevated temperatures has to be dealt with carefully. Using Monte Carlo simulations, we are able to show that a carrier gas stabilizes mass-selected clusters at and above melting by increasing the evaporation time scale. The objective of the present work is to establish how the thermodynamics of clusters is influenced by a carrier gas at different densities.

Results: We use the hard sphere model for the carrier gas interactions and the carrier gas cluster interactions, and the Lennard-Jones potential for the interaction between cluster particles. Cubic periodic boundary conditions are used for the carrier gas particles while the walls of the cube are perfectly reflecting for the cluster. Parallel tempering⁶ is used to reduce quasi-ergodicity in the Metropolis algorithm.

In Figure 1, two areas of rapid change can be identified. The first, which peaks around $T^* = 0.18$, is associated with the melting of the cluster. The second feature, associated with the cluster evaporation, is visibly affected by the carrier gas density and decreases in intensity dramatically. The data demonstrates that the melting range becomes better defined, and the evaporation of the cluster is shifted to higher temperatures as the density of the carrier gas increases.

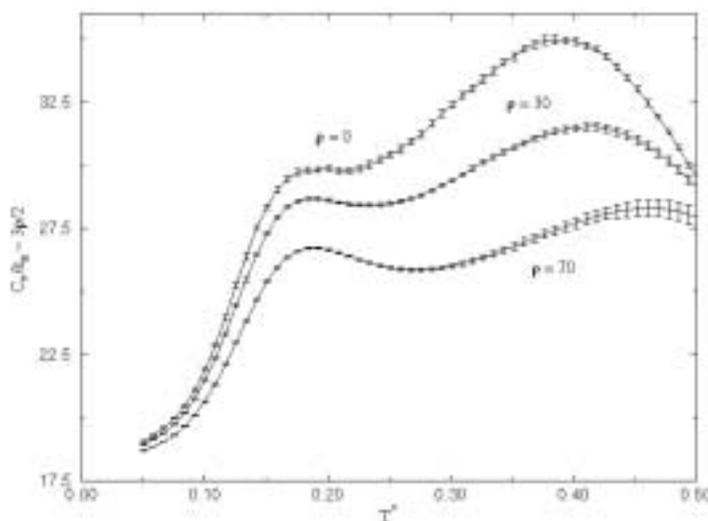


Figure 1. The dimensionless heat capacity of LJ_7 as a function of the reduced temperature ($T^* = T/119.4$ K which is the dissociation energy of Ar_2 divided by Boltzmann's constant) for several values of the gas density. The carrier gas contribution to the heat capacity was subtracted from the graphed quantities for ease of comparison.

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Author and Contact: Curotto Emanuele

Organization: Department of Chemistry & Physics, Arcadia University, 450 South Easton Road, Glenside, PA, 19038-3295

URL: <http://www.arcadia.edu>

Resources: IBM SP at MHPCC and Silicon Graphics O2 workstation at Arcadia University

Acknowledgement: The Stacy Ann Vitetta '82 Professorship Fund and The Ellington Beavers Fund for Intellectual Inquiry are greatly acknowledged. This research has also been supported in part by the Air Force Research Laboratory, Air Force Materiel Command, USAF, through the use of MHPCC resources.

MHPCC Assists Project EAST Students in Mapping Ground Features at Kealia Pond National Wildlife Refuge, Maui, Hawaii

Scott Splean

Project EAST (Environmental And Spatial Technology) is a four-year-old national educational initiative with more than 10,000 student participants. Project-oriented learning is used to encourage students to think creatively and critically. Technology is used as a tool to focus the intellectual skills of students, and to prepare the students for the Information Age.

Project EAST students recently began research projects at the Kealia Pond National Wildlife Refuge (NWR), assisted by the Maui High Performance Computing Center (MHPCC) Geographical Information System (GIS) specialist. Project EAST student research at Kealia Pond NWR includes hydrologic and vegetation modeling, and endangered native waterbird and migratory waterfowl surveys. Using hand-held Global Positioning System (GPS) data receivers, students geo-reference important ground features

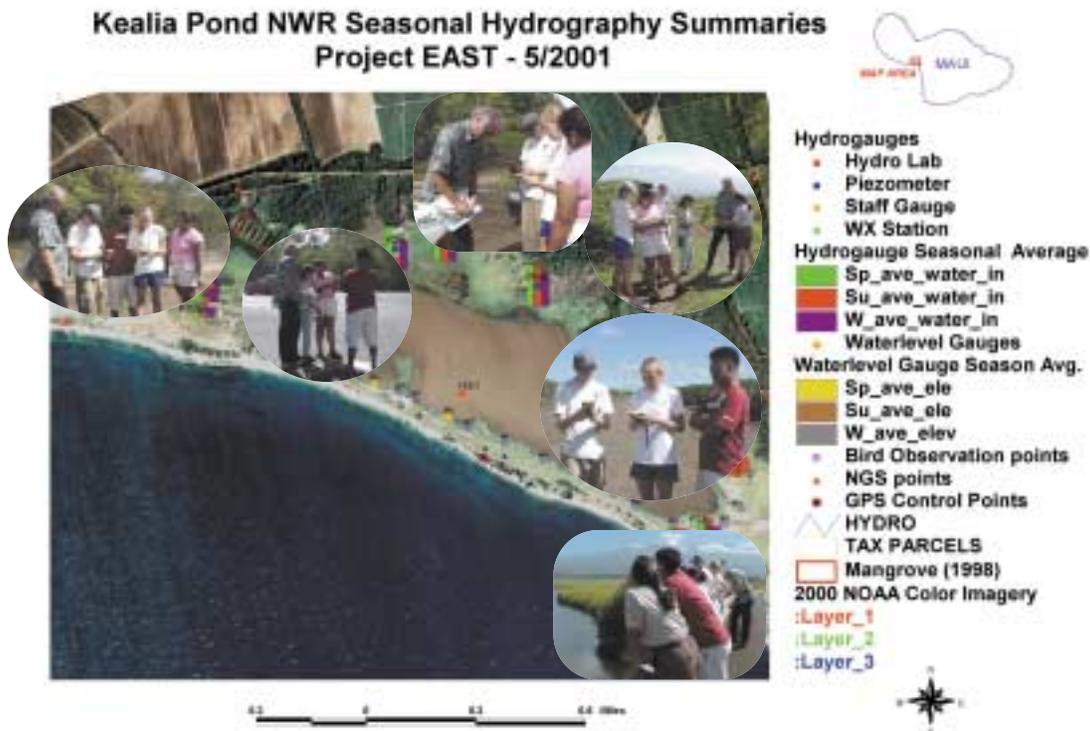
in and around the refuge. Geographic coordinates from GPS orbiting satellites of the Department of Defense's GPS were captured for each feature. Geo-referenced data include permanent features such as intersections, bridges, towers, roads, and buildings, as well as key research features such as hydrographic gauges, bird transects, and vegetation plots. The information gathered is uploaded to a GIS, a computer-mapping program that allows for data storage, analysis, and mapping. Important refuge ground features are cataloged by the EAST students and combined with historical and contemporary digital data, including aerial and satellite imagery. These data will later be merged with current GPS benchmark surveys of the area.

Objective: Students solve real world problems in their schools and communities by:

- Working in teams and individually
- Becoming productive participants in the community
- Enhancing their intellectual growth and creative thinking skills
- Employing the use of cutting-edge technologies
- Completing projects that provide solutions to real-world problems

MHPCC Project EAST Support Includes:

- Staff scientific expertise and mentorship
- GPS/GIS application development
- Computer storage of GIS data
- Computer server use for web-based projects
- Wireless Internet capability for field projects
- Streaming media capabilities
- Spatial technologies training



Author and Contact: Scott Splean

Organization: Maui High Performance Computing Center (MHPCC), 550 Lipoa Parkway, Kihei, Maui, Hawaii, 96753

URL: www.mhpcc.edu

Resources: Trimble GeoExplorer3 GPS receivers and MHPCC GIS resources and servers

Sponsorship: MHPCC

Novel Ultra-Lightweight Space Telescopes Using Optically Active Polymer Membrane Mirror Shape Control

Joe Ritter, James Newhouse, Debi Evans, Jim Brozik

The development of novel lightweight space qualified optics and support structures is of vital importance to science, to industry, and to national defense. High-resolution space imaging requires the production of lightweight large aperture optics, subject to design tradespace constraints based on nanometer physical tolerances, low integrated system aerial density, control authority, deployment, thermal and mechanical properties, launch vehicle volume constraints, as well as production cost and schedule risk mitigation. The new generation of deployable-segmented large aperture systems imposes an even tougher set of requirements on segment alignment, wavefront phasing, deployment, and mass constraints. Primary mirrors are one of the main drivers of the mass of space based optical systems, as the other spacecraft masses scale proportionally with the optical system mass. Therefore lightweight optics are an essential component of SAIC's commitment to reducing launch costs while increasing payload utility. Ongoing experiments are providing a foundation the development of light-activated shape control of deployable ultra-light space telescope mirrors. This technology will enable large diffraction limited membrane optics, as well as multiconjugate super adaptive optics.

Research Objectives: Proposed missions like the Next Generation Space Telescope, and Larger Gossamer optics supporting the NASA Origins program, as well as proposed space and air based laser systems depend on the successful development of ultra-lightweight mirrors. In diffraction limited systems resolution is inversely proportional to the aperture diameter. This requirement, along with the need for gathering many photons from distant and dim sources, drives the requirement for ultra-low density large aperture telescope primaries.

In order to achieve a million-fold improvement in area/density, 100-fold improvement in light gathering capability, 10-fold improvement in spatial resolution, and factor of 10 reduction in production and deployment cost, photoactive isomers have been incorporated

into space durable polyimide membrane optics (as well as other polymers) to construct nanomachine "laser controlled molecular actuators" to provide non-contact active figure control, allowing a robust response to pointing, slewing, and thermal perturbations. This project joins technologies at vastly different scales, the nanoscale "photonic muscles" studied by Professors Debi Evans and Jim Brozik (University of New Mexico), and a project of Dr. Joe Ritter (SAIC/University of Hawaii) utilizing a different class of photonic muscles to fabricate ultra-thin, ultra-light ultra-large optics for deployment in space. The ongoing research is to merge these two technologies to develop a completely novel approach to the production and figure control of ultra-lightweight (< 0.1 kg/m²) diffraction limited active optics.

The research team is seeking to develop technology to build telescopes with apertures from 20 to 60 meters in diameter. Future missions (Terrestrial Planet Imager) which require up to 4000 square meters of primary mirror and multiple apertures, can only be implemented by substantially reducing mirror density, as well as by lowering fabrication costs, both of which are addressed by the enabling optically active polymer mirror laser shape control technology. Most importantly, reducing payload mass means reducing launch costs. The goal is to produce an Ultra-light-weight membrane optic (<100g/m²) whose shape can be remotely controlled using lasers. This will eliminate the need for actuators thus providing significant mass reduction. This also provides a way to excite vibratory modes to couple with and damp out normal modes of oscillation induced by motion and thermal changes, thus allowing a robust response to slewing. Polymers have low density, high packing efficiency, and can be fabricated out of space durable polyimides having a low CTE. A prototype photoactive polymer mirror was developed by Joe Ritter

Photonic Muscles: Recently it has become apparent that it will soon be possible to build molecular-scale machines and devices. This new technological thrust is partly inspired by biology and partly by the decreasing dimensions of semiconductor devices, and will result in novel devices set apart from any others currently used and understood. Work on molecular machines today is as important and fundamental as work on semiconductors was 50 years ago.

Early work by Ritter later funded by NASA under the Gossamer initiative investigated use of Cis-Trans isomerization to effect figure change in membrane optics. As an extension of this, the research group proposes to design, construct, and characterize a new class of excimer based polymeric muscles. The simplest photonic muscle is a polymer molecule with chromophore pendant groups spaced along its length that forms tightly bonded excimer pairs which when excited by light contracts and thus converts radiant energy into mechanical work. A photonic polymer has been synthesized, and first experiments demonstrating its ability to contract when illuminated have been performed.

Adaptive Optics: Current AO correctors for 4 meter class telescopes cost several million dollars, burn out when stressed, and limit the field of view that can be well corrected. Larger and multi-aperture telescopes require higher than currently available actuator density and number, and larger deformable mirrors, which cannot currently be produced at any price. Current efforts are scale limited by the size of silicon wafer technology. Prototype supercorrectors with a few thousand corrective elements have been produced at very high cost, and they are far from the large aperture "virtual megapixel correctors" proposed by Ritter. This novel research effort presents both a completely new production technique along with a potentially vastly superior novel non-contact control technique. This technology opens up the possibility of a light based physical computer closed loop correction of secondary optics which in turn control wavefront phasing, i.e., an adaptive optics system with a physical as opposed to computer processor. This amazing possibility of having enormous bandwidth has never been proposed, and is a likely spin-off of this effort.

Methodology: Dr. James Newhouse is using parallel machines at MHPCC to calculate parameters for the Effective Hamiltonian of the polymer/pyrene excimer/excimer system via *ab initio* calculations using Gaussian 98 A.11, and Q-Chem 2.0.1/1.2. The Effective Hamiltonian is used by Prof. Debi Evans in molecular dynamics simulations to simulate the force and throw of different variants of the molecular muscles, and the behavior of energy transport along the polymer/pyrene system to the site of excimer formation by means of Frenkel excitons. The excited states of the molecules are obtained using the Time-Dependent Density Functional Theory method in Q-Chem.

The exciton model requires calculation of the adiabatic surfaces and the coupling between them. Given that an *ab initio* electronic structure calculation for the entire polymer is not feasible, a small fragment of the polymer (most likely a chromophore dimer) will be used to generate this data on the assumption that the dimer units are essentially uncoupled. Initially, distortion of only one mode will be considered. If more than one mode is strongly coupled to the dynamics, subsequent wavepacket propagation will be done using the time-dependent Hartree approximation, which scales favorably with the nuclear degrees of freedom.

Exciton dynamics: Exciton properties in the absence of coupling to the polymer backbone will be accessed from electronic structure calculations. The Frenkel model describes a general aggregate made out of L interacting two-level chromophores. For localized excitations, the Frenkel-exciton model is directly applicable, and can be used to generate the Hamiltonian for the dynamical processes. To describe its electronic states one introduces the exciton creation (annihilation) operators (B_n^\dagger / B_n) which add (eliminate) an excitation on the nth chromophore that satisfy the fermion commutation relations. Using these operators, the Frenkel Hamiltonian reads:

$$\hat{H} = \sum_{kn} A_{kn} B_k^\dagger B_n + \sum_j H_{vib}(x_j) + \sum_{jkn} x_j \Delta_j B_j^\dagger B_n$$

The first term represents the purely excitonic system: $A_{kn} = \omega_k \delta_{kn} + J_{kn}$

where ω_k are the on-site exciton energies, and J_{kn} are the site-to-site exciton transfer matrix elements. Diagonalization of A_{kn} gives the one-exciton eigenstates and energies of the system in the absence of coupling to the polymer vibrational modes. *Ab initio* simulations of chromophore dimers and trimers will be used to obtain the above matrix elements for the exciton states in the absence of nuclear interactions. The polymer vibrational modes are taken to be harmonic (the second term in the Hamiltonian), and the coupling to the exciton motion is taken to be a bilinear coupling (the third term in the Hamiltonian). Dissipative effects of the polymer distortion are more difficult to obtain.

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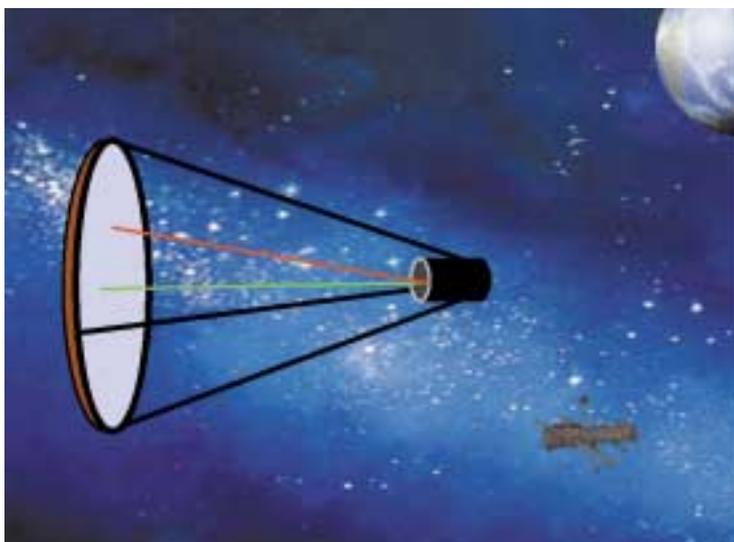


Figure 1. Future space telescope, approximately 1,000 times the size of the Hubble spacecraft.



Author and Contact: Joe Ritter
 Organization: SAIC, Technology Research Group, 590 Lipoa Parkway, Building B, Kihei, HI, 96753
 University of Hawaii Institute for Astronomy
 Author: James S. Newhouse
 Organization: Maui High Performance Computing Center, 550 Lipoa Parkway, Kihei, Maui, HI, 96753
 Author: Debi Evans and Jim Brozik
 Organization: University of New Mexico, Department of Chemistry, Albuquerque, NM, 87131
 Resources: IBM SP3 and SGI Octane dual R12000 at MHPCC

Imaging of Nuclear Motion Using Ultra-Short Intense Laser Pulses

André D. Bandrauk and Szczepan Chelkowski

Non-Born Oppenheimer supercomputer simulations of dissociative-ionization of H_2^+ are used to illustrate the nonlinear, nonperturbative response of electrons and nuclei to intense ($I > 10^{15} \text{ W/cm}^2$) ultrashort ($t_p < 15 \text{ fs}$) laser pulses resulting in Coulomb Explosion (CE) and Above Threshold Ionization (ATI). We demonstrated that it is possible to reconstruct nuclear vibrational wave functions from either experimentally measured proton or electron kinetic energy spectra.

Research Objectives: The nonlinear, nonperturbative response of atoms in intense laser fields has been extensively studied both experimentally and theoretically in the past twenty years. This has led to new unexpected effects, such as Above Threshold Ionization, ATI, high order frequency generation, etc., and these are documented in a recent book¹. The similar studies of molecules is a new chapter in the pursuit of laser control and manipulation of molecules. The nonlinear, nonperturbative response of molecules to intense ($I > 10^{15} \text{ W/cm}^2$) and ultra-short ($t_p < 10 \text{ fs}$) laser pulses² is expected to yield new effects due to the extra degrees of freedom of nuclear motion, as compared to

atoms³, such as creation of Laser Induced Molecular Potentials (LIMP's), Charge Resonance Enhanced Ionization (CREI⁴), and molecular High Order Harmonic Generation⁵. These nonlinear, nonperturbative effects were seen in experiments⁶, and were predicted and confirmed by high-level numerical simulations of appropriate Time-Dependent Schrödinger Equations^{3-5,7} (TDSE's) for molecules in laser fields.

Our recent supercomputer simulations of H_2^+ molecule dynamics in intense laser fields^{7,8,9} based on TDSE, also allowed us to propose two new molecular imaging techniques: a) LCEI, (Laser Coulomb Explosion Imaging⁸), and b) LPEI, (Laser Photoelectron Imaging⁹). The first technique is based on the analysis of the kinetic energy of molecular fragments after Coulomb Explosion, CE, whereas the latter imaging uses the shape of ATI electron peaks, produced by an intense laser pulse. We describe summarily in the present communication these two imaging methods which were developed using high level supercomputer simulations.

Computational Details and Results: Following the method discussed⁷, we have numerically solved the complete three-body, 1-D, TDSE for the H_2^+ one-electron molecular ion in the field of strong, ultra-short, linearly polarized laser pulse,

$$i \frac{\partial \Psi(z, R, t)}{\partial t} = H(z, R, t) \Psi(z, R, t)$$

where z is the electron coordinate and R is the distance between two protons, each lying on a line parallel to the laser field $E(t)$. Our methodology involves split-operator, spectral numerical methods. We execute our code using 32 processors, with a total 1.5 GB of memory, and use frequent communication calls between the processors. We choose the H_2^+ molecule to be prepared, at time $t=0$ (before the turn-on of laser pulse) in the vibrational state $\phi_v(R)$ on the Σ_g ground electronic surface. Next, we perform, numerically, the time evolution of $\Psi(z, R, t)$ described by TDSE until $t=t_f$, well after the turn-off of the laser pulse. Then, projecting $\Psi(z, R, t_f)$ onto electronic plane waves (and) or onto nuclear Coulomb wave functions, yields the electron kinetic energy (or ATI) spectra, $S_e(E_e)$ and (or) proton relative kinetic energy (or CE) spectra, $S_N(E_N)$.

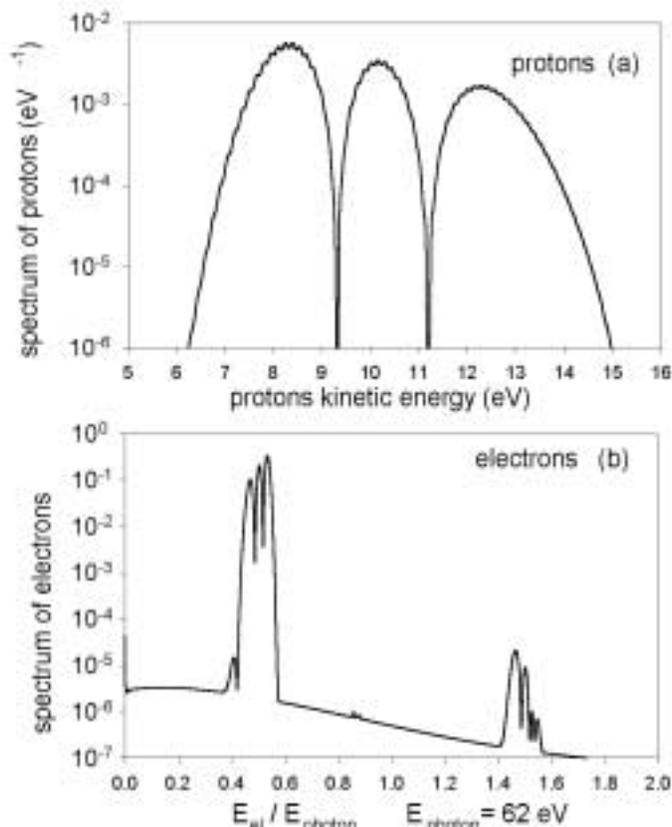


Figure 1. (a) Proton Coulomb Explosion energy spectra; (b) Photoelectron ATI kinetic energy spectra. Both for wavelength $\lambda=20 \text{ nm}$, laser intensity $I=10^{15} \text{ W/cm}^2$ and the pulse duration (half-width of a Gaussian intensity profile) $t_p=12.8 \text{ fs}$.

As an example, we illustrate results for such calculation in Figure 1, for an intensity $I=10^{15}$ W/cm², $\lambda=20$ nm, and pulse length 12.8 fs, for an initial $v=2$ vibrational state. Both spectra show clearly the double nodal structure of the $v=2$ vibrational state. Reconstruction of the initial wave function $\phi_v(R)$ from the protons spectra is obtained by a classical inversion procedure⁸, whereas its reconstruction from the electron spectra $S_e(E_e)$ is in addition, based on energy conservation applied for the one photon absorption process, leading to the sharing of energy between exploding protons and ionizing electron⁹.

Our previous simulations of LCEI were done for current high power T-Sapphire laser technology, $\lambda=800$ nm number⁸. The results illustrated in Figure 1 show that VUV ultrashort intense laser pulses should allow for a more complete LCEI procedure with nuclear wave functions now appearing in both CE and ATI spectra. We demonstrate, as well, that both imaging methods, LCEI and LPEI, also allow imaging of dissociating wave packets⁹.

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Author and Contact: André D. Bandrauk

Author: Szczepan Chelkowski

Organization: Laboratoire de Chimie Théorique, Université de Sherbrooke, Sherbrooke, Québec, Canada, J1K 2R1

URL: www.cacpus.usherb.ca

Resources: IBM SP at MHPCC

Acknowledgements: Natural Sciences and Engineering Research Council of Canada and Canadian Institute for Photonics Innovations

Spatially Adaptive Neural Nets with Exotic Topology

Frank L. Gilfeather and John A. Holbrook

Most earlier work on spatially adaptive neural nets (sometimes called self-organizing feature maps) has been limited to linear or planar nets. Here we explore the phenomena that arise when the topology of the net is more exotic. Our main motivation is the problem of sorting Electron Micrographs (EM) designed to reveal the 3-D structure of biological macromolecules.

Methodology: Electron Micrographs must be sorted according to the spatial orientation of the object being studied. Thus the topology most appropriate for the EM application is that of $SO(3)$, the special orthogonal group of rotations in space. Spatially adaptive nets are trained from an initial random state by items from the data set to be organized. The process is designed to converge to a continuity-preserving map between the data set and the topology of the net. If the group of self-maps of the net is complex,

convergence to a "wild" self-map is a dangerous possibility. Some of the difficulties in applying this method to $SO(3)$ arise in this way. Here we report numerical studies of a simpler case, where data and net have the topology of a torus.

Results: A comparison of computational experiment with the mathematical possibilities in the case of a toroidal net allows us to estimate the danger of convergence to various "wild" self-maps of the net. Some of the possible phenomena are seen in the figures. Figure 1 gives the reference position (identity map id), while Figures 2-4 show examples of convergence to "tame" maps (in the connected component of id) and to the "wild" maps (diagonal flips and twists) that are more problematic for applications. A failure of convergence due to locked-in "metastable" states may also occur, as in Figure 5. Figures 6-10 illustrate the convergence of the net under training from an initial random state to a well-organized one (though with a twist, in this case).

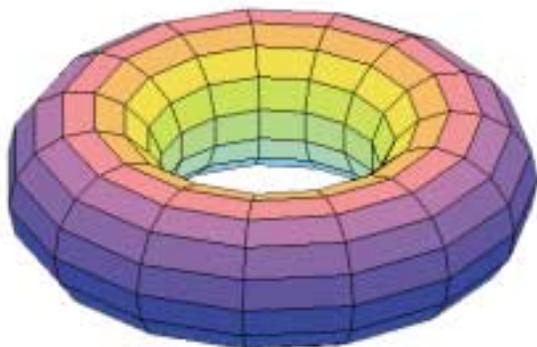


Figure 1. Reference position (id)

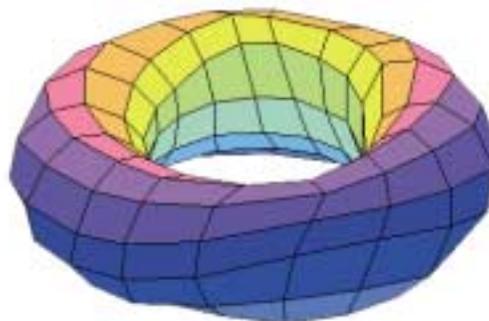


Figure 2. Tame adapted state (connected component of id)

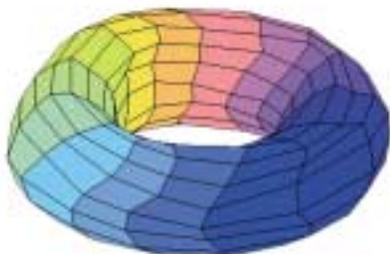


Figure 3. Wild adapted State (diagonal flip)

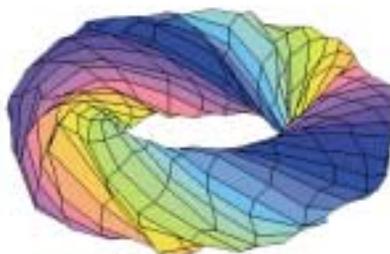


Figure 4. Wild adapted state (torsion-2)

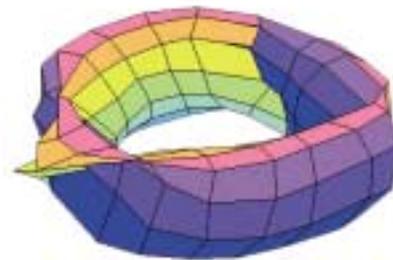


Figure 5. Maladapted "metastable" state

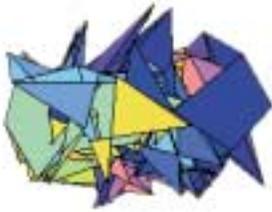


Figure 6. *Initial random state*

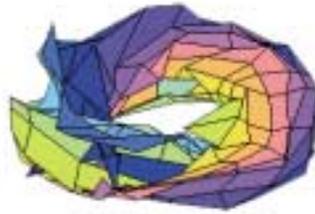


Figure 7. *Early adaptive state*

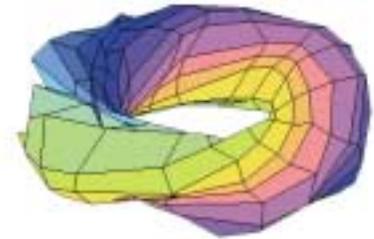


Figure 8. *Later adaptive state*

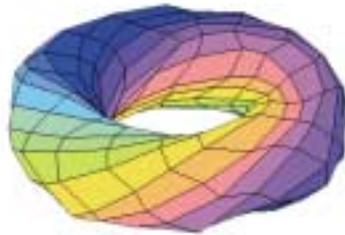


Figure 9. *Yet later adaptive state*

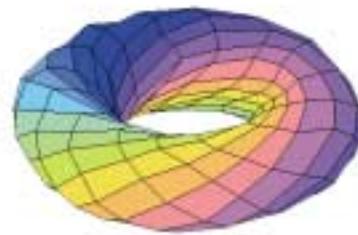


Figure 10. *Adapted state with torsion*

Significance: The techniques of spatially adaptive nets have many potential applications to sorting visual and other spatial data. In particular, the orientation problem for electron micrographs has bedeviled molecular biologists for decades. Any advance on this problem will allow more valuable 3-D structural information to be extracted from the mountains of data collected by microscopists.

Summary: Experimental data often have a known geometric structure, which is masked by the method of collection. For example, electron microscopy of very small biological structures seriously degrades the target molecules, so that it is not feasible to capture many views at known relative orientations. Instead, we collect many views of identical particles at orientations that must somehow be obtained by comparing the images themselves. We explore new techniques for solving this orientation problem through adaptive neural nets. These nets try to fit the given data into a geometric structure that reflects the variation to be expected in such data.

Author and Contact: John A. Holbrook

Organization: University of Guelph, Guelph, Ontario, Canada, N1G 2W1

Author: Frank Gilfeather

Organization: University of New Mexico, Galles Building, Albuquerque, NM, 87131

URL: www.mathstat.uoguelph.ca

Resources used: IBM SP at MHPCC and NSERC (Canada) research funding at the University of Guelph

Sponsorship: NSERC (Canada) research funding at University of Guelph

Performance Modeling of Data Parallel Applications

Daniele Tesserà and Anshu Dubey

In this research we have investigated widely used communication policies available in the MPI standard which have identical data volumes and range of communications. The results of this research were very surprising in that the non-blocking version of the communication strategy turns out to be the worst performing, while the kernel using a single collective operation is the fastest. Knowledge of comparative performance of different strategies can be very useful for programmers when several strategies are available.

Methodology: Within the framework of multidimensional FFT algorithms, we have investigated five widely used communication policies, available in the MPI standard, which have identical data volumes and range of communications. Two of them use point-to-point blocking communication (i.e., Send-Recv and Replace), one uses point-to-point non-blocking communication (i.e., Overlap), one has a set of collective communications (i.e., Oneplane), and the last one (i.e., Allplanes) uses a single collective operation.

The non-blocking version of the communication strategy turns out to be the worst performing, despite the fact the IBM SP2 has dedicated communication processors. On the other hand, the kernel using a single collective operation is the fastest, where normally one would have expected a lot of contentions and, hence, degradation in performance. To substantiate the actual behavior of the various FFT kernels, we have derived, by means of fitting techniques, analytical models of the times each kernel spent in communication and computation activities. These models, shown in Figure 1, represent the times spent in computation and communication activities by the various communication policies, as functions of the number of allocated processors executing an FFT computed on a 128 x 128 x 128 matrix.

The models have the following structure:

$$t(p) = a_0 + \frac{a_1}{p} + a_2 p$$

where $t(p)$ is either the communication or computation time, and p being the number of allocated processors. In the computation time models, parameter a_0 corresponds to the amount of sequential work, whereas a_1 is related to the concurrent computation, and parameter a_2 is always negligible.

On the other hand, in the communication time models, a_0 corresponds to the communication setup time, whereas a_1 is related to the volume of exchanged data. The last parameter a_2 takes into account the overhead costs due to managing the parallelism and plays a critical role only when modeling the communication times of the kernel, based on point-to-point exchanges (i.e., Send-Recv, Replace, and Overlap). These models have been validated with measurements related to different problem sizes. An in-depth analysis^{1,2} has shown that the unexpected behavior of these kernels can be explained in terms of the overhead costs required to manage their communication strategies. These costs also result in increased wall-clock times of pure computation routines, due to concurrent tasks executed by the operating system to manage the point-to-point protocols.

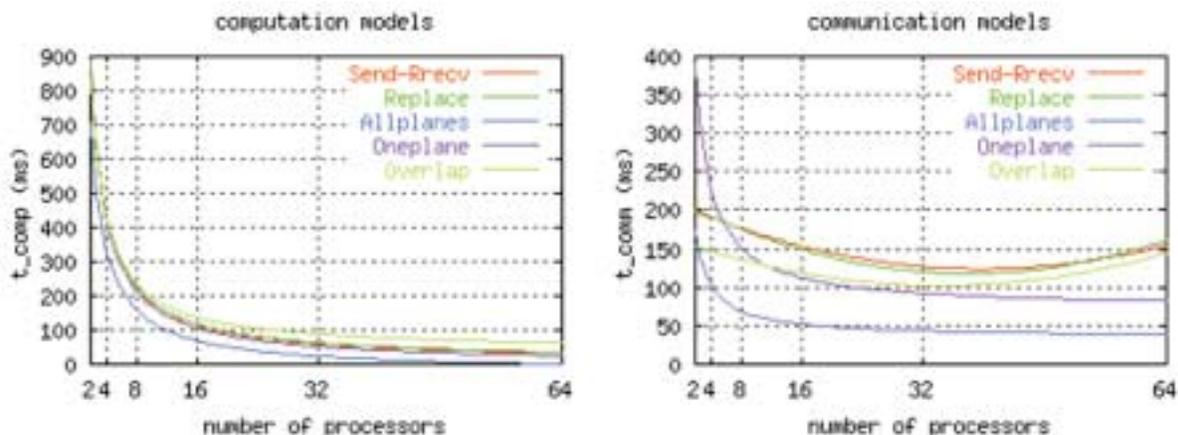


Figure 1. These models represent the times spent in computation and communication activities by the various communication policies, as functions of the number of allocated processors executing an FFT computed on a 128 x 128 x 128 matrix.

Significance: Communication activities are among the most critical factors for the performance of parallel applications, and usually limit the number of processors that can be profitably allocated. Hence, the choice of communication strategy (e.g., point-to-point versus collective exchanges, blocking versus non-blocking protocols) plays a critical role on the overall application performance, because it impacts setup and overhead costs due to buffering and/or contentions. Knowledge of comparative performance of different strategies can be very useful for programmers when several strategies are available.

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Author and Contact: Daniele Tessaera

Organization: Department of Computer Science, University of Pavia, Via Ferrata, 1, I-27100, Pavia, Italy

Author: Anshu Dubey

Organization: Astronomy & Astrophysics, University of Chicago, 5640 Ellis Ave., Chicago, IL, 60637

URL: <http://mafalda.unipv.it>

Resources: IBM SP at MHPCC and workstations at the University of Pavia and the University of Chicago

Sponsorship: Partially funded by the Italian Research Council under the grant CNRG0032FB "Argenzia 2000"

Assessing the Utility of Patient Simulation Using Immersive Virtual Reality to Enhance Distance Learning in a Medical Education Curriculum: Project T.O.U.C.H.

Joshua Jacobs M.D., Stanley Saiki M.D., Dale Alverson M.D.

This project was conceived as a response to challenges in healthcare education faced by the State of Hawaii and the State of New Mexico. This paper will review the similar circumstances found in both States, and describe how Project T.O.U.C.H. is addressing these circumstances. The project aims to augment medical school teaching methods, done over distance, to provide access to quality medical education to people in remote locations. The project began as a feasibility study, and has evolved into a proof of concept, with plans for widespread implementation.

Research Objective: Project T.O.U.C.H. is an acronym for Telehealth Outreach for Unified Community Health. It brings together a multidisciplinary, inter-institutional group of faculty members. The University of Hawaii and the University of New Mexico have a lot in common. Both serve to educate a multicultural population, including native peoples. Both States have large areas of medically underserved populations who face geographic barriers to access—the ocean in the case of Hawaii, and the desert in the case of New Mexico. The two States have similar curricula in their medical schools; that of Problem Based Learning (PBL). Both Universities are committed to training students in rural settings, with

continuing efforts to attract and retain providers in rural settings. There are several programs underway in both States to train local ethnic minorities in healthcare professions.

Methodology: With so many similar challenges, the two Universities are collaborating on a similar solution; Project T.O.U.C.H. This project includes immersive virtual reality, patient simulation, and volumetric image manipulation utilizing high-performance computing methods to enhance PBL, and to do so over distance. The project is creating a model that can be applied to different disciplines, cases, and situations.

This enhanced learning package is based on the concept that experiential learning will enhance the overall learning process. The mantra for the project team has become this Chinese proverb: "I hear and I forget, I see and I remember, I do and I understand."

In the current setting, PBL focuses on small group interaction and experiential, case-based learning. The clinical problem is the vehicle for learning. It is peer-taught, and tutor-mediated. The components of PBL are listed in Table 1.

Case scenario	Paper-based	Graphical, Immersive virtual reality patient simulator
Data sets	Paper-based books	Graphical, 3-D, Animations
Communication	Face-to-face with whiteboard	Face-to-face and remote, with shared electronic whiteboard

Table 1. *Traditional PBL components and their formats, compared to Project T.O.U.C.H. formats.*

A specific case scenario was developed to serve as a model for application of the technology. The case is of a neurological trauma, resulting in epidural hematoma formation, with an appropriate clinical picture. Data sets include animations of intracranial processes and intracranial anatomy.

Faculty at the University of New Mexico designed Flatland software. It allows construction of, and interaction with arbitrarily complex graphical and aural representations of data and systems. Flatland is written in C/C++ and uses the standard OpenGL graphics language extensions to produce all graphics. Flatland is the graphical environment within which the students can view and manipulate three-dimensional data sets, and interact with the patient simulator. (Figure 1)

An interactive patient simulation engine will allow a new dimension in PBL, in which the students can dynamically determine the direction of the case scenario. Realism will be heightened by use of immersive virtual reality technology. This project utilizes emerging Access Grid technology, developed by the National Computational Science Alliance (NCSA). It employs TCP/IP-based video conferencing using multicasting for simultaneous interactions with multiple applications, and with multiple sites. The Access Grid will be employed to conduct multi-site student group interactions.



Figure 1. "Toma", a Virtual Patient, demonstrates the 3-D Flatland graphic environment that allows students to view and manipulate 3-D data sets.

Results: During the first phase of this project the feasibility of employing advanced computing methods to enhance education in a PBL format currently being used in a medical school curriculum, by applying a specific clinical case (traumatic brain injury) as a model, and deploying to remote sites/workstations, was demonstrated.

During the second phase of this project the goals include assessing the effects of the technology on the learning process. Development of virtual reality tools, including the patient simulator, will continue. The evaluation component of this phase will examine students using the technologies and compare them to those who use traditional methods. In this manner, differences in educational value and impediments to education will become evident.

Significance: Project T.O.U.C.H. will serve as a model for future case development, allowing expansion to other systems, environments, and disciplines. Future phases will also explore PC-versions of the model for increased distribution. Currently, the immersive virtual reality experience is limited to one person at a time. In the future, this will be expanded to a group setting. Additional case scenarios and clinical models will be developed, along with additional 3-D images. Evaluation will be expanded to better assess impact on learning. If evidence indicates a clearly superior learning outcome, then the current model under development may indeed become the standard for medical education.

Author and Contact: Joshua Jacobs

Author: Stanley Saiki

Organization: University of Hawaii

Author: Dale Averson

Organization: University of New Mexico

Resources: Access Grid at MHPCC, SGI Onyx 2, SGI Octane, SGI 02, IBM Intellistations, Linux Cluster, Windows machine, and Access Grid at AHPCC, HP workstations at Sandia National Labs

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Electron-Impact Ionization of Helium

Igor Bray

In a recent Rapid Communication to the Physical Review A, Baertschy, et. al., reported excellent agreement between two diverse theories of electron-hydrogen ionization. We compare our own theory for this problem and find surprising results.

Research Objectives: Electron-impact ionization of atomic hydrogen is a prototype Coulomb three-body problem. Its solution has recently been claimed by Rescigno, et. al. (1999). They use their Exterior Complex Scaling (ECS) method to solve the problem and yielded generally excellent agreement with experiment.

Methodology: Another candidate for the solution of this problem is the Time-Dependent Close-Coupling (TDCC) method of Pindzola and Schultz (1996), and our own Convergent Close-Coupling (CCC) method (Bray and Stelbovics, 1995). To carefully check theories against each other, a small component of the full problem was presented by Baertschy et. al. (2001). They found excellent agreement between the ECS and TDCC theories for the zero-th partial wave of 17.6 eV e-H Singly Differential Cross Section (SDCS), and hence the Total Ionization Cross Section (TICS).

Results: In the figure, we compare the CCC-calculated results obtained on the *Tempest* system at the Maui High Performance Computing Center and compare with those of ECS and TDCC. Surprisingly, we find excellent agreement for the TICS, but not the SDCS, even though convergence with 'N' has been achieved.

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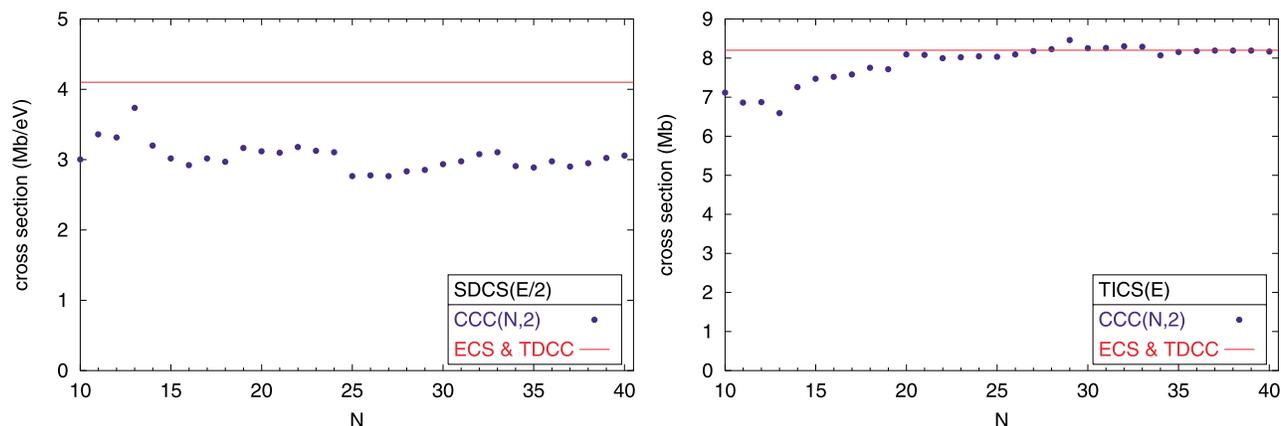


Figure 1. 17.6 eV e-H ionization SDCS and TICS for total energy $E=4$ eV.



MURDOCH
UNIVERSITY
PERTH, WESTERN AUSTRALIA

Author and Contact: Igor Bray

Organization: School of Mathematical and Physical Sciences, Murdoch University, 90 South Street, Murdoch, Perth, Western Australia, 6150

URL: <http://wwwstaff.murdoch.edu.au/~ibray>

Resources: IBM SP at MHPCC and SUN E450 and SGI Power Challenge at the University of South Australia

Sponsorship: Australian Research Council

Density Functional Study of the Retrocyclization of Norbornadiene and Norbornene Catalyzed by Fe⁺

Michael L. McKee

The theoretical study of organometallic ion chemistry provides important insights into catalytic systems and may allow the design of more selective and benign catalysts in the future. The present study considers the catalytic effect of an iron cation on the retrocyclization of norbornadiene and norbornene. This system was chosen because experimental mass spectrometric data is available for comparison. The mechanism is controlled by the relative strengths of metal-hydrogen and metal-alkyl bonds, as well as σ versus π metal-ligand interactions.

bornadiene (NBD) and norbornene (NBN) is considered. Both reactions are predicted to be stepwise. However, for norbornene (NBN), the Fe⁺-catalyzed retro reaction is 8.5 kcal/mol lower than the uncatalyzed stepwise reaction, but 3.8 kcal/mol higher than the concerted reaction. The intermediates from the NBD and NBN retro Diels-Alder reactions, C₅H₆FeC₂H₂⁺ and C₅H₆FeC₂H₄⁺, are predicted to have low activation barriers for ligand-to-ligand hydrogen transfers (through an iron hydrido intermediate) to form CpFeC₂H₃⁺ and CpFeC₂H₅⁺ and, ultimately, vinyl- and ethyl-substituted cyclopentadiene-iron complexes, respectively.

Results: Molecular plots of stationary points are given in Figure 1 and reaction profiles of the retrocyclization of NBD and NBN are shown in Figure 2. In both reactions, a bicyclic metalocycle is formed. Ligand-to-ligand hydrogen migrations in C₅H₆FeC₂H₂⁺ and C₅H₆FeC₂H₄⁺ lead to CpFeC₂H₃⁺ and CpFeC₂H₅⁺, respectively, in near-thermoneutral reactions that have low activation barriers. A pathway for dehydrogenation of C₅H₆FeC₂H₄⁺ has been calculated leading to C₅H₆FeC₂H₃⁺. While there is no evidence for a dihydrido intermediate, a monohydrido intermediate is predicted in both mechanisms. In hydrogen/deuterium exchange for C₅H₆Fe/C₂D₄⁺, the first exchange occurs with facile formation of a CpFeC₂D₄H⁺ intermediate. Subsequent H/D exchanges require 1,2-hydrogen migrations in the complexed cyclopentadiene of C₅H₅DFeC₂D₃H.

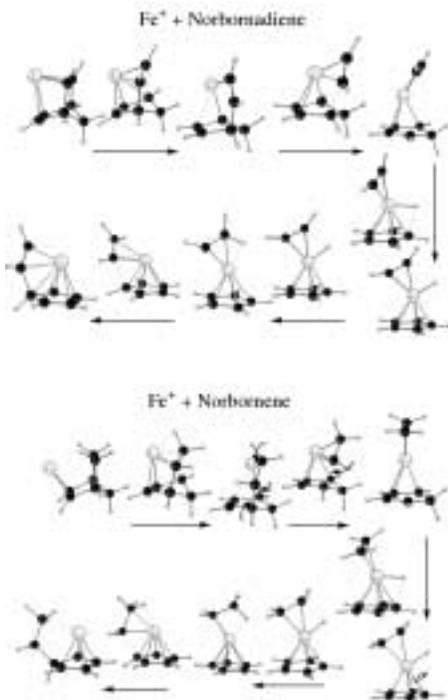


Figure 1. Molecular plots of stationary points

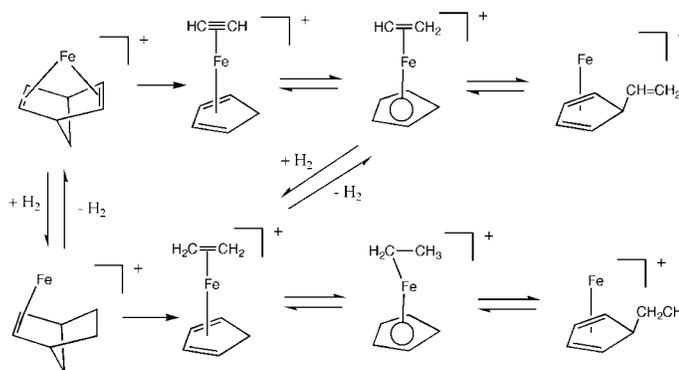


Figure 2. Reaction Profiles

Author and Contact: Michael L. McKee

Organization: Department of Chemistry, Auburn University, Auburn, AL, 36849

URL: www.auburn.edu/~mckeeml

Resources: IBM SP at MHPCC

Sponsorship: DOE/EPSCoR, MHPCC, Alabama Supercomputer Network

INDEX OF AUTHORS

A

Farid Abraham17
Dale Alverson38

B

Andre Bandrauk32
Alfred Brandstein6
Igor Bray40
Bob Brem4
Jim Brozik30
Steve Businger16
Eric Bylaska10

C

Emily Carter2
Szczezan Chelkowski32
Margaret Chen8
Flo Cid4

D

Andrea Donnellan24
Roland Draxler16
Anshu Dubey36
Bruce Duncan4, 6, 14

E

Curotto Emanuele28
Debi Evans26, 30

F

D. J. Fabozzi6, 14
Francis Fujioka20
Derek Funayama20

G

Frank Gilfeather34
Steve Gima4
Apostol Gramada10

H

Jongil Han20
Michele Hershey4
John Holbrook34
Carl Holmberg14
Gary Horne6

J

Joshua Jacobs38
Emily Jarvis2
Joel Johnson12

K

George Karniadakis1
R. M. Kirby1
John Kresho6

M

Carol McCord18, 20
Mary McDonald6
Michael McKee41
Ted Meyer6
Maria Murphy4, 6

N

James Newhouse26, 30

P

John Porter16

R

Thomas Reichler22
Joe Ritter26, 30
John Roads20, 22
Kevin Roe18, 20
John Rundle24

S

Stanley Saiki38
Kathy Schulze4
Scott Splean29
Duane Stevens18, 20
Bob Swanson6, 14
Brent Swartz6

T

Daniele Tessera36
Kristy Tiampo24
David Tyler4

U

Steve Upton6

V

Ron Vitoria6

W

John Weare10
Brian Widdowson6

INDEX OF ORGANIZATIONS

A

Aerospace Corporation 8
Air Force Research Laboratory 4, 28
Albuquerque High Performance Computing Center
. 4, 34, 38
Arcadia University 28
Auburn University 41

B

Boeing LTS 4
Brown University 1

I

IBM Research Division 17

J

Jet Propulsion Laboratory 24

K

KJS Consulting 4

L

Lawrence Livermore National Laboratory 17

M

Marine Corps Combat Development Command 6
Maui High Performance Computing Center
. 4, 6, 14, 18, 20, 26, 29, 30
Mitre Corporation 6
Murdoch University 40

N

NOAA Air Resources Laboratory 16

O

Ohio State University 12

P

Pacific Northwest National Laboratory 10

R

Riverside Fire Laboratory 20

S

San Diego Supercomputer Center 10
Science Applications International Corporation . 26, 30
Scripps Institute of Oceanography 20, 22

U

Université de Sherbrooke 32
University of
California at
Los Angeles 2
San Diego 10
Chicago 36
Colorado 24
Guelph 34
Hawaii 16, 18, 20, 38
New Mexico 26, 30, 34, 38
Pavia 36
Saskatchewan 17