High Performance Computing

contributions to

DoD Mission Success

2002

Report Documentation Page

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Backgrounds (front and back cover):

Forecasting the Weather Under the Sea: NAVO MSRC Scientific Visualization Center Allows Navy to See the Ocean Environment for Undersea Recovery Operations by Pete Gruzinskas (pg. 89)

Still image showing Ehime Maru retrieval over real bathymetry data. The animation was designed to conceptualize/visualize what the recovery would look like in the context of the real data collected by the USNS SUMNER.

Front cover captions (clockwise from left to right):

Identification of "Hot-Spots" on Tactical Vehicles at UHF Frequencies by Anders Sullivan and Lawrence Carin (pg. 119)

Impulse response mapped on T-72

Novel Energetic Material Development Using Molecular Simulation by John Brennan and Betsy Rice (pg. 103)

Molecular configuration snapshot of reacting system at P=28.47 GPa (blue: N_2 molecules; red: O_2 molecules; green: NO molecules)

Multidisciplinary Applications of Detached-Eddy Simulations of Separated Flows at High Reynolds Numbers by J. Forsythe, S. Morton, R. Cummings, K. Squires, K. Wurtzler, and P. Spalart (FY 03 DoD Challenge Project)

Development of a High-Fidelity Nonlinear Aeroelastic Solver by Raymond Gordnier (pg. 100)

Acoustic radiation due to travelling wave flutter of a flexible panel

Simulation and Redesign of the Compact A6 Magnetron by Keith Cartwright (pg. 121)

This shows the Titian/PSI A6 magnetron simulated in ICEPIC. This snap shot shows the electric field and particles 50 ns after the start of the applied voltage. The camera is pointing upstream toward the pulse power. The iso-surfaces in this figure are the electric field pointing around the cathode (theta direction). Red is in the clockwise direction when facing upstream, green is in the counter clockwise direction. The power extracted from the magnetron into the wave-guides shows a pi phase advance between the two cavities. The desired mode has a 2pi phase advance for the extractors, this magnetron is operating in the wrong mode. The phase advance from cavity to cavity is not constant in this design. The phase advance for the extracting cavities and the cavity between is pi/2. The rest of the cavities have a 3pi/4 advance, which makes the average phase advance 2pi/3.

Novel Electron Emitters and Nanoscale Devices by Jerry Bernholc (pg. 159)

Electron distribution near a tip of a BN/C nanotube in a field emitter configuration

For more information about the DoD HPC Modernization Program Office and the DoD HPC Modernization Program, visit our Web site at http://www.hpcmo.hpc.mil

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High Performance Computing

contributions to

DoD Mission Success 2002

March 2003

ACQUISITION,
TECHNOLOGY
AND LOGISTICS

OFFICE OF THE UNDER SECRETARY OF DEFENSE

3000 DEFENSE PENTAGON
WASHINGTON, DC 20301-3000

MAR 18 2003

The Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) provides world-class, commercial, high-end high performance computing capabilities to the DoD science and technology and test and evaluation communities. The program supports over 600 high performance computing projects. The user base exceeds 4,000 scientists and engineers, who are located at more than 100 DoD laboratories, test centers, contractor, and academic sites. In an era of Homeland Security and the War on Terrorism, the contributions made by the HPCMP community are of increasing importance, providing the answers to tomorrow's questions.

These success stories focus on the contributions made by the HPC community to the transformational goals of the Department. Whether through long-term research or more immediate support to address critical operational issues, our scientists and engineers are now routinely using HPCMP resources in a pervasive environment to assist in the transformation of our military forces. They are assisting in the protection of critical bases of operations by simulating chemical warfare agents and their antidotes, as well as blast protection from explosions. Others are conducting research that will ensure the integrity of our information systems in the face of attack. HPCMP supported research will allow the projection and sustainment of US forces in distant hostile environments through better weapons system design. DoD scientists are using HPCMP resources to improve synchronization within the battlespace environment and to develop the next generation of tools needed to deny enemies sanctuary. Still others are developing new materials to enhance the capability and survivability of space systems, leveraging information technology and innovative concepts to develop joint operational pictures. Enhancing our response to terrorist threats, improving the design of structures and weapons systems, conducting robust testing programs, and comprehensively evaluating the structural design of entire platforms – all are represented in this technical report, and all require high performance computing.

The threat environment of the 21st century requires a defense posture that is flexible, innovative, and fully capable of superior response across the spectrum of conflict. The Department of Defense's scientific, engineering, and testing communities are fulfilling those challenges using HPCMP resources.

Ronald M. Sega
Director
Defense Research and Engineering

Charles J. Holland
Deputy Under Secretary of Defense
(Science and Technology)

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Section 1

Introduction

Introduction

The Department of Defense (DoD) High Performance Computing Modernization Program (HPCMP) was initiated in 1992 by a Congressional directive to modernize the DoD laboratories high performance computing (HPC) capabilities. The HPCMP operates under the auspices of the Deputy Under Secretary of Defense for Science and Technology. Since its inception, the program has realized great success in its efforts to modernize the Department's laboratories and test centers to levels on par with other world-class organizations.

This technical report, *HPCMP Contributions to DoD Mission Success 2002*, will provide insights into how the program has evolved and chronicle some of the near term and long term national defense work done by the science and technology (S&T) and test and evaluation (T&E) communities using HPCMP resources. The High Performance Computing Modernization Program is placing critical enabling 21st century technology into the hands of the Department's science, technology, test, and evaluation communities that allows them to realize the Department's transformational goals.

This report is organized into four sections. The first section provides an overview of the program and its accomplishments as well as an explanation of how the stories are grouped. The second section consists of a selection of stories detailing the scientific research and engineering work done by the scientists and engineers in the Department's laboratories and test centers, working with academia and industry in seamless high performance computing environments. The third section provides a detailed discussion of the structure of the HPCMP and the fourth section is a list of acronyms used throughout the publication.

Overview of the High Performance Computing Modernization Program

The Department of Defense High Performance Computing Modernization Program was established as a Joint Program Office in 1993. This mandate was subsequently expanded to include the Department's test and evaluation community as well as the Missile Defense Agency (MDA) [formerly the Ballistic Missile Defense Organization]. In the following years, the Program has taken fragmented, Service-oriented research and engineering efforts and transformed them into a nearly seamless, joint operating environment that leverages the best practices of all of the Services and Agencies as well as the national academic and industrial infrastructure.

Mission and Vision

The High Performance Computing Modernization Program's mission is to

> *"Deliver world-class, commercial, high-end, high performance computational capability to the DoD's science and technology (S&T) and test and evaluation (T&E) communities, facilitating the rapid application of advanced technology into superior warfighting capabilities."*

The Director of the HPCMP has articulated that mission in the following vision for the Program:

> *[To create] "A pervasive culture existing among DoD's scientists and engineers where they routinely use advanced computational environments to solve the most demanding problems."*

Today's HPC Modernization Program supports over 4,000 scientists and engineers working through resources located at sites throughout the United States, including Alaska and Hawaii. As Figure 1 illustrates, the Program has provided a phenomenal increase in the computational power available to the community, along with the tools and intellectual expertise needed to fully use the resources effectively. The innovative and groundbreaking work being done using program resources is found throughout the Program's components — of the current 41 DoD Challenge Projects (listed in Section 3), over 90% are directly or indirectly related to one or more transformational objectives (see page 7). The software applications support initiative contributes daily to the expanding software suite available to the scientific and engineering efforts. The Defense Research and Engineering Network (DREN) is a premier departmental example of leveraging information technology as well as providing groundbreaking defensive input/output (I/O) through its work with network intrusion devices and multi-tiered access.

HPCMP Organization

The HPCMP has three components, which are detailed in Section 3. These components – HPC Centers, Networking, and Software Applications Support — provide a technologically advanced computational environment to support the ongoing and emerging needs of the Department's laboratories and test centers. The High Performance Computing Centers, shown in Figure 2, provide local and generalized support to the HPCMP community based on Service and Agency-validated requirements and priorities. The centers also support outreach to the communities in which they reside, encouraging students to become involved with engineering and scientific disciplines.

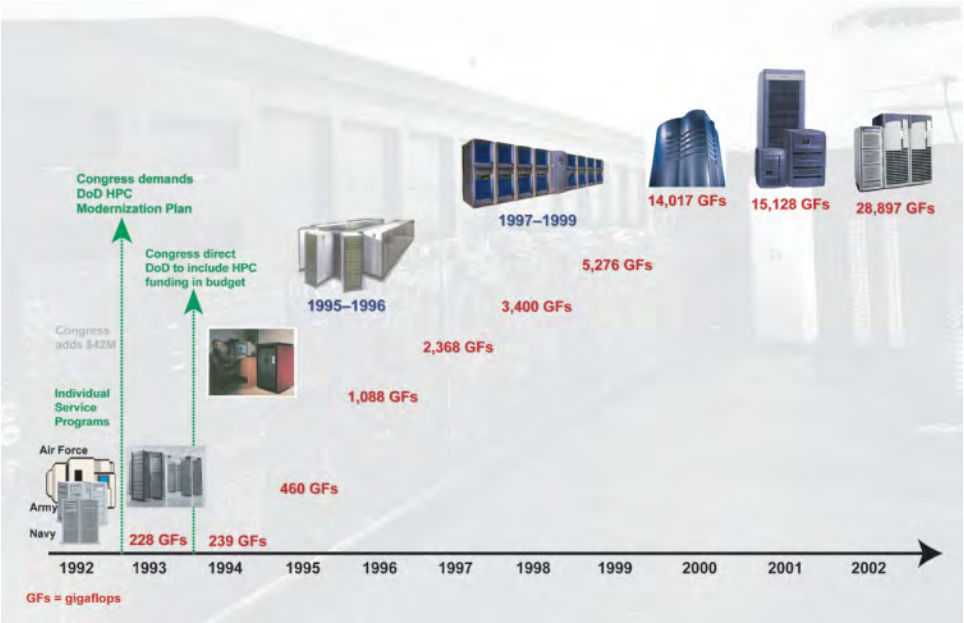


Figure 1. DoD S&T and T&E growth in computational capability

The HPCMP Community

The HPCMP community consists of over 4,000 scientists, engineers, computer specialists, networking specialists, and security experts working throughout the United States. All three Services and several Defense Agencies participate in the program.

Figure 2. HPC Centers (As of December 2002)

As shown in Figure 3, the user base is diverse, drawing from the government workforce, academia, and industry.

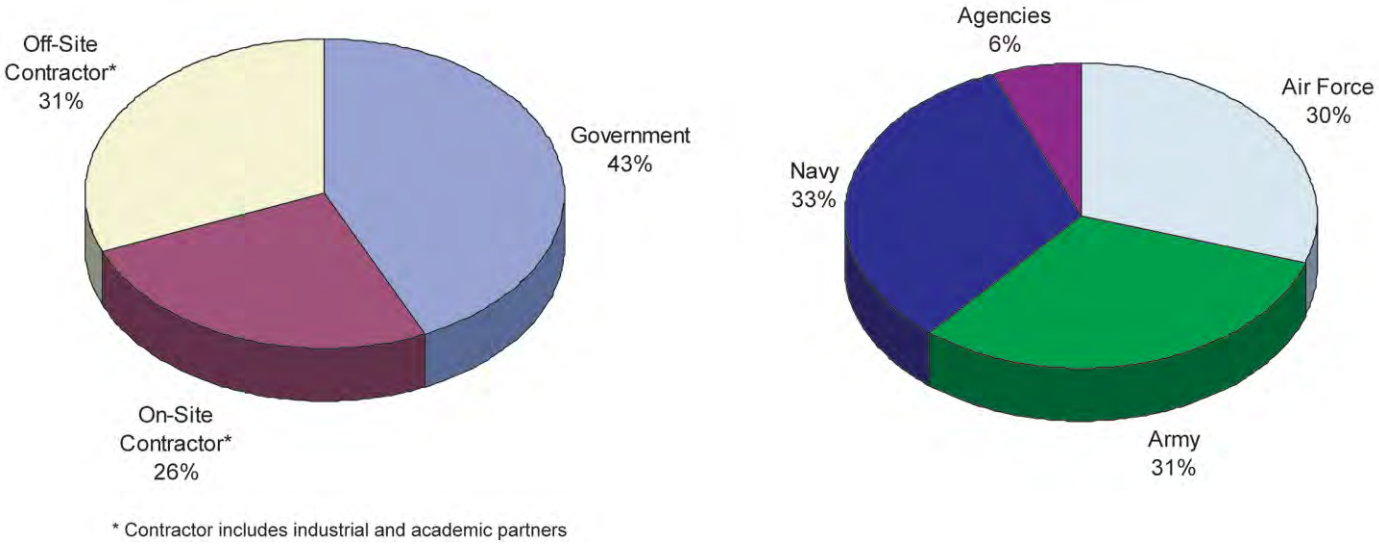


Figure 3. User Demographics

The community is organized around 10 computational scientific disciplines, which are known as Computational Technology Areas (CTA). The CTAs are described in Table 1. A nationally recognized expert in that discipline leads each CTA. In addition, there are a subset of projects which focus on the Department's highest priority, most computationally demanding work — the DoD Challenge Projects.

Table 1. Computational Technology Areas

	CTA	Description
CSM	**Computational Structural Mechanics**	Covers the high resolution, multi-dimensional modeling of materials and structures subjected to a broad range of loading conditions including static, dynamic, and impulsive. CSM encompasses a wide range of engineering problems in solid mechanics such as linear elastic stress analysis. CSM is used for basic studies in continuum mechanics, stress analysis for engineering design studies, and structural and material response predictions to impulsive loads.
CFD	**Computational Fluid Dynamics**	Covers high performance computations whose goal is the accurate numerical solution of the equations describing fluid and gas motion. CFD is used for basic studies of fluid dynamics for engineering design of complex flow configurations and for predicting the interactions of chemistry with fluid flow for combustion and propulsion.
CCM	**Computational Chemistry and Materials Science**	Covers the computational research tools used to predict basic properties of new chemical species and materials which may be difficult or impossible to obtain experimentally. Within DoD, quantum chemistry and molecular dynamics methods are used to design new chemical systems and solid state modeling techniques are employed in the development of new high-performance materials.
CEA	**Computational Electromagnetics and Acoustics**	Covers the high-resolution, multi-dimensional solutions of Maxwell's equations as well as the high-resolution, multi-dimensional solutions of the acoustic wave equations in solids, fluids, and gases. Some DoD applications include calculating the electromagnetic fields about antenna arrays, the electromagnetic signatures of tactical ground, air, sea and space vehicles, the electromagnetic signature of buried munitions, high power microwave performance, as well as the interdisciplinary applications in magnetohydrodynamics and laser systems.
CWO	**Climate/Weather/Ocean Modeling and Simulation**	Is concerned with the accurate numerical simulation of the earth's climate including the simulation and forecast of atmospheric variability and oceanic variability. CWO includes the development of numerical algorithms and techniques for the assimilation of in-situ and remotely sensed observations into numerical prediction systems.
SIP	**Signal/Image Processing**	Emphasizes research, evaluation, and test of the latest signal processing concepts directed toward these embedded systems. This will enable the traditional expensive, military-unique 'black boxes' required to implement high-speed signal/image processing to be replaced by commercial-off-the-shelf HPC-based equipment.
FMS/ C4I	**Forces Modeling and Simulation**	Focuses on force level modeling and simulation for training, analysis, and acquisition. The acquisition domain includes research and development, test and evaluation, and production and logistics. The overarching Simulation Based Acquisition domain is included.
EQM	**Environmental Quality Modeling and Simulation**	Covers the high-resolution, three-dimensional Navier-Stokes modeling of hydrodynamics and contaminant and multi-constituent fate/transport through the aquatic and terrestrial ecosystem and wetland subsystems, their coupled hydrogeologic pathways, and their interconnections with numerous biological species.
CEN	**Computational Electronics and Nanoelectronics**	Uses advanced computational methods to model and simulate complex electronics for communications, command, control, electronic warfare, signal intelligence, sensing, and related applications. Use of high performance computing assets enables the DoD electronics community to solve complex problems, explore new concepts, gain insight and improved understanding of the underlying physics, perform virtual prototyping, and test new ideas.
IMT	**Integrated Modeling and Test Environments**	Addresses the application of integrated models, simulation tools and techniques with live tests and hardware-in-the-loop simulations. IMT also provides proof-of-concept by using technology-based war gaming modeling and software integration tools for the simulation of weapon component subsystems and systems in a virtual operational context.

Within the DoD Challenge Projects, scientists and engineers are using program resources to work on projects such as the evaluation and retrofit for blast protection in urban terrain; three-dimensional modeling and simulation of bomb effects for obstacle clearance; the active control of fuel injectors in full gas turbine engines; and the seismic signature simulations for tactical ground sensor systems and underground facilities. Others are working on improving naval capabilities through unprecedented modeling of the climate, oceans, and weather conditions of the world as well as investigating littoral environments. Still others directly support the airborne laser and missile defense programs. Program resources helped to develop thermobaric weapons and to provide forensic data for investigation of terrorist bombings and consequence management. Additionally, program scientists and engineers are developing codes to help development of new materials that will enhance our capabilities and survivability in space.

HPCMP Support of Transformation and the War on Terrorism

Transformation Operational Goals

The stories included in this Technical Report are grouped to reflect the Department's transformation operational goals. The 2001 Quadrennial Defense Review Report states that "the purpose of transformation is to maintain or improve US military preeminence in the face of potential disproportionate discontinuous changes in the strategic environment." It also states that "the transformation must therefore be focused on emerging strategic and operational challenges and the opportunities created by these challenges." The 2001 Quadrennial Defense Review Report lists the six critical operational goals that provide the focus for DoD's transformation efforts:[1]

1. Protecting critical bases of operations (US homeland, forces abroad, allies, and friends) and defeating chemical, biological, radiological, nuclear, or high-yield explosive weapons and their means of delivery;
2. Assuring information systems in the face of attack and conducting effective information operations;
3. Projecting and sustaining US forces in distant anti-access or area-denial environments and defeating anti-access and area-denial threats;
4. Denying enemies sanctuary by providing persistent surveillance, tracking, and rapid engagement with high-volume precision strike, through a combination of complementary air and ground capabilities, against critical mobile and fixed targets at various ranges and in all weather and terrains;
5. Enhancing the capability and survivability of space systems and supporting infrastructure; and
6. Leveraging information technology and innovative concepts to develop an interoperable, joint Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance architecture and capability that includes a tailorable joint operational picture.

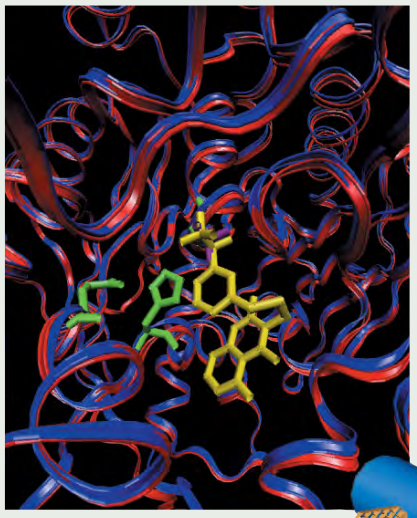
[1] 2001 Quadrennial Defense Review Report, September 30, 2001, pg. 30; www.defenselink.mil/pubs/qdr2001.pdf

"Our challenge in the 21st century is to defend our cities and our infrastructure from new forms of attack while protecting our forces over long distances to fight new adversaries"

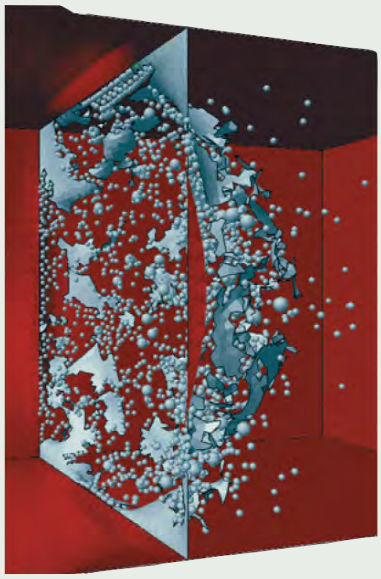
— Defense Secretary Donald Rumsfeld in a speech to students at the National Defense University, January 21, 2002

Section 2
Success Stories

Protect Bases of Operation



Chemical Defense
Combating Terrorism
Consequence Management



Missile Defense
Biological Defense

References (from top to bottom):

Defense Against Chemical Warfare Agents by Margaret Hurley, Jeffery Wright, William White, and Gerald Lushington
Overlaid crystal structures of Torpedo californica AChE with reversible (red) and irreversible (blue) inhibitors bound to active site residues (green)

Effect of Planar and Grid Tail Fins on Canard Roll Control Effectiveness on a Generic Missile by James DeSpirito
Canard-controlled missile with grid fins

Dispersion of Biological or Chemical Aerosols in Cities by Shahrouz Aliabade, Robert Bafour, Jalal Abedi, and Andrew Johnson
Geometric model of downtown Atlanta, GA, to be used for fine-scale (1 to 5 meter) numerical simulations of biological/chemical dispersion

Modeling Structural Response to Blasts by Joseph Baum
Airblast/fragments impact on a steel plate

Protect Bases of Operations

Since the Cuban missile crisis in 1962, no single event has shocked the nation into the reality of our vulnerability as did the events of September 11, 2001. The need to defend the US homeland and overseas bases has spurred increased attention to developing defenses against chemical warfare agents, cleaning up contaminated soils and groundwater, strengthening the resistance of buildings to blast events, and developing technologies to detect potential terrorist attacks from land or sea. The following success stories share a common theme — the unprecedented challenge of protecting our infrastructure and warfighters by taking advantage of the invaluable HPC resources made available through the High Performance Computing Modernization Program.

The threat of nerve and other chemical warfare agents, a major concern, has been the focus of studies such as those by Margaret Hurley and her associates ("Defense Against Chemical Warfare Agents"). In this investigation, HPC resources are being used to model the interaction of nerve agents and the enzyme acetylcholinesterase (AchE), enabling numerous advancements over previous simulations based on classical molecular dynamics techniques. In another research effort, Robert Bernard et al. ("Pore-Scale Contaminant Transport") describe improved measurement and modeling systems for the study of chemical and biological agent transport in permeable media. Advances in HPC technologies have made possible the complex computations necessary for these improved systems and subsequent successful applications on military sites.

Contamination of soils and groundwater from explosives, fuels, or other agents can be hazardous to the environment and to human beings, as well as costly to clean up. Computational simulation methods were employed in a project led by Jerry Leszczynski ("Exploring Cleanup Technologies for Explosives in Soils and Groundwater") to develop remediation technologies for soils and groundwater contaminated by explosives. Using a quantum-chemical (QC) approach, Dr. Leszczynski's team investigated the breakdown of nitrobenzene through interaction with the surface of an iron oxide (FeO) mineral normally found in soil. Parallel supercomputing resources significantly enhanced the study. In another contamination study, J.D. Nieber and his associates ("Promoting Environmental Stewardship: Understanding Fingering Flow in Unsaturated Porous Media") focused on the movement of fluids in porous media in order to determine effective remediation processes. Dr. Nieber's team used a new approach to solve the multi-phase fluid problem.

Simulations on high performance computers are invaluable in the development of technologies to protect the nation's infrastructure from blasts or explosives. Joseph Baum ("Modeling Structural Response to Blasts") describes the use of HPC and a coupled Computational Fluid Dynamics (CFD)/ Computational Structural Dynamics (CSD) code to model the processes involved in a blast event, and specifically the interactions of the blast and the structural response. Starting with a "glued-mesh" approach, Dr. Baum and his team of researchers have developed a more effective "embedded-mesh" technique. The computational simulations using this approach illustrate the structural responses to be expected in a car or truck bombing. These findings will enable the design of structures that are more resistant to blast events. Tommy Bevins et al. ("Evaluation of Blast Response to the Pentagon") provide an in-depth description of the retrofit designs for repair of the Pentagon after the September 11, 2001, attack. A number of factors had to be taken into consideration, including the loads on the components of the structure, the response of these components to the loads, and improved safety for the occupants. The complex computations required millions of equations and thousands of time steps.

Defense measures include protection and surveillance devices that are essential to homeland security. Modeling approaches being developed by John Starkenberg and Toni Dorsi ("Modeling Methods for Assessment of Gun-Propellant Vulnerability") will be used to analyze the reactive responses of propellant beds to unplanned stimuli. Simulation results will be used in the design of propellant beds

with the goal of reducing the violence of these reactive responses. The modeling approaches developed in this study are being used for the Army's Future Combat System in the design of high-loading-density gun-propellant charges. In another research effort, infrared search and track systems under development offer improved surface and air defense capabilities ("A Highly Parallel, Scalable Environment for Developing Search and Track Algorithms," Cottel, Douma, and Henderson). These systems require highly computationally intensive spatial, spectral, and temporal processing for real-time applications. Jeffery Dugan and his associates ("Robust Scalable Information Processing for Multistatic Sonars") describe improved algorithms that increase the performance of acoustic sonar, enhancing the ability to detect submarine threats and reducing false pings. HPC resources were used to test and validate the algorithm for an improved range rate estimator for the Hyperbolic Frequency Modulated (HFM) waveform, thus reducing the percentage of high-speed clutter as well as the algorithmic and operator resources.

The significance of these projects and their reliance on HPC technologies cannot be underestimated. The large storage and processing capabilities made possible by HPC resources have enabled the robust testing, accuracy, and time and cost effectiveness that are essential to homeland defense.

Lee Byrne

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US Army Corps of Engineers, Engineer Research and Development Center (ERDC), Vicksburg, MS

Defense Against Chemical Warfare Agents

Margaret Hurley
Army Research Laboratory (ARL), Aberdeen Proving Ground, MD
Jeffery Wright
Soldier and Biological Chemical Command (SBCCOM), Natick, MA
William White
Edgewood Chemical and Biological Center (ECBC), Aberdeen Proving Ground, MD
Gerald Lushington
University of Kansas, Lawrence, KS

The threat of nerve agents and other chemical warfare agents has been a constant specter over the last century, and will continue to be so. Despite international conventions banning their use, confirmed or alleged incidents have occurred over the last two decades alone in Afghanistan, Iraq, Iran, and Japan. Defense against and therapy for exposure to chemical warfare agents will remain a cornerstone of protection for the warfighter (as well as civilians) in years to come.

Investigating Nerve Agents

While much information has been obtained on the function of nerve agents and one of their primary targets, the enzyme acetylcholinesterase (AChE), substantial questions remain. Researchers continue to investigate the mechanism of their interaction, as well as the mechanism of related compounds used for therapy and prophylaxis. Experimental studies on these systems are, by their very nature, dangerous and expensive, making this an ideal target for theoretical investigation. Dr. Margaret Hurley and her associates are attempting to understand the key molecular features leading to reversible and irreversible binding in the active site of acetylcholinesterase (and related reactions). In doing so, they will develop a solid basis for devising chemical prophylaxis and therapeutics techniques, as well as developing a reliable technique for prediction of new, possibly dangerous, compounds.

Understanding the Chemistry

Previous simulations of these systems have been performed by using classical molecular dynamics techniques, or by quantum mechanical study of a severely truncated section of the active site residues. Classical techniques are extremely useful tools in understanding gross structural features contributing to the active site chemistry, but cannot provide the detailed energetics necessary to understanding the chemistry involved. Truncated models may leave out surrounding residues and other features that play a key role in determining the mechanism. Mixed quantum/classical (QM/MM) methods have been generally accepted as a reasonable compromise, capable of simultaneous representation of both the subtle reactive (QM) phenomena and the bulk (MM) environment dependence.

"Experimental studies on these systems are, by their very nature, dangerous and expensive, making this an ideal target for theoretical investigation."

Applying HPC to Higher QM/MM Models

Access to HPC resources (both hardware and software) has allowed the research community to make numerous improvements over previous treatments of AChE systems. They are able to treat substantially larger and/or higher accuracy QM models, and to run larger and/or higher accuracy

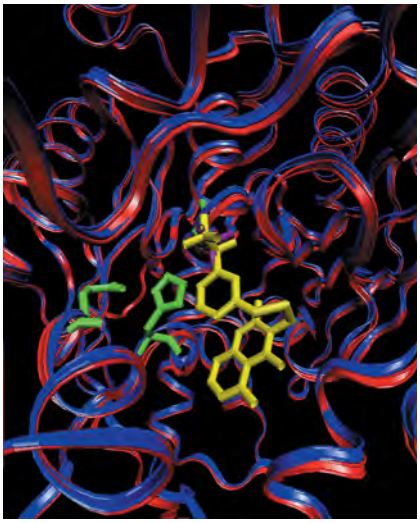

Figure 1. Overlaid crystal structures of *Torpedo californica* AChE with reversible (red) and irreversible (blue) inhibitors bound to active site residues (green)

QM/MM models. High performance computing resources supported one of the first systematic comparisons of competing QM/MM methodologies to determine the effect of the algorithm on results. The program also provided sufficient resources to perform a mapping of model details (size, method, level of accuracy, etc.) and their effect on results.

Reproducing the Short Strong Hydrogen Bond

The results to date have demonstrated the effectiveness of these models. The research team has been able to reproduce the Short Strong Hydrogen Bond (SSHB) in the active site residues seen experimentally in the bare AChE enzyme. In addition, the models confirm greatly reduced energy barriers to the phosphylation reaction in enzyme relative to related calculations of phosphonate hydrolysis in aqueous solution. They have also demonstrated the charge transfer between agent and oxyanion hole residues of enzyme, thus showing importance of quantum effects in non-active site residues to the reaction.

Currently, the team is conducting a detailed mapping of the aging reaction (by which the agent becomes irreversibly bound to the enzyme) and the origin of stereospecificity in these systems, as well as implementation of new higher accuracy QM/MM methods.

References

Hurley, M.M., Wright, J.B., Lushington, G.L., and White, W.E., "QM and Mixed QM/MM Simulations of Model Nerve Agents with Acetylcholinesterase," *Theoretical Chemistry Accounts (Special Issue on QM/MM)*, 2002. [Accepted]

Hurley, M.M.,Wright, J.B., Lushington, G.L., and White, W.E., Studies of Acetylcholinesterase and Model Nerve Agent Interactions: a QM/MM Approach. Presented at the 10th Conference on Current Trends in Computational Chemistry, Jackson, MS, November 1–3, 2001.

CTA: Computational Chemistry and Materials Science

Computer Resources: SUN E10000 and SGI Origin 3000 [ARL], IBM SP P3 [ASC], and Cray T3E [ERDC]

Pore-Scale Contaminant Transport

Robert Bernard, Stacy Howington, and John Peters
Engineer Research and Development Center (ERDC), Vicksburg, MS
Robert Maier
Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN
Daniel Kroll and H. Ted Davis
University of Minnesota, Minneapolis, MN

Modeling gas and liquid flows in permeable media is important in understanding the dispersal and persistence of chemical and biological agents. Until recently, the direct numerical simulation (DNS) of flow and transport in permeable media was regarded as a computationally intractable problem. Resolving flow even in a small sample requires an enormous computational effort due to the complex physical boundaries. However, recent advances in the application of HPC technologies have demonstrated that such computations are not only feasible, but can be performed on a reasonable production schedule, leading to improvements in measurement and modeling systems.

Pore-Scale Simulations

DNS in permeable media is often referred to as pore-scale flow and transport because flow is resolved on the length scale of typical pore spaces, using the three-dimensional Navier-Stokes equations. Species transport is modeled on the same length scale by solving a convection-diffusion equation, either coupled with the flow calculation or, more typically, using a steady-state flow field. As shown in Figure 1, no tunable parameters are needed to solve these equations; only the molecular viscosity and diffusion coefficients need be specified.

$$\rho\left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right] = \rho F - \nabla p + \mu\nabla^2\mathbf{v}$$

$$\frac{\partial c}{\partial t} = \nabla\cdot(D_m\nabla c) - \nabla\cdot(\mathbf{v}c)$$

Figure 1. Navier-Stokes (top) and convection-diffusion equations (bottom) where **v** denotes the fluid velocity, *p* the pressure, c the species concentration, ì the viscosity, D_m the coefficient of molecular diffusion

Early examples of pore-scale simulation were conducted for civilian projects, including research on oil recovery conducted at Los Alamos National Laboratory (LANL) in the early 1990's. The technology was subsequently applied to DoD projects within the Environmental Quality Modeling and Simulation (EQM) Computational Technology Area, including modeling of subsurface contamination on military sites. These simulations required up to 512 processors, 200 gigabytes main memory, and three days of wall-clock processing time.

"Until recently, the direct numerical simulation (DNS) of flow and transport in permeable media was regarded as a computationally intractable problem. Recent advances in the application of HPC technologies have demonstrated that such computations are not only feasible, but can be performed on a reasonable production schedule, leading to improvements in measurement and modeling systems."

Modeling Flow Columns

One application of pore-scale simulation is the modeling of physical experiments in laboratory flow columns. This type of simulation has revealed artifacts inherent in experimental measurements and protocols. Simulations predicted the existence of a damping effect in Nuclear Magnetic Resonance (NMR) velocity measurements caused by molecular diffusion. Simulations also predicted that in flow column experiments, the confining wall enhances experimental measurements of the hydrodynamic dispersion coefficient compared to an unconfined permeable medium (Figure 2).

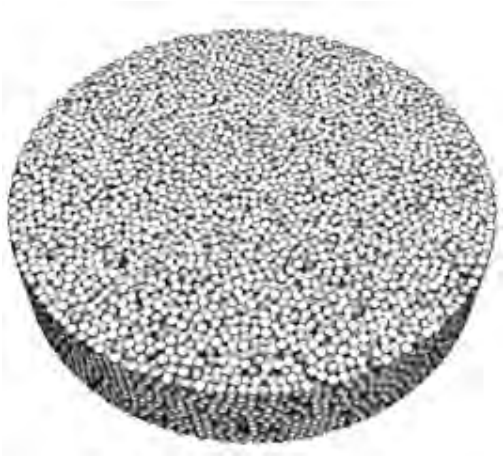

Figure 2. An example of permeable media: thin section of a cylinder ($r = 25d$) packed with monodisperse spheres of diameter d (full cylinder includes over one million spheres)

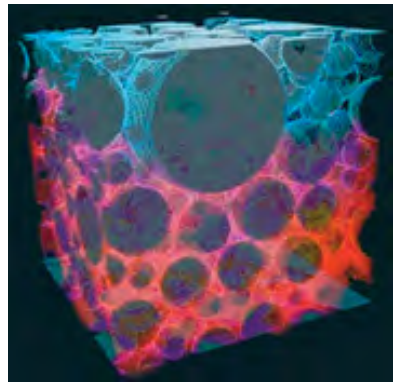

Figure 3. Three-dimensional view of dissolved chemical concentration in a polydisperse packed bed. Flow is from top to bottom, dissolving a thin chemical film from the solid surfaces. The intensity of red color denotes the relative concentration.

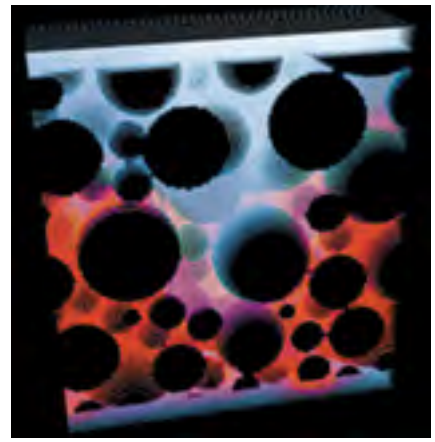

Figure 4. Quasi-2D view (thin section) of dissolved chemical concentration in polydisperse bed

Further applications of the pore-scale simulation have been identified, including the flow of combustion gases in ceramic foams, particle residence time in chromatographic columns and spectrographic sampling chambers, and shear stress calculations in saturated soil microstructures (Figures 3–6). A new challenge is to extend the technology to the flow of colloidal suspensions, including aerosols.

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CTA: Envionmental Quality Modeling and Simulation
Computer Resources: Cray T3E [AHPCRC, NAVO] and IBM SP [ERDC]

Figure 5. Contours of dissolved chemical concentration in cross section of a three-dimensional monodisperse packed bed. Flow of water is from top to bottom, washing a thin chemical film from solid surfaces. Darker contours denote higher concentration.

Figure 6. Residual chemical film on solid surfaces after washing is highlighted in black

Exploring Cleanup Technologies for Explosives in Soils and Groundwater

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Sponsor: Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN

Computational simulation methods have become powerful research tools for developing effective, passive, in situ clean-up technologies for explosives in soils and groundwater within the US Army environmental restoration mission. Among these computational methods, the quantum-chemical (QC) approach is one of the fastest growing and most powerful. The status of QC models permits the determination of numerous properties of molecules and molecular complexes involving hundreds of atoms. It is important to note that QC predictions for small- and medium-sized molecules and molecular complexes (tens of atoms) approaches the same accuracy as that achieved from high-quality experimental data. This suggests that computational studies can be more feasible and more cost efficient than experimental investigations.

QC Simulations of the Decomposition of Nitrobenzene

A team of AHPCRC/Jackson State University researchers led by Dr. Jerzy Leszczynski performed a computer simulation of the decomposition of the nitroaromatic compound, nitrobenzene, through interaction with the surface of an iron oxide (FeO) mineral typically found in soil. This process included the formation of the adsorbed state, the decomposition of nitrobenzene to nitrosobenzene, and the formation of the adsorbed complex between the nitrosobenzene and the surface of FeO mineral. The simulation has been performed using the density functional theory level of theory. The parallel version of the Gaussian-98 package, updated for the Cray T3E, was employed. The computer time necessary for completion of this project was an estimated 50,000 node hours using up to 64 nodes per job on the Cray T3E.

It was concluded that the adsorbed molecule undergoes destruction by transferring one of its oxygen atoms to a surface iron atom in FeO. This transfer is possible because the surface iron atoms are not fully coordinated. The probability of such a reaction pathway was determined by calculating a value of the activation energy for the separation of an oxygen atom from nitrobenzene and subsequent formation of a new FeO chemical bond. It was predicted that the transition of an oxygen atom to the surface of iron oxide is accompanied by the rotation of the aromatic ring to form the most energetically favorable orientation. This orientation stabilizes the structure by means of the formation of a new nitrogen-iron (N…Fe) bond. The calculated activation energy is 22.4 kcal/mol. The relatively small size of the activation barrier suggests that the proposed mechanism for the decomposition of nitrobenzene is realistic.

> "It is important to note that QC predictions for small- and medium-sized molecules and molecular complexes (tens of atoms) approaches the same accuracy as that achieved from high quality experimental data. This suggests that computational studies can be more feasible and more cost efficient than experimental investigations."

The final step of this project involved simulation of the product of nitrobenzene decomposition: nitrosobenzene adsorbed onto iron oxide. The adsorbed nitrosobenzene interacts with the iron oxide surface through its oxygen and nitrogen atoms forming an adsorption complex with an adsorption energy of 12.5 kcal/mol. This is almost one half of that calculated for the adsorption of nitrobenzene. This result suggests that nitrosobenzene will be desorbed from the surface of iron oxide easier than nitrobenzene after the chemical reaction of

decomposition has occurred. The total scheme of the described transformation is presented in Figure 1.

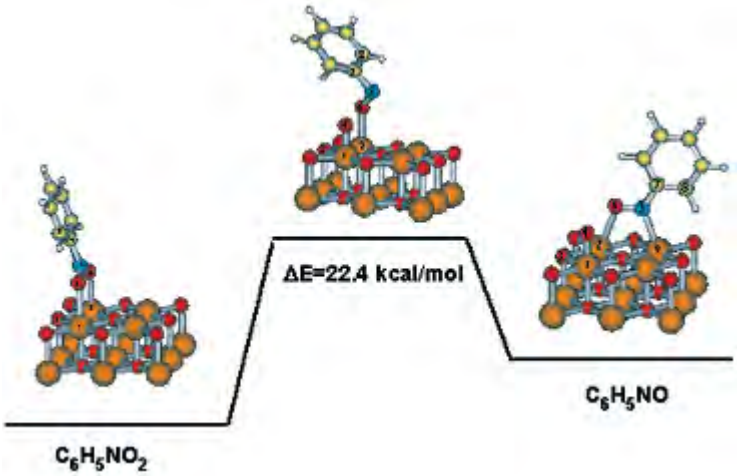

Figure 1. Reduction of nitrobenzene by (001) face of iron oxide

Applying QC methods allows computational chemists to successfully investigate not only simple molecules but also to extend their studies to problems of industrial and environmental importance. The power of QC investigations is increased dramatically when modern parallel supercomputers are used. In particular, these simulations allow iron oxide containing minerals to be considered as possible catalysts for the degradation of nitroaromatic compounds.

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CTA: Envionmental Quality Modeling and Simulation

Computer Resources: Cray T3E, IBM SP2, and Cray SV1 [AHPCRC]

Promoting Environmental Stewardship: Understanding Fingering Flow in Unsaturated Porous Media

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In 1998, the DoD cleanup budget already exceeded one billion dollars[1]. While promoting good stewardship, this also diverts scarce resources from other Defense priorities. Research that lowers cleanup costs, and anticipates potential hazards, will have a long ranging impact on both the Department and the welfare of US citizens.

Many US military sites have been contaminated by fuels, cleaning fluids, and munitions. Researchers working for the ARL are seeking to understand the movement of fluids through the soil and the deep unsaturated zone; this is important to the remediation of contaminated sites, and to predict the behavior of fluids in any new contamination events. Modeling fluid movement in soils and deep unsaturated zones involves solving coupled, nonlinear mass balance equations that quantify the movement of individual fluids in multi-phase fluid conditions.

"Unstable flow of fluids in soils and the deep unsaturated zone is important because the unstable flows lead to inefficient remediation of contaminated sites and faster movement of contaminants."

Solving the Multi-Phase Fluid Problem

Conventional approaches to solving the multi-phase fluid problem have used mass balance equations and assumed equilibrium capillary pressure-saturation relationships. The typical mass balance equation is represented by

$$\frac{\partial S}{\partial t} - \nabla \cdot K(S)\nabla p + \frac{\partial}{\partial z} K(S) = 0$$

where p is the fluid pressure, $K(S)$ is the hydraulic conductivity, and S is the fluid saturation. In the conventional method, the fluid pressure is related directly to the equilibrium capillary pressure-saturation relation by

$$p = \mathrm{P}(S)$$

where P is the equilibrium capillary pressure.

In the new approach, the ARL team of research scientists kept the mass balance equation but replaced the equilibrium relation with the non-equilibrium relation

$$\tau \frac{\partial S}{\partial t} = p - \mathrm{P}(S),$$

where τ is a relaxation parameter.

The solution of the unconventional equations leads to a completely new realm of flow characteristics. The conventional equations yield solutions that are unconditionally stable (in the physical sense). The new equations lead to flows that can become unstable for a wide range of conditions. Researchers concluded that the conditions leading to stability are a special case of the more general case where non-equilibrium conditions prevail.

Unstable flow of fluids in soils and the deep unsaturated zone is important because the unstable flows lead to inefficient remediation of contaminated sites and faster movement of contaminants.

High performance computing resources are important to the study of fluid flow processes such as unstable flows in porous media. For two-dimensional domains, it is sufficient to use scalar processor computations, but for three-dimensional domains, it

[1] Guide to the DoD Environmental Security Budget, October 1998, DUSD(I&E)

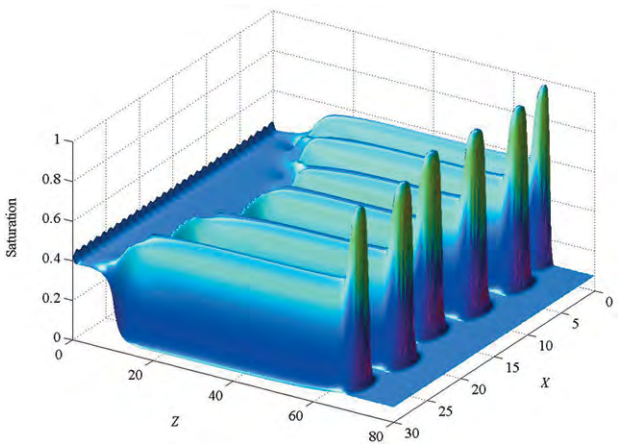

Figure 1. Distribution of fluid saturation in a two-phase situation showing the invasion of a wetting fluid into a porous medium originally saturated with non-wetting fluid. The invading fluid moves in a fingered flow pattern, representing a condition of unstable flow. The fluid flow solution was derived using a conventional mass balance equation for two-dimensional flow with a non-equilibrium model for the capillary pressure – saturation relationship.

is necessary to perform computations on parallel computer platforms. At present, the ARL team has investigated the physical process for only the two dimensional case, and for homogeneous porous media. In the future, the ARL research team will continue to use HPCMP resources to consider heterogeneous media, and three-dimensional domains.

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CTA: Environmental Quality Modeling and Simulation
Computer Resources: Cray T3E [AHPCRC]

Modeling Structural Response to Blasts

Joseph Baum
Defense Threat Reduction Agency (DTRA)/SAIC, Alexandria, VA

The White House, the Capitol, and the Pentagon are three of the most prestigious, recognizable, and powerful symbols in the United States. After the events of September 11, 2001, these buildings have also become prime targets for a terrorist attack in the form of a car or a truck bomb. Structural response of these structures to large-size charges is currently being simulated on high performance computers.

Dr. Joseph Baum and a group of research associates, sponsored by the Defense Threat Reduction Agency (DTRA), are using high performance computers and a coupled CFD and Computational Structural Dynamics (CSD) code to model all the relevant physical processes controlling these scenarios. These processes include: 1) detonation wave initiation and propagation within the explosive; 2) CSD modeling of the car/truck/case fragmentation; 3) blast wave expansion through the breaking case, diffracting about the flying fragments; 4) blast and fragment propagation and impact on the target; 5) target structural response to the blast and fragment loading; and 6) the resulting new blast and fragment environment.

Using High Performance Computers to Accurately Model Fluid-Structure Interactions

This HPCMP DoD Challenge Project is addressing an inability to accurately model fluid-structure interactions that require simultaneous modeling of such events as a blast near a building and the resulting structural response, or blast near a ship, and the resulting holing and blast penetration. Researchers gain a better understanding of fluid-structure interactions by coupling CFD and CSD codes. For a typical blast problem, the CFD portion models the detonation process within the explosive using the appropriate equation-of-state for the specific explosive, and at the same time, models the air blast that has started propagating. If this is a cased explosive (i.e., an explosive in some steel casing—such as a pipe), the CSD part will model the breakup of the case. The CFD will then model the propagation in the air of both the expanding shock wave and the fragments until they impact an object (a wall of a structure, a car, etc.). At that point, the CSD code will model the response of the impacted structure to this air blast and fragment loading. If, for instance, the CSD model is a ship, the CSD code will model the hull holing and fragmentation and then the air blast going through the breaking/fragmenting structure into the next compartment.

The "Glued-Mesh" Approach

The initial coupled CFD/CSD algorithm used the so-called "glued-mesh" approach, where the CFD and CSD faces match identically. Failure of this approach to model severe structural deformation, as well as crack propagation in steel and concrete, led the team over the last year to develop the so-called "embedded-mesh" approach. Here, the CSD objects float through the CFD domain. While each approach has its own advantages, limitations, and deficiencies, the embedded approach was proven to be superior for the class of problems modeled here. The embedded approach enables easier modeling of the response of civilian structures, which include a variety of structural materials, such as brick, stone, steel, aluminum, concrete, and glass.

"The embedded approach enables easier modeling of the response of civilian structures, which include a variety of structural materials, such as brick, stone, steel, aluminum, concrete, and glass."

Comparison to the Embedded Approach

Figure 1 shows a comparison between the glued approach (Figure 1a) and the embedded approach (Figures 1b to 1e). The first approach did not allow

for the application of a physically correct crack propagation model, as each crack had to be modeled with at least 4–6 fluid elements across the narrow gap, at a prohibitive computational cost. The fragments had to be pre-defined, hence precluding the modeling of weapons for which there are no arena data. In addition, the break-up of each fragment was a topology-changing event, requiring global remeshing at a fairly high computational cost, even when performed in parallel using a parallelized grid generation scheme. In comparison, the embedded approach allows both the treatment of crack propagation and the formation of small fragments. Thus, the cracking model automatically determines the size of the fragments. The results shown in Figures 1c-e demonstrate: 1) the randomness of the size of the fragments; 2) the narrow cracks between the fragments, some of which are very small; 3) The large number of fragments modeled, a simulation that would have been computationally prohibitive with the glued approach; 4) mesh adaptation to both the structure (smaller elements within the cracks will yield more accurate pressure relief and detonation products expansion) and density gradients; and 5) most fragments reach about the same velocity (within a range of about 15%), in agreement with available experimental data. After being applied to the study of blast and fragment interaction with reinforced concrete (military) structures, the new methodology is applied to the survivability study of important US Government centers as well as major transportation links and infrastructure centers.

A second simulation modeled fragment/airblast interaction with a steel wall chamber. Similar to the weapon case breakup case, three levels of mesh refinement were used in the CSD model. The standard DYNA3D element erosion model was used to eliminate failed CSD elements.

The numerical predictions show that the impacting weapon fragments arrive ahead of the airblast, punching holes through the plate (Figure 2a). Next, the pressure blast from the detonation tears the weakened plate apart (Figure 2b). The eroded plate elements were converted into particles that can interact with the rest of the structure. Contact conditions were enforced between all entities to avoid fragment interpenetrations and therefore a failure in meshing.

The results will give researchers a better understanding of the structural response of a variety of materials to a car or truck bomb. This will enable engineers to design buildings which are more resistant to these types of blasts.

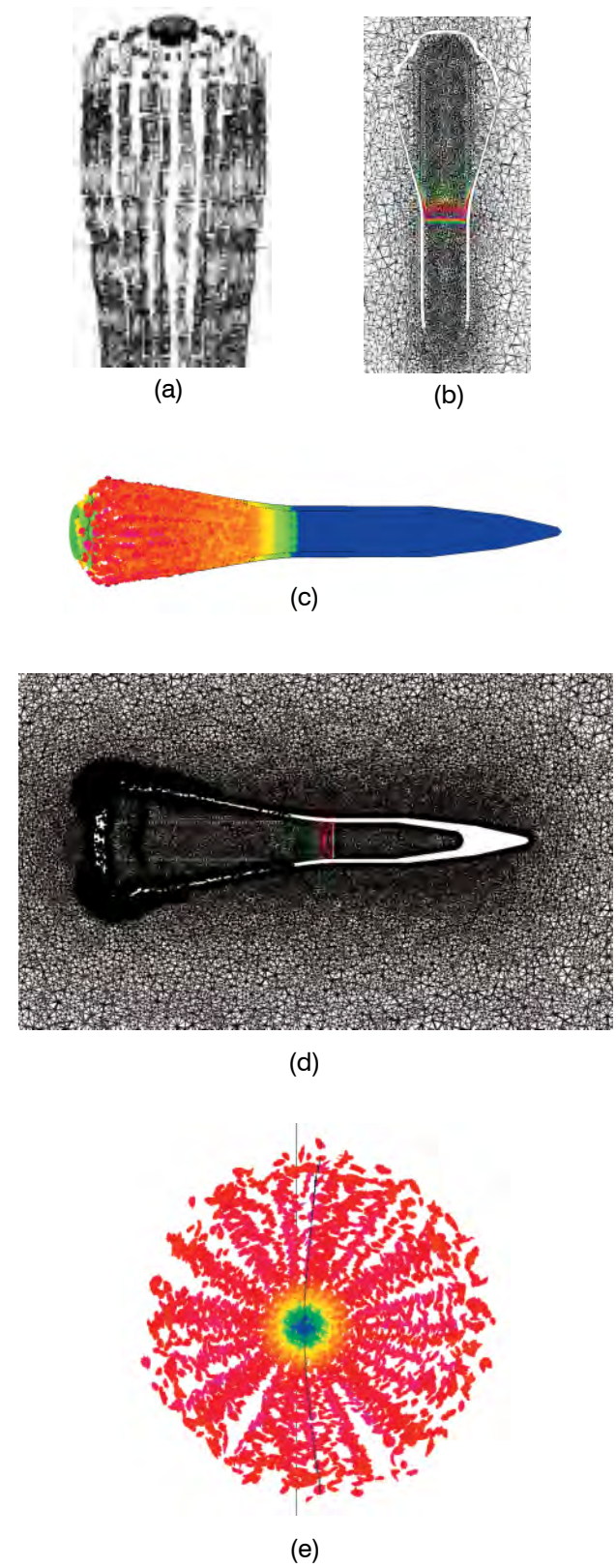

Figure 1. Comparison of glued and embedded CSD schemes applied to the weapon fragmentation study

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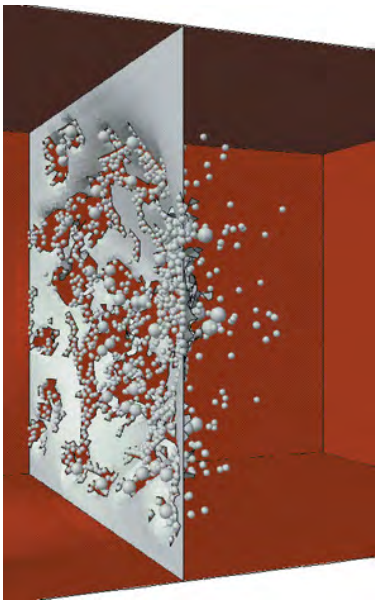
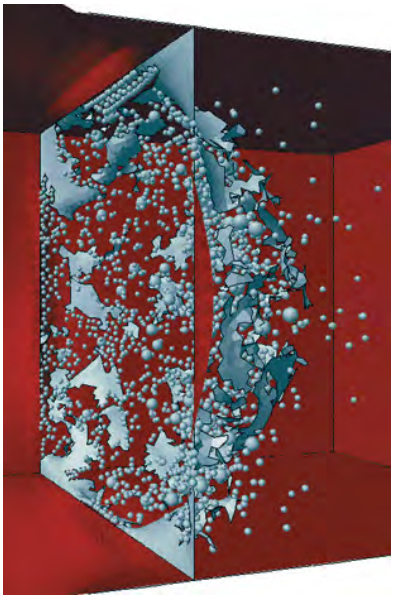
CTA: Computational Fluid Dynamics
Computer Resources: SGI Origin 3000 [ERDC]



(a)



(b)

Figure 2. Airblast/fragments impact on a steel plate

Evaluation of Blast Response of the Pentagon

TOMMY BEVINS, BYRON ARMSTRONG, JAMES BAYLOT, AND JAMES O'DANIEL

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Protecting our military personnel from terrorist attacks is critical to DoD mission success. Real life scenarios rarely consist of simply an explosion, the propagation of the blast load over a flat terrain, and its impact on a structure. The blast environment is affected by the presence of other structures, as well as the natural topography. A complete understanding of this complex blast environment, including the effects of adjacent structures on the blast loads on a structure, is needed to protect building occupants in an urban environment. These effects were studied in a combined experimental/analytical study conducted at the Engineer Research and Development Center (ERDC). The analytical study used high-priority HPC processing hours provided under the HPCMPO DoD Challenge Project: "Evaluation and Retrofit for Blast Protection in Urban Terrain." Simulations of several different experiment geometries and combinations of structures have been performed as part of this DoD Challenge Project. The analyses have compared very well with experimental results, giving credibility to these analysis methods for use in further blast propagation studies.

The Defense Department placed a high priority on the rapid repair of the damages to the Pentagon resulting from the September 11, 2001, terrorist attack. The US Army Corps of Engineers had been tasked with providing possible retrofit designs to the Pentagon in order to improve its response to a range of terrorist threats. Because of the desire to rapidly repair the Pentagon, the Corps of Engineers recommendations for improvements had to be finalized and presented to the Pentagon Renovation Office (PenRen) within eight weeks. This effort involved determining the loads on the components of the Pentagon and the response of these components to the loads. It also involved developing, analyzing, and evaluating retrofit concepts to improve safety of building occupants.

Prediction of Loads and Response of Pentagon

The Pentagon is a complex structure and in some respects behaves like a group of structures rather than one. There are five concentric pentagonal rings separated by a lightwell (air space) over the top three floors of adjacent rings. The lightwell walls contain hundreds of windows. If a terrorist bomb is detonated outside the Pentagon, the blast pressures will propagate over the top of the Pentagon and into the lightwells, thus loading the windows. The propagation of blast into the lightwells is similar to the propagation of blast over, around, and between structures. An accurate determination of the loads on these lightwell windows will allow the Department to improve the structure and consequently, protect its occupants. Figure 1 shows that airblast propagation into the lightwells could be a hazard to occupants of rooms near the lightwells.

"This research is important to DoD because it transitions technology needed to improve the survivability of the Pentagon to those responsible for its blast retrofit. The research also decreases costs by helping to determine the critical areas of the Pentagon so that resources are expended in those locations where they are most needed."

The Pentagon is a concrete frame structure with nonstructural exterior in-fill walls. The in-fill walls of the structure are two-layer brick walls clad with large limestone blocks. Many large windows are present on the first four floors of the outer wall of the Pentagon. Multiple scenarios were evaluated, including the existing Pentagon exterior walls, the current Pentagon retrofit walls, and the enhanced retrofit designs.

Research conducted under the challenge project has demonstrated that the HPC simulations match the experiments well. Further simulations will be performed beyond those for which experiments will

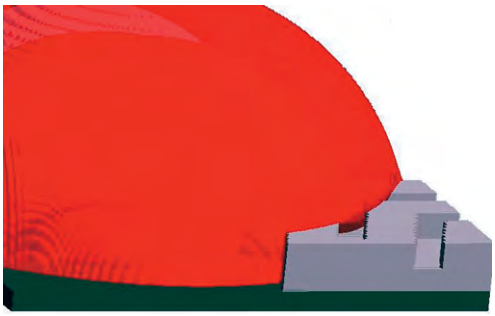

Figure 1. Blast propagation into lightwells

be conducted. The results will be used to develop engineering models for blast in urban terrain.

HPC simulations were used to evaluate the safety of the Pentagon occupants to a range of terrorist threats. The retrofits currently installed in portions of the Pentagon as well as other improved retrofits were evaluated. Figure 2 shows that the bricks of the exterior wall will be a hazard to occupants for the threat analyzed. The brick walls of the retrofitted Pentagon will fail as shown in Figure 3, but will be captured by the geotextile fabric and will not be a hazard. The results of the study were presented to PenRen, and PenRen has asked the ERDC to participate in a study to enhance the safety of Pentagon occupants.

This research is important to DoD because it transitions technology needed to improve the survivability of the Pentagon to those responsible for its blast retrofit. The research also decreases costs by helping to determine the critical areas of the Pentagon so that resources are expended in those locations where they are most needed. This research promotes the understanding of experiments and the phenomenology of the blast environment, which will in turn lead to better engineering models for predicting blast loads.

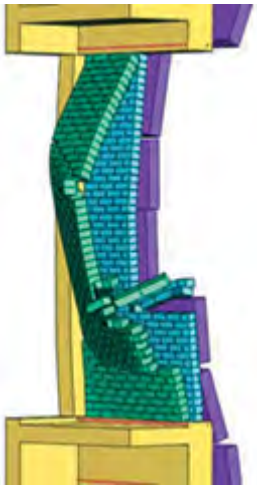

Figure 2. High-hazard failure of original Pentagon wall

Figure 3. Response of successfully retrofitted Pentagon wall

Engineering Models Too Simple

Blast loadings on structures have typically been evaluated using empirical equations that relate blast pressure characteristics (incident pressure, incident impulse, reflected pressure, reflected impulse, shock front velocity, time of arrival, and dynamic pressure) to known physical parameters (explosive charge weight, standoff, and the angle between the shock front propagation direction and the normal to the structure). These relationships have been determined for both hemi-spherical surface bursts and for spherical bursts in free air. These equations assume that there are no obstacles between the explosive source and the target. The simplest approach to determine the loads on a structure behind an obstacle is to assume that the obstacle has no effect on the pressure on the structure behind it. A second approach adjusts the standoff distance to account for the distance that must be traveled to go around the obstacle. Neither of these methods provides reliable or precise estimates of the pressures time-history on a shielded target. One problem is that the relationship between the incident pressure, the shock front velocity, and the reflected pressure is not the same for a clear path to a target as it is for an obstructed path to a target. Recent experiments have demonstrated that even if the incident pressure at a target point is essentially the same with and without an obstruction, the shock front velocity at the target may be significantly different, leading to a significantly different reflected pressure.

The response of masonry walls to blast is typically modeled using single-degree-of-freedom (SDOF) representations of the wall to determine a pressure-impulse (P-I) diagram. The applied pressure and impulse can then be plotted on the diagram. If that pair is above and to the right of the curve, then the response exceeds the damage level associated with the P-I curve. This type of analysis is valid and easily applicable to simple masonry walls such as a single layer brick wall. For complicated structures where a brick wall interacts with another wall, these methods can only be used as a guideline, unless validated by some other means.

Explicit Time-Stepping Method Models Blast Response

With the availability of HPC, it is possible to calculate the problem of shock propagating through the air by dividing the large volume — including the structure, the air, and the explosives — into a large number of small cells. The propagation of shock is modeled in an explicit time-stepping method. The method conserves mass and momentum and represents the correct equations of state for the air and the explosives. Determining the solution requires the computation of millions of equations for each of thousands of time steps. HPC resources allow these calculations to be performed in a finite length of real-time for significant amounts of simulation time. The advantage of this method over the usual method for obtaining loads is that the incident pressure, shock front velocity, dynamic pressure, and reflected pressure are all computed based on the physics of the problem rather than on the combination of empirical equations that are not actually valid for the problem being solved. Historically, how to computationally solve the governing equations was known, but there was not enough computer power to solve significant problems in a practical length of actual time.

Simplified methods provided an overall answer to the response of the structure, whereas these methods provide a solution with detailed information about the response. HPC makes it possible to explicitly model the interaction of individual bricks of a brick wall. Using procedures that have been developed at ERDC, the model of the complex wall system of the Pentagon was developed. The model included the two-layer brick wall, the concrete frame, and the limestone façade. Models were also developed for several retrofit designs. Approximate P-I diagrams for several wall configurations were validated using HPC simulations. Scientific visualization has been used extensively to assist in understanding the phenomenology of blast interacting with structures and the response of those structures to blast.

Initial Blast Load Evaluations Completed

The availability of high-priority HPC time has allowed ERDC to complete initial evaluations of the methods being used to study blast loads on structures in urban terrain. These initial evaluations have been done in time to impact the PenRen Program. The evaluations are also very encouraging and give credibility to the analyses to determine the survivability of the Pentagon to a terrorist attack. The PenRen asked the ERDC to assist in overcoming some of the deficiencies identified by the HPC analyses performed in the original study. Experimental results are very useful for studying blast loads on structures, but are not sufficient to completely understand the phenomenology of blast passing around an obstacle and then loading a structure. HPC results were used to fill in gaps in the data and to visualize how the physical process evolves.

"Historically, how to computationally solve the governing equations was known, but there was not enough computer power to solve significant problems in a practical length of actual time."

Continued expansion of HPC resources, including number of processors available and the compute speed of those processors, allowed the size of the models to expand. By allowing the use of a larger number of cells or elements, more detail could be inserted into the models and fewer simplifications needed to be taken. All of these models were approximations, and the capability to more explicitly model the subject allowed more accurate solutions to be obtained.

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CTA: Computational Structural Mechanics
Computer Resources: SGI Origin 3000 and IBM SMP [ERDC] and IBM SMP [ASC]

Modeling Methods for Assessment of Gun-Propellant Vulnerability

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Army Research Laboratory (ARL), Aberdeen Proving Ground, MD

In order to increase the muzzle energy in medium- and large-caliber guns (and consequently their lethality), approaches involving increasing the available mass of gun propellant are being pursued by scientists at the ARL. This generally means packing more propellant into the available volume, which may adversely affect the vulnerability of associated weapons systems by allowing the propellant bed to support detonation.

"The modeling approaches developed in this program are being used for the Army's Future Combat System to help design high-loading-density gun-propelling charges to provide maximum performance with minimum impact on systems survivability."

Starkenberg and Dorsey are developing modeling approaches for assessing the violence of the reactive responses of propellant beds to unplanned stimuli, emphasizing the tendency for detonation to spread from one part of a bed to another. Their results will be applied to emerging propellant technologies to determine how to design beds to minimize reactive response violence.

Studying Detonation Propagation Models

Traditionally, gun-propellant vulnerability has been assessed through experiments, not simulations. Now explosive initiation models such as those included in the Eulerian finite-volume continuum mechanics solver CTH may also be used to model detonation propagation and failure. A detailed computational study of the use of these models for detonation propagation was undertaken. Based on the understanding gained in that study, large three-dimensional simulations of the spread of detonation between propellant grains and between parts of more advanced charge designs were undertaken using CTH's History Variable Reactive Burn (HVRB) model.

The fundamental study showed that extremely fine computational resolution and special calibrations of the HVRB model are required to accurately determine the smallest propellant grain diameter that allows a detonation to propagate. This is referred to as the failure or critical diameter. Eight different propagation and contact modes for propagation between pairs of cylindrical propellant grains in a bed were identified and simulated. Figure 1 shows the results of a simulation of grains in side-to-side point contact with the detonation spreading directly from one grain to the other. The results show that diameters larger than the critical diameter are required for grain-to-grain propagation and explain experimental observations. This indicates that

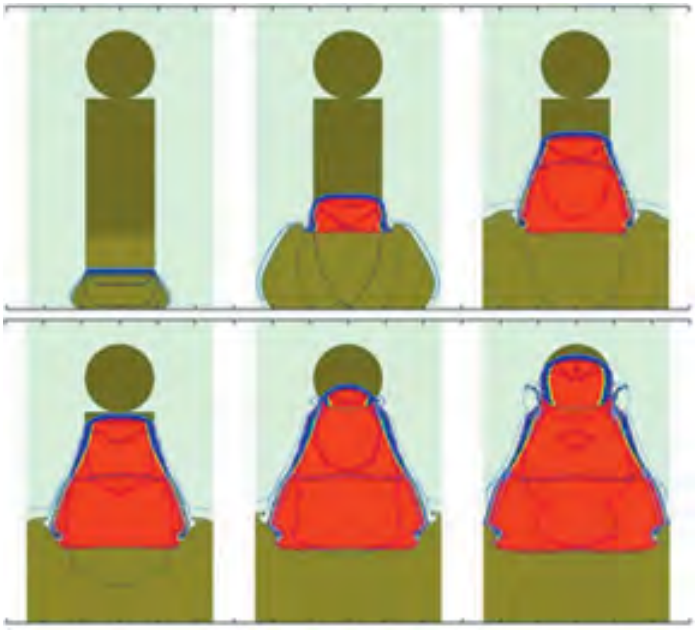

Figure 1. Sequence of plots showing propagation of detonation between propellant grains

detonation can be prevented from spreading throughout a bed even when the grains are larger than the critical diameter. Results from simulations of more advanced propellant bed designs also show how the beds can be designed to minimize the violence of the reactive response.

Modeling Used to Design Propellant Charges

The modeling approaches developed in this program are being used for the Army's Future Combat System to help design high-loading-density gun-propellant charges to provide maximum performance with minimum impact on systems survivability. The approach is suitable for evaluating special propellant configurations even when samples for testing are unavailable. This helps in understanding the system vulnerability implications of using specific propellant configurations on proposed weapons platforms.

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CTA: Computational Structural Mechanics

Computer Resources: SGI Origin 2000, SGI Origin 3000, and IBM SP Power3 [ARL]

Robust Scalable Information Processing for Multistatic Sonars

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Acoustic sonar performance for various Anti-Submarine Warfare programs benefits from improved algorithms that increase detection of the submarine threat, as well as reduce the false alarms caused by misclassified clutter detections. Current algorithm development achieves robustness by analyzing data from a large number of at-sea tests, which represent different environments, target dynamics, and transmitted signals (Figure 1).

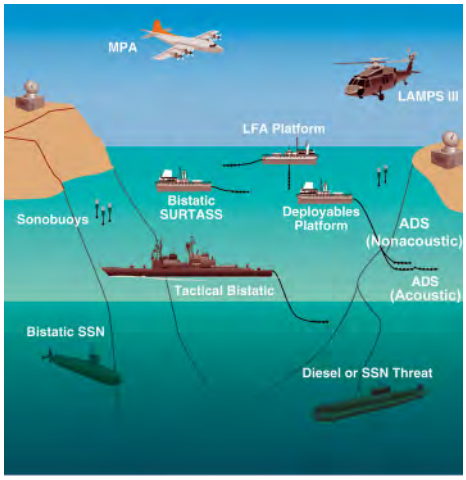


Figure 1. Surveillance Platforms

Active sonar systems benefit from the ability to estimate target range. Complex pings can be used to improve the target state estimation by providing a range-rate estimate. One algorithm tested and validated using the HPC resources is an improved range rate estimator for one of the mainstay waveforms in active sonar, the Hyperbolic Frequency Modulated (HFM) waveform. Improved range rate estimation reduces the percentage of high-speed clutter thus reducing both the algorithmic and operator resources.

Correlation-Based Algorithms

Traditionally, range rate estimates for HFM waveforms have been calculated using a correlation based algorithm. The range rate estimates from the correlation-based algorithm tended to incorrectly estimate the range rate of bottom-induced clutter. In the system, there are multiple channels. The correlation-based algorithm uses pair wise correlation of the HFM echo returns to update the time delay of the HFMs. The correlation information is reduced to two time delays. The two time delays are then used in a line fit, and the slope of the line is used to estimate the range rate. The existing method loses the shape information of the echoed HFM, and spurious noise spikes can cause the line fit to fit at an inappropriate speed estimate.

Improved Algorithm Analysis

The HPC resources are used to improve algorithm analysis, with a goal of transitioning the algorithms into fleet use. The Space and Naval Warfare (SPAWAR) System Center (SSC) Signal Processor and the ORINCON Information Processor (IP), hosted on the HPC HP-V2500 Multiprocessor Computer, are flexible and can be configured for processing data from various acoustic arrays (Figure 2).

The HPC resources enable efficient and robust algorithm evaluation due to the amount of data that can be stored and processed. The Scalable

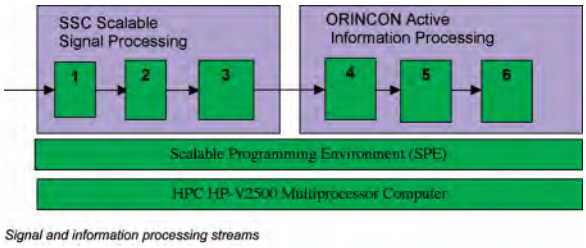


Figure 2. Signal and Information Processing Streams

Programming Environment (SPE) available on the V2500 provides a well-defined interface, portability, and reduced development time. The SPE layer allows for modularization, and adding a module to the system is relatively easy. Algorithms that are being compared may be run in parallel, and their classifier Receiver Operating Characteristics (ROC) curves can be analyzed quickly.

"The HPC resources are used to improve algorithm analysis, with a goal of transition of algorithms into fleet use. The HPC resources enable efficient and robust algorithm evaluation due to the amount of data that can be stored and processed."

HPC allowed this research project to robustly test and evaluate the improvement in active sonar detection and classification when applying ORINCON's improved range rate algorithm.

The SPAWAR System Center, San Diego (SSCSD) Advanced Visualization for Intelligence, Surveillance, and Reconnaisance (ADVISR) visualization tool has been used in some of the work as well as in MATLAB. MATLAB has been an invaluable tool for data analysis and prototyping. The ADVISR simulations allowed for viewing the evolution of the situation over time and provided improved viewer comprehension.

Target Detections Improved

Processing within the Scalable Signal Processor and Active Information Processor consists of several steps. The echoes for the HFM transmissions are beam formed, matched filtered, noise normalized, and thresholded. The IP receives the threshold crossings and attempts to group together crossings that are from the same echo source. This is the clustering portion of the IP. The next step is to combine the multiple HFM waveforms that were transmitted into detections. Detections use an M-out-of-N criterion where M is the minimum number of the multiple HFM sweeps and N is the number of HFM sweeps transmitted. These HFM detections can be combined with other waveform types, such as continuous waveform, to form wave train detections (Figure 3). The wave train detections are sent to the tracker for linking over time. At all stages, classification calculations are performed and target or clutter likeness is determined.

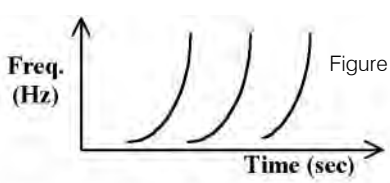
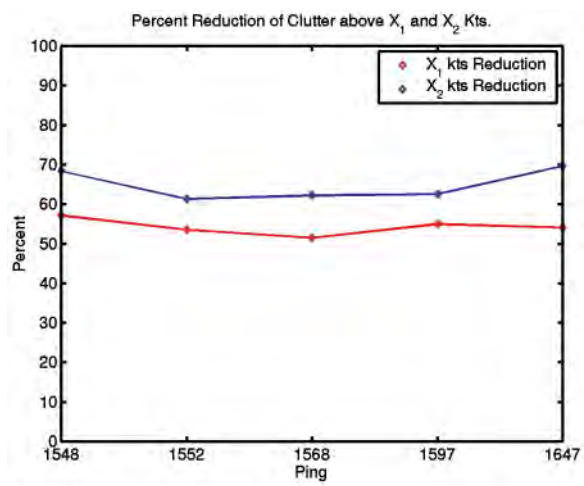


Figure 3. HFM Wavetrain

Wavetrain comprised of three HFM waveforms

For the data analyzed, target detections for surface and sub-surface detections were achieved at tactical ranges. The improved range rate parameter is calculated in the detection portion of the IP. Analysis of the improved range rate parameter has shown a marked reduction in the range rate of high-speed clutter detections while preserving the range rate of targets of interest. As shown in the results plot (Figure 4), the algorithm provides a minimum 61 percent reduction in "high-speed" clutter detections. At a lower range-rate X1, which is half of X2, over 50 percent of the clutter detections are removed. This improvement reduces the single-ping false alarm rate when alerting the operator to detections that are thought to be from moving objects. The importance of this project is the capability to robustly test candidate algorithms. The availability of the HPC resources allowed use of the SPE. The SPE allowed for the design of the processing components in a modular, scalable fashion. This architecture provided a test bed for active signal processing that allows easy replacing of various candidate classification algorithms. The large storage and computing capabilities allowed very large quantities of data to be processed, allowing robust testing.



Range rate estimation results

Figure 4. Range Rate Results

Estimating Target Range Rates

In this environment and architecture, Navy researchers have tested a novel approach to estimating target range rate with HFM waveforms that are not typically associated with providing range rate. In addition to estimating the range rate of a detection, they also computed a new classification clue "t-ratio" which is the speed estimate divided by the standard deviation of the speed estimate. The t-ratio

computation represents the confidence of the range rate estimate. Adding t-ratio to the classification clue set resulted in a very significant reduction in the number of clutter detections that would be classified as targets and sent to an operator, thus reducing their workload and allowing them to focus on other detections, while preserving the range rates of targets of interest.

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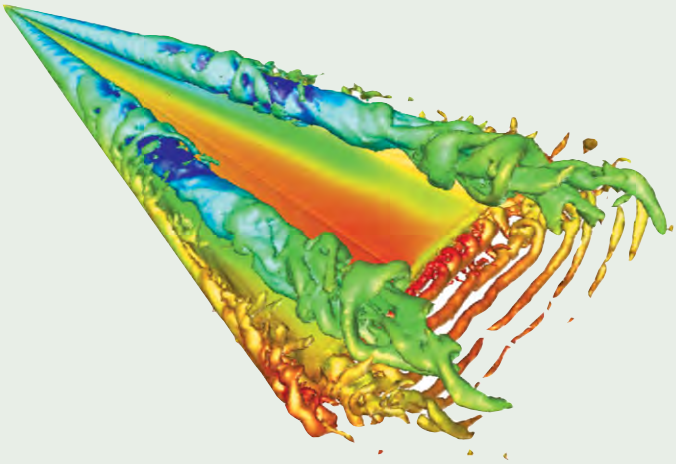
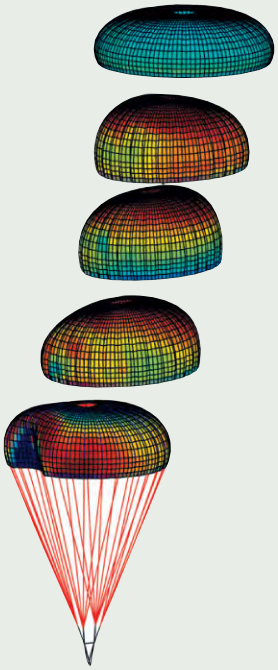
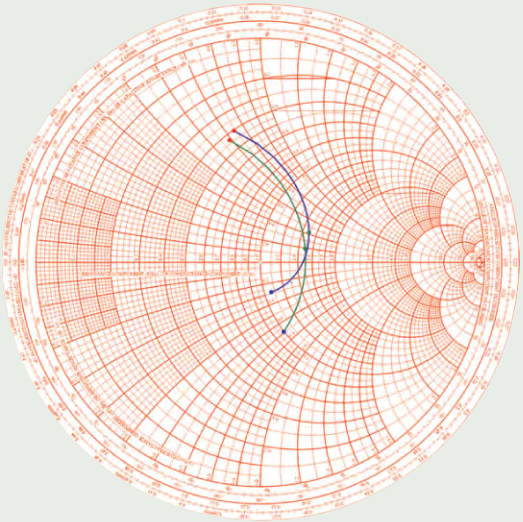
CTA: Signal/Image Processing
Computer Resources: HP V2500 [SSCSD]

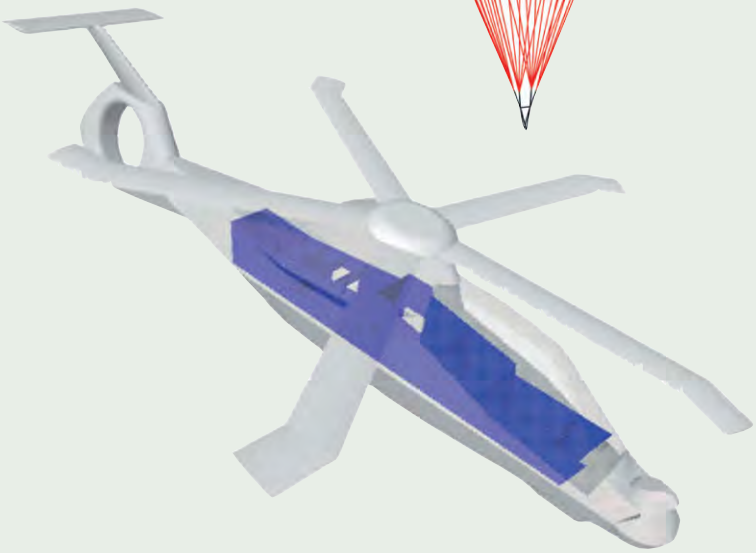
Project and Sustain US Forces

Anti-Access Capabilities Minimize Logistics Footprint









References (from left to right):

Detached-Eddy Simulation of Massively Separated Flows over Aircraft by Kyle Squires, James Forsythe, Scott Morton, Kenneth Wurtzler, William Strang, Robert Tomaro, and Philippe Spalart

Flow over the delta wing at 27° angle of attack. Isosurface of vorticity

Airdrop Systems Modeling: Fluid-Structure Interaction Applications by Richard Benney, Keith Stein, Tayfun Tezduyar, Michael Accorsi, and Hamid Johari

This figure shows the structural response of the upper canopy as it deforms and interacts with the surrounding flow field. The colors on the canopy correspond to the differential pressures, which are a part of the fluid dynamics solution.

Absolute Scalability of Space/Time Domain Decomposition in Computational Structural Dynamics for Virtual Modeling and Testing Applications by R. Kanapady and K. K. Tamma

Solid modeling of keel beam

Accurate Modeling of Lossy Frequency Selective Surfaces for Real-Time Design by John Meloling, Wendy Massey, and David Hurdsman

Smith chart of boundary admittance using past approximations (green) and more accurate solutions (blue)

Project and Sustain US Forces

"All warfare is based on deception. Hence, when able to attack, we must seem unable; when using our forces, we must seem inactive; when we are near, we must make the enemy believe we are far away; when far away, we must make him believe we are near."[1] The following success stories describe some important efforts to use HPC for the design and analysis of military platforms and the battlespace environment to help project and sustain US forces.

High performance computing is critical to the research, design, acquisition, and testing of military platforms with superior warfighting capabilities. One of the primary goals of these warfighting platforms is to project US forces into hostile situations and sustain them in that situation.

High performance computing contributes significantly to the design of these weapons platforms in a variety of ways, as chronicled by the first group of seventeen success stories. What is particularly impressive is the breadth of computational work represented in terms of length scales. They range from the nanoscale as detailed in the Jarvis and Carter accomplishment of using quantum mechanics to investigate thermal barrier coatings on jet engine turbine blades to the size of large vehicles as discussed in the Gorski, Hyman, Taylor, and Wilson article on hydrodynamics on entire ships. Component level simulations of armor and composites are discussed in articles by Holmquist and Johnson, and Shires, Henz, and Mohan. Analysis of components such as turbomachines and full systems such as modern airplanes is performed with Computational Fluid Dynamic (CFD) simulations in articles by Moin, You, Wand, and Mittal; by Jurkovich, Rittinger, and Weyer; by Polsky; by Rizzetta; by Green and Ott; and by Forsythe, Morton, Squires, Wurtzler, Strang, Tomaro, and Spalart. Pushing the computational frontiers downward in size to the nanoscale to model specific surfaces atomistically or upward in size to model aerodynamic flow in a time-dependent fashion around whole aircraft represents an expansion of the computational capability envelope that is now just becoming possible with present-day systems.

Along another dimension, this set of success stories represents several of the program's major computational areas. In addition to CFD, there are also stories in computational chemistry and materials science, computational structural mechanics, and computational electromagnetics and acoustics. The stories by Hill, Navale, and Sancer, and by Mark, Clarke, Namburu, Le, and Nehrbass employ the techniques of computational electromagnetics (CEM) to compute the electromagnetic signatures of electromagnetically large combat vehicles. Of particular interest is interdisciplinary computational work, as presented in the Soo, Feiz, and Menon contribution on incorporation of finite rate chemistry into computational fluid dynamic studies of fuel injectors for propulsion systems, and the coupled fluid/structure investigations of aircraft wing response to artillery damage of Hinrichsen. The interaction of structures with the surrounding land, air, and sea environments is investigated in the article by Prakash on testing armor, in the article by Benney, Stein, Tezduyar, Accorsi, and Johari on airdrop systems, and in the article on the effects of mines by Landsberg.

All in all, these seventeen stories make impressive contributions to solving real DoD problems. Every single one of them addresses a real mission need, ranging from a specific, short-term problem on a current weapon system through basic research and design work on future weapons systems.

Synchronization and coordination within the battlespace to project and sustain US Forces are key transformational military goals. The 2001 Quadrennial Defense Review states that DoD will "… develop an interoperable, joint C4ISR architecture and capability that includes a tailorable joint operational battlespace." This battlespace is defined by "layers" of information where some layers are static (e.g.,

[1] Sun Tzu, *The Art of War*

land, buildings, space) and others are dynamic (e.g., weather, ocean, foliage, weapons locations). The battlespace environment itself is the subject of study the next group of five stories that discuss specifically how the Common High Performance Computing Software Support Initiative (CHSSI) and DoD HPC efforts help build the dynamic weather/ocean layers.

Characterizing the environmental battlespace is the most important goal in building dynamic weather/ocean layers. But what does "characterizing the environmental battlespace" really mean? It is the ability to take real-time weather/ocean observations, combine the observations with numerical model fields, and create a volumetric dataset where weather/ocean layers are defined in space and time. Allard et. al., provides an overview on how their CHSSI portfolio efforts are building the ocean, tide, wave, estuarine, and riverine layers for littoral regions. Through new techniques in coupling different models to create a synthesized environment, the littoral battlespace layers will constantly provide the warfighters with the appropriate readiness to conduct their missions.

The Fleet requires wave and surf hind-casts and short-term forecasts for accurate mission planning. Successful amphibious assaults are enabled by accurate wave modeling along the beach. Smith describes how HPC resources were critical to building the "wave" layer within the littoral battlespace portfolio. The integration effort described by Allard et. al., involves the coupling of the wave layer to other littoral layers, and the fuzing of the layers (in time and space) to create a volumetric dataset. Burnett focuses on the atmospheric layer and describes a successful story of how HPC resources allowed the operational community to continue providing operational weather layers to the warfighter while the Production Center converted from vector to scalable architectures. The story by Hughes, Wegiel, McAtte, Michalakes, Barker and LaCroix discusses integration of data from real-time weather observations with HPC forecast models.

The final critical part in developing the environmental battlespace is the visualization and understanding of the various layers. Gruzinskas describes how HPC efforts in visualizing the battlespace environment will ensure that planners and decision-makers have an in-depth understanding of the constantly changing environmental conditions. He describes a particular case where the Navy supported the Ehime Maru salvage operations using virtual environments and on-scene data. The effort actually went a step further and integrated real-time observations with the virtual environment.

Characterizing the battlespace environment is an on-going effort. These success stories show that the Meterology and Oceanography Community is only a third of the way toward reaching their goal of creating a volumetric battlespace. Initial steps in building the littoral environmental battlespace and crucial DoD HPC support of CHSSI, Programming Environment and Training (PET), and MSRCs will allow the community to reach their goal within the next five years.

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How Quantum Mechanics Can Impact Jet Engines: Improving Aircraft Design at the Nanoscale

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Sponsor: Air Force Office of Scientific Research (AFOSR)

Thermal barrier coatings (TBCs) of jet engine turbines afford thermal and oxidative/corrosive protection of the underlying metal superalloy that is crucial to aircraft performance. This coating must withstand temperature cycling over a range exceeding 1000 °C, as the engine is taken from rest to maximum operating capacity. The highest temperatures accessed within the combustion chamber are even beyond the melting point of the superalloy substrate. Nevertheless, such high temperature combustion is required to attain optimal engine power and maximum fuel efficiency.

For years, the TBC of choice has been zirconia with ~7–8% yttria (yttria-stabilized zirconia, YSZ) added to stabilize the tetragonal/cubic phases of zirconia over the relevant temperature cycling range. This Y_2O_3-ZrO_2 coating affords significant thermal protection, exhibiting very low thermal conductivity. Unfortunately, it is not well suited to oxidative/corrosive protection. Furthermore, its materials properties are not optimally matched to the single crystal nickel alloy substrate. As a result, an intermediate protective layer, commonly called the "bond coat" and typically consisting of a NiCrAlY alloy, is deposited on the nickel superalloy prior to deposition of the YSZ. This layer provides an intermediate thermal expansion coefficient to that of the superalloy and the YSZ. It also is designed to promote YSZ adhesion, and must supply a source of oxidative/corrosive protection from the harsh combustion gases. The Al content in the bond coat is responsible for this latter task. The oxidation product of aluminum, Al_2O_3, forms a nearly continuous layer that serves as a slow-growing, effective barrier against further oxidation of the underlying metal alloy.

"Only with the recent advent of high performance computing capabilities is it feasible to explore the detailed interactions at metal-ceramic interfaces."

TBC Spallation

Unfortunately, a process known as spallation, whereby the TBC peels off the underlying substrate, limits a TBC's operational lifetime. TBC spallation is catastrophic because: 1) the superalloy composing the turbine blade is left unprotected; and 2) large spalled coating pieces may pose additional danger during engine operation. Turbine blades with failed TBC's must be recoated or replaced. To help minimize spallation, a nickel alloy bond coat is deposited on the superalloy substrate before the TBC is applied. This bond coat can promote adhesion, serve as a graded thermal expansion layer, and limit hot oxidation/corrosion resulting from high temperature oxygen diffusion through zirconia. As a result of the TBC's transparency to high temperature oxygen diffusion, most bond coat alloys in current production form a thermally grown oxide layer of primarily Al_2O_3. The thickening of the thermally grown oxide with repeated thermal cycling is accompanied with increased spallation. Research, sponsored by AFOSR, is being conducted to suggest chemical modifications to the bond coat alloy that will improve adhesion at the ceramic/metal interface. It will inhibit oxide formation or form oxide products more ideally suited to the imposed interface and thermal cycling requirements. In addition to jet engine turbine applications, improved TBCs might permit more efficient running of stationary power plants—providing benefit both by decreasing pollution and cost.

Trial and Error Methods

The physical and chemical complexity of TBCs has required "trial and error" empirical engineering methods for most material advances. From a

theoretical standpoint, the rich physics underlying the fundamental nature of metal/oxide interfaces is only recently being explored. Before this, the strong attractive force at nonreactive metal/ceramic interfaces had been attributed to classical electrostatic effects. Although it is likely these electrostatic forces are important, a theory emphasizing these contributions to the exclusion of chemical bonding mechanisms provides an incomplete picture of interface adhesion. More importantly, the logical conclusions that can be inferred from such a theory result in counter-productive materials design predictions.

Exploring Metal-Ceramic Interfaces

Only with the recent advent of high performance computing capabilities is it feasible to explore the detailed interactions at metal-ceramic interfaces. In many instances, quantum mechanical effects may dominate the interface adhesion. Treating the quantum mechanical problem in metal/ceramic interface studies is very computationally challenging, requiring extensive computing power and memory. Neglecting to treat the quantum mechanical problem, or treating these effects at a very approximate level, is far less computationally expensive but excludes the effects necessary for crucial insights into materials advancements.

Researchers at the University of California, Los Angeles, employ density functional theory (using planewave bases and pseudopotentials within the Vienna Ab Initio Simulation Package) to investigate atomic-level interactions at ideal ceramic/metal interfaces designed for TBC applications. These calculations are computationally intensive but can be run efficiently on parallel platforms. Although the system size is limited to a few hundred atoms due to computational size constraints, the three-dimensional (3-D) periodic boundary conditions simulate an effective "infinite" interface neglecting long-ranged relaxation effects. They have performed both static calculations, where the ionic coordinates are relaxed to a local minimum energy configuration using a conjugate-gradient algorithm, and molecular dynamics simulations of high-temperature annealing to better approximate the extreme environment in jet engine combustion chambers.

Previously, the calculations provided insight into atomic-level contributions to the observed spallation of TBCs. They found the ideal interface between Al_2O_3 and the bond coat alloy, as well as the Al_2O_3 interface with the zirconia topcoat, is unfavorable from the standpoint of interfacial adhesion and chemical bonding. In particular, the ceramic/metal interface adhesion dramatically decreases with increasing oxide thickness. Their calculations indicated a fundamental weakness of such interfaces could be linked to the high ionicity, and thus closed-shell-like behavior, of the Al_2O_3 interface with an alloy primarily composed of Ni, an element with a mostly filled d-shell. Such electronic structure results in effective "closed-shell repulsions" at the interface instead of strong bonding interactions.

Investigating Chemical Modifications

Accordingly, the team investigated chemical modifications to the metal alloy bond coat designed to promote a strong interface by permitting bonding interactions at the ceramic/metal rather than closed-shell repulsions. They explored the atomic-level impact of early transition metal dopants at the ceramic/metal interface currently relevant in TBCs Al_2O_3/Ni (Figure 1). Their initial results indicated that early transition metal doping of the bond coat alloy effect a dramatic increase in adhesion. Their calculations showed this bond coat alloy "doping" resulted in a ~45% increased adhesion, relative to nickel, at the ZrO_2/Ni interface and a dramatic 100% increase in adhesion at the Al_2O_3/Ni interface.

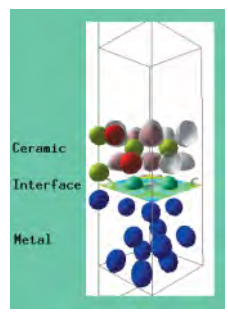

Figure 1. This figure displays the doped metal-ceramic interface structure from atomic-level calculations. Although the actual number of atoms in the simulation is fairly small, periodic boundary conditions allow the team to simulate an "infinite" interface.

Over the past year, the team has performed detailed studies exploring how the electron density is modified as a result of early transition metal interface doping. They also investigated the effects of modifying the interface electronic structure through altering the oxygen states of the ceramic. They calculated the ideal adhesion at the SiO_2/Ni and ZrO_2/SiO_2 interfaces and found it to be much greater than the adhesion at the corresponding interfaces with Al_2O_3 instead of SiO_2. Similar to early transition metal interface dopants, the dramatically increased adhesion is a result of quantum mechanical interactions at the interface. The Si-O bond in SiO_2 is less ionic than the Al-O bond in Al_2O_3, thus the oxygen in SiO_2 does not contribute local interface repulsions like those seen in the Al_2O_3/Ni couple. Local bonding interactions are essential; using only electrostatic considerations as the means to predict

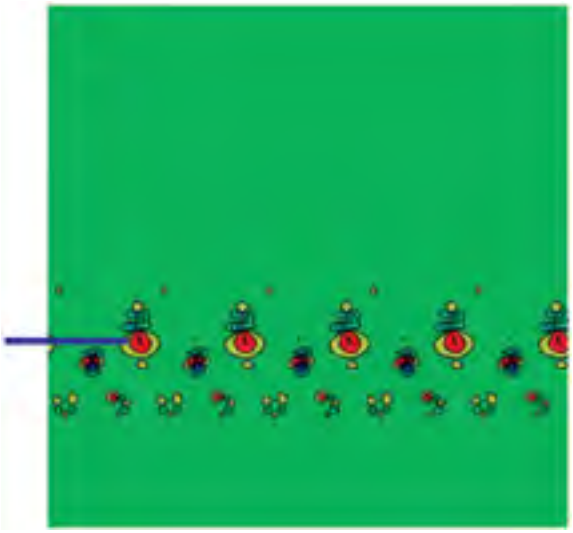

Figure 2. Contour plot of the electron density difference between the sum of the isolated metal substrate and ceramic coating densities and the metal-ceramic interface (Al_2O_3/Ti-Ni) electron density. The color scale runs from red to violet with red showing increased density in the interface and violet indicating decreased density. The yellow "circles" in the horizontal region indicated by the blue line display a region of metal-metal bonding as a result of interface formation.

strong metal-ceramic interfaces for TBC applications results in the wrong physics. Their calculations indicate chemical bonding effects are responsible for strong heterogeneous interface adhesion.

Predicting Materials Improvements

Previous studies have concentrated on achieving a detailed understanding of atomic-level weaknesses at idealized interfaces related to those found in TBCs and predicting materials improvements to these interfaces. The team's predictions that quantum mechanical effects play the dominant role in strong interface adhesion may allow new materials design paradigms that permit informed engineering modifications to real TBCs. Predictions for improving materials performance should significantly decrease the "trial and error" phase of materials design for these applications.

Although current results may provide fruitful avenues for materials improvements, additional challenges remain. In the future, the team plans to study the effect of diffusion and segregation of harmful dopants to the metal alloy/oxide interface. A detailed understanding of how interface adhesion is reduced by undesirable segregants, such as sulfur, may suggest means by which the detrimental impact of such elements could be limited or eliminated.

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CTA: Computational Chemistry and Materials Science
Computer Resources: IBM SP P3 [MHPCC]

Modeling "Smart" Fuel Injector Designs

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Georgia Institute of Technology, Atlanta, GA
Sponsor: Army Research Office (ARO)

The Army needs lightweight, compact, fuel-efficient propulsion systems for helicopters and tanks for the Army After Next. This will require significant improvement in the performance of the next generation gas turbine engines. Reduction in engine size and weight will also reduce the logistics burden for rapidly deployable forces. Reduced fuel consumption is especially critical since fuel is a major logistics burden. Under the leadership of the Army Research Office (ARO), scientists are developing advanced fuel-efficient systems to reduce fuel consumption without sacrificing performance. However, experimental investigations of such systems are complicated by the difficulty in obtaining non-intrusive access to the hot, turbulent reacting region in the combustor. Numerical tools that can predict the unsteady combustion processes may be able to provide a new, previously unavailable capability to investigate the mixing enhancement process. This, in turn, will advance the design process.

Revolutionizing the Design of Fuel Injectors

The department's engineers and scientific researchers must revolutionize the design of fuel injectors to increase fuel efficiency and reduce the environmental impact of combustion-powered vehicles. Fuel injectors are designed to rapidly and thoroughly mix fuel with the surrounding air (oxidizer) before the mixture is burnt. Ineffective or incomplete mixing produces sooty flames and heat loss, which causes a substantial performance drop. Traditional injectors are designed with circular or round jets since they generally deliver a symmetric (though not necessarily uniform) fuel mixture. Geometries such as square jets (Figure 1), however, may offer increased mixing rates. Fuel injectors that employ active control of fuel dispersion may offer even more enhanced mixing efficiency. For example, synthetic microjet forcing of fuel injectors has shown a remarkable ability to increase and control mixing. Synthetic jets do not add additional fuel to the mixture but, instead, work with fluid already injected into the mixing environment. Synthetic jets can be used to increase fuel/air mixing rates and/or to actively control the primary jet flow or boundary layers by periodically sucking and blowing fluid into and out of their micro-scale storage chambers, as shown in Figure 2. Innovative techniques based on micro-electro-mechanical systems (MEMS) technology are currently being studied where the fuel jet is actively forced using embedded synthetic micro-jets. Significant enhancement of fuel-air mixing appears to be occurring due to these MEMS

"Numerical tools that can predict the unsteady combustion processes may be able to provide a new, previously unavailable capability to investigate the mixing enhancement process. This, in turn, will advance the design process."

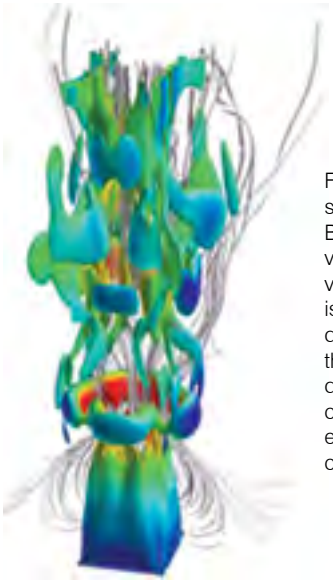

Figure 1. Simulation of square jet using Lattice-Boltzman method. Square vortices, depicted by the vorticity magnitude isosurface, are propelled downstream (upwards) with the flow. The streamlines are drawn from outside the jet core reveal the high mass entrainment rates characteristic of square jets.

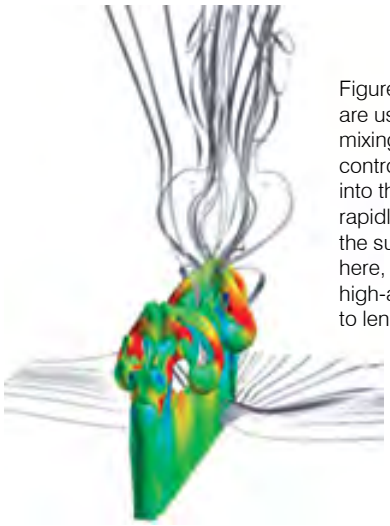

Figure 2. Synthetic microjets are used to increase fuel/air mixing and boundary layer control. Outside air is sucked into the jet cavity and then rapidly expelled outwards into the surround mixture. Shown here, is the simulation of a high-aspect-ratio (high width to length ratio) synthetic jet.

devices, however, detailed observation of the flow field generated by these micro-scale actuators is difficult, if not impossible.

High Performance Modeling of Synthetic Jets

Modeling of fuel injectors is a challenging task due to their small size. The small dimensions restrict the maximum allowable time-step that may be taken in a traditional CFD simulation. Time-accurate (unsteady) simulations are required to capture the dynamics of the unsteady nature of jet motion and fuel/air mixing. The restrictive time-step effect is even more pronounced for micro-scale synthetic jets, which have to be small enough to actually fit inside the primary fuel jets. A new modeling technique, Lattice-Boltzman Equation (LBE), is used to simulate the small-scale flow in one synthetic jet and other novel fuel injector designs. Unlike traditional CFD, which represents the working fluid as a continuous system (macroscopic view), LBE treats the fluid as a collection of particles governed by a single statistical distribution equation (microscopic view). This technique is advantageous when simulating small-scale fluids since its time-step limitations are not restrictive. Additionally, LBE is easily parallelized and is highly scalable on a parallel high-performance computing system.

In the current studies, various 3-D non-circular and synthetic jets are simulated using the LBE method. The objective of this study is to investigate the turbulent dynamics of these jets and to evaluate the effectiveness and accuracy of the 3-D, parallel LBE method. Typically, 2–3 million grid points are used to resolve the resulting unsteady flow. This complexity requires 600 CPU hours and nearly 2 gigabytes of memory on a distributed shared-memory parallel machine. The extreme efficiency of the LBE algorithm coupled with the high-performance computing resources available at the DoD MSRCs allows high-resolution parametric jet simulations with rapid turn-around times.

Excellent results have been obtained from the LBE simulations. Simulations of free and forced square jets have been able to capture phenomena such as axis switching (vortices inverting as a result of the non-uniform flow) and increased mass entrainment. Similarly, direct comparisons with experiments on a series of synthetic jets have also been conducted. The simulations show good agreement with the experiments, adding credibility to the numerical method. Finally, the interaction of a square jet with a steady cross-flow (as would be used for boundary-layer control or combustor wall cooling) has been investigated. Complex flow structures such as “horse-shoe” and “hairpin” vortices have been observed.

Several extensions to the LBE method are currently underway. These include extending this promising method to combustion (which requires the modeling of chemical reactions and heat-release) and coupling the LBE simulations to Large-Eddy Simulations (LES). LES is an effective tool for simulating unsteady, complex flows such as those found inside gas turbine combustors. The coupled LBE/LES method would allow the simulation of both the fuel injectors mixing regions and the combustor at an affordable computational cost. The combined LBE/LES approach provides a unique simulation capability that can be used to investigate the performance of these fuel injectors under realistic operating conditions. In the future, many other issues of practical interest to DoD such as high-pressure combustion, supercritical fuels, and combustion instability can be addressed with these codes.

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CTA: Computational Fluid Dynamics

Computer Resources: IBM P3 SMP, Cray T3E, and Mass Storage [NAVO]

Computational Modeling of Ceramic Armor

Timothy Holmquist and Gordon Johnson
Army High Performance Computing Research Center (AHPCRC)/NetworkCS, Minneapolis, MN

The United States Army is developing advanced lightweight armor to increase vehicle protection and reduce vehicle weight. One class of materials that has been considered for armor applications in recent years is ceramics. Ceramic materials are very strong in compression, relatively weak in tension, and tend to be lightweight when compared to more traditional armor materials such as metals. Certain ceramics have also exhibited a phenomenon called "ceramic dwell". Ceramic dwell occurs when a high velocity projectile impacts a ceramic target and then dwells on the surface of the ceramic with no significant penetration. These characteristics make ceramics well suited for armor applications, but also present a significant design challenge when incorporated into armor systems.

Ballistic Testing Used to Develop Ceramic Armor

Historically, ceramic armor has been developed by rigorous use of ballistic testing. Although much advancement has been made in ceramic armor design primarily using ballistic testing, it is a time consuming and very expensive process. A better approach is to use ballistic testing along with computations. Effective armor design can be enhanced, cost can be reduced, and the behavior better understood by the use of HPC resources if the computational models adequately represent the material behavior. Furthermore, the HPC systems have the memory and speed required to perform these computations in a timely and efficient manner.

Recent advancements in the development of ceramic material models and numerical algorithms at AHPCRC, allows for accurate representation of ceramic material behavior. Specifically, the ability to model the phenomenon of ceramic dwell has been developed and computations have been performed to investigate ceramic dwell and how it is affected by target geometry.

Figure 1 presents the computational results for three target configurations. All three targets are comprised of a ceramic core surrounded by metal. The baseline geometry is a configuration that was investigated experimentally. The computational results accurately represent the behavior exhibited in the experiment. The other two target configurations, slight modifications of the baseline geometry, were performed to investigate the effect of diameter and cover plate attachment. The penetration results are presented as a function of time at the bottom of Figure 1. The results indicate that the best performing design is the large diameter configuration (least amount of ceramic penetration at 60 microseconds) and the worst performing design is the detached cover (most amount of ceramic penetration at 60 microseconds). Computations such as these can be performed to provide insight into the complex behavior of ceramic armor and aid the armor designer in developing improved armor systems.

"Effective armor design can be enhanced, cost can be reduced, and the behavior better understood by the use of HPC resources if the computational models adequately represent the material behavior. Furthermore, the HPC systems have the memory and speed required to perform these computations in a timely and efficient manner."

The ability to accurately simulate the ceramic dwell phenomenon allows the Army reseachers to design ceramic armor in an efficient, cost effective manner. This new capability is currently being used by the ARL and the Tank Automotive Research, Development and Engineering Center (TARDEC) to help design ceramic armor for the Future Combat System (FCS).

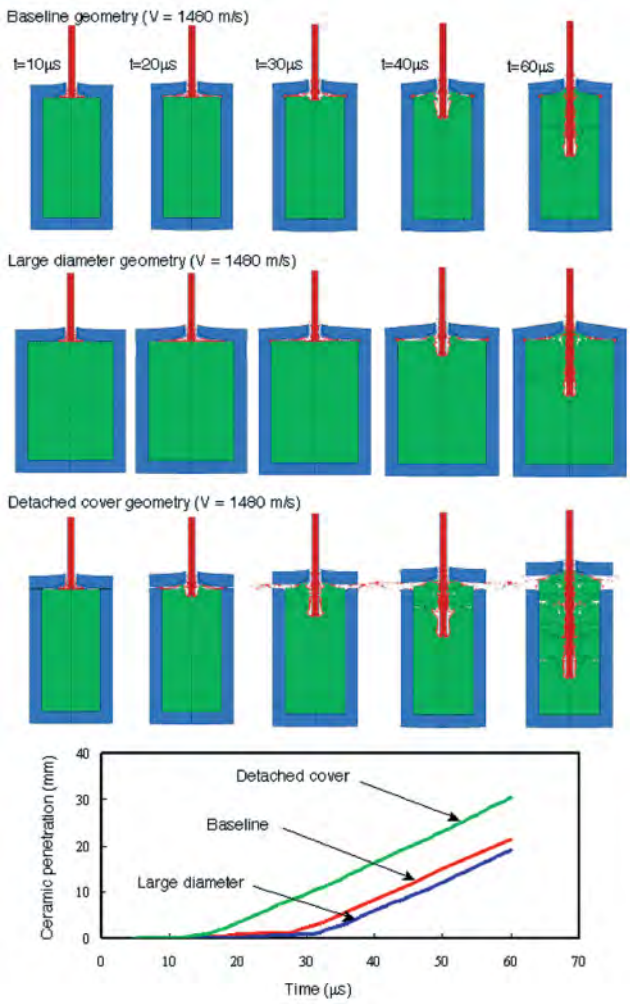

Figure 1. Computational results for a baseline ceramic target geometry, a large diameter geometry and a detached cover geometry. For all three geometries, the ceramic material is encapsulated by metal. Also shown are the ceramic penetration time histories.

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CTA: Computational Structural Mechanics
Computer Resources: SGI Onyx2 [TARDEC]

Parallel Computing Enables Streamlined Acquisition for Composite Materials

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Ram Mohan
University of New Orleans, New Orleans, LA

As composite materials are increasingly used in weapon and combat systems (both retrofitted and new components), it is increasingly important to fully understand the complexities associated with their manufacture. Structural materials used in the past, such as metals, have well-established design, manufacturing, and testing protocols. The same cannot be said of composites. Even after years of use, the structures remain risky in terms of cost and difficulties associated with manufacture. Traditionally, experienced process engineers have manufactured these parts using "best guess" approaches. However, the complexities of the new designs being developed to support FCS significantly highlight the limits of that approach. Composites with embedded structures, for example, significantly increase the level of difficulty in producing a viable part on the first manufacturing attempt.

Modeling Composites and the Manufacturing Process

The best solution to overcome these problems is a physics-based modeling and simulation approach. Liquid injection molding of composites usually involves some fiberglass or organic matrix fiber structure being placed into a mold and being injected with a thermosetting resin. Darcy's law governs the flow of resin through a porous media. It relates the velocity field to the pressure gradient through fluid velocity and the fiber preform permeability. Darcy's law is defined as

$$\vec{u} = \frac{K}{\mu}\nabla P$$

where $\vec{u}$ is the velocity field, μ is the fluid viscosity, and P is the pressure. Permeability K is a measure of the resistance experienced by a fluid as it flows through a porous media and is an important material characteristic involved in the flow simulations. Complex structures are discretized using finite element meshes to model the geometric complexities. Material regions in the model are defined based on the permeability characteristics of the fiber preforms.

"Now, large-scale process simulations of even the most detailed and complex parts are possible with results available in hours rather than weeks or even months."

Traditional numerical approaches to model the manufacturing phenomena, such as the finite element-control volume method, were considered and found inadequate. The stability conditions associated with the solution required computer times exceeding weeks of single processor or parallel computer time. However, the newer methodologies, found in the COmposite Manufacturing PrOcess Simulation Environment (COMPOSE) suite of tools, were developed with a focus on parallelism and fundamental algorithmic changes. Now, large-scale process simulations of even the most detailed and complex parts are possible with results available in hours rather than weeks or even months. Process engineers can perform parametric studies to identify potential manufacturing problems and optimize the manufacturing process before capital investment in mold tooling is made. COMPOSE developers are working to expand these capabilities by adding sensitivity analysis and thermal and cure modeling to the parallel solutions. Recent additions such as a cross-platform Java-based user interface are putting

the technology in the hands of process engineers and manufacturers even faster.

COMPOSE has been used to model numerous geometries found in rotorcraft applications. These parts include fuselage components, stabilizers, and interior components. Recent work with Sikorsky United Technologies was directed toward manufacturing improvements for composite seat fittings found in the RAH-66 Comanche helicopter (shown in Figure 1). This part, shown in Figure 2, is thin-shelled, made from a graphite woven fiber, and injected with a polymer resin. By using computer modeling, it was possible to verify the injection scheme anticipated in production and to suggest improvements. Process simulations were conducted using various numbers of processors (Figure 3 shows a 16-processor partition). Vent locations, optimally placed near areas that are last to fill, were also determined from the model. Detailed parametric studies and numerous white papers addressing the manufacturing practices of this part were possible thanks to the quick turn-around time provided by the parallel COMPOSE suite of tools. One example showing resin flow progression through the part, based on injection into a channel along the bottom edge, is shown in Figure 4.

Figure 1. RAH-66 Comanche heavily features composite materials (Image courtesy of Sikorsky)

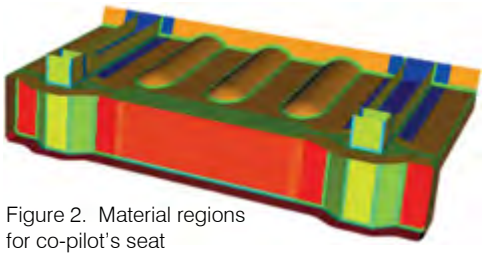

Figure 2. Material regions for co-pilot's seat

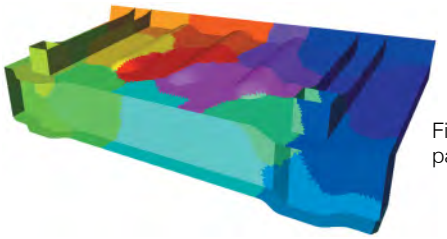

Figure 3. 16-processor partition of co-pilot's sea

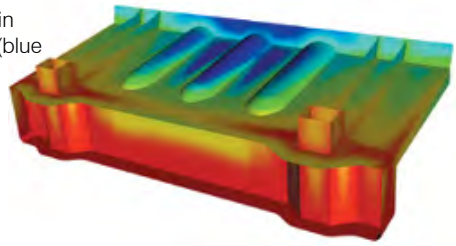

Figure 4. Plot of resin impregnation times (blue is last to fill)

Transitioning to DoD Industrial Partners

This work is part of a larger effort directed towards facilitating and enhancing the use of composite materials in military systems. ARL and the Universities of New Orleans and Minnesota are conducting the basic research behind process modeling. Transition to DoD industrial partners such as Boeing and Sikorsky is being conducted through the Aviation Applied Technology Directorate (AATD), Weapons and Materials Research Directorate-ARL, and the US Army Aviation and Missile Command. These process models are one of the significant manufacturing technology advancements found in the Rotary Wing Structures Technology Demonstration project managed by AATD.

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CTA: Integrated Modeling and Testing

Computer Resources: SGI Origin 2000, SGI Origin 3800, and IBM NH-2 [ARL, AHPCRC]

Large-Eddy Simulation of Tip-Clearance Flow in Turbomachines

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RAJAT MITTAL
The George Washington University, Washington, DC

Cavitation is "the formation of partial vacuums in a liquid by a swiftly moving solid body (as a propeller) or by high-intensity sound waves." [1] In liquid handling systems like turbomachinery pumps and propellers, low pressure fluctuations downstream of the rotor can induce cavitation, leading to acoustic noise, loss of performance, and structural damage. This complex, highly unsteady flow phenomenon is poorly understood and cannot be predicted by the traditional CFD methods. In the present work, sponsored by the Navy, researchers employ LES to study the flow past a stator (stationary)-rotor combination with tip leakage, with the objective of understanding, predicting, and eventually controlling cavitation. The LES code developed for this project has the potential to be a useful research and design tool for other future weapons systems design efforts.

"The simulations conducted to date have shown encouraging results in terms of predicting both the qualitative and quantitative features of the rotor tip-leakage flow as observed experimentally."

Understanding the Underlying Causes of Cavitation

Traditionally, scientists used experiments to study tip-leakage flow in turbomachines. There is evidence suggesting that low-pressure events and cavitations are strongly related to the turbulence associated with the tip-leakage vortex near the endwall (Figure 1). However, knowledge of the detailed mechanisms is still quite limited. Computational studies of this flow have customarily relied upon Reynolds Averaged Navier-Stokes (RANS) models, which cannot describe the highly unsteady flow and pressure characteristics. In addition, the tip-gap region has presented CFD practitioners with considerable challenges in terms of grid topology and resolution.

Figure 1. Example of a ducted propeller with tip-clearance

Introduction of the Large-Eddy Simulation

The HPCMP resources allow scientists to use LES, which is computationally much more intensive than RANS calculations. As shown in Figure 2, the present LES research attempts to resolve a wide range of flow scales associated with the stator wake, the rotor tip-leakage vortex, and the turbulent boundary layers. The computational domain is quite long since the region of interest extends several chord lengths into the wake. The flow is three-dimensional without a statistically homogeneous direction, requiring extremely long sampling time to obtain converged flow statistics. A full simulation requires more than 25 million grid points and 100,000 time steps. A typical production run requires over 50,000 single-node CPU hours and 10 gigabyte (GB)

[1] Merriam Websters Collegiate© Dictionary

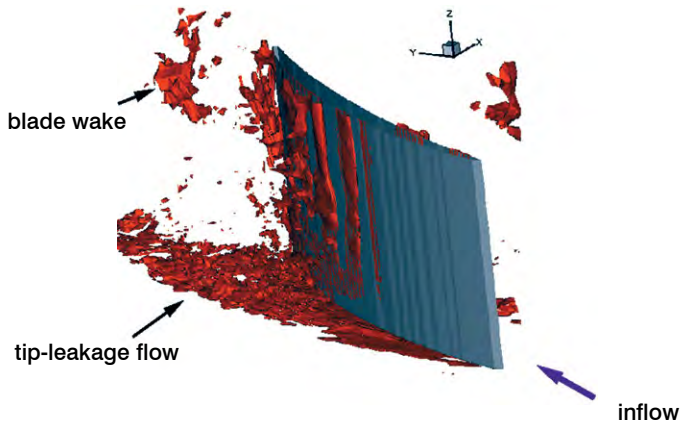

Figure 2. Instantaneous streamwise velocity iso-surfaces revealing the tip-leakage flow and rotor-blade wake

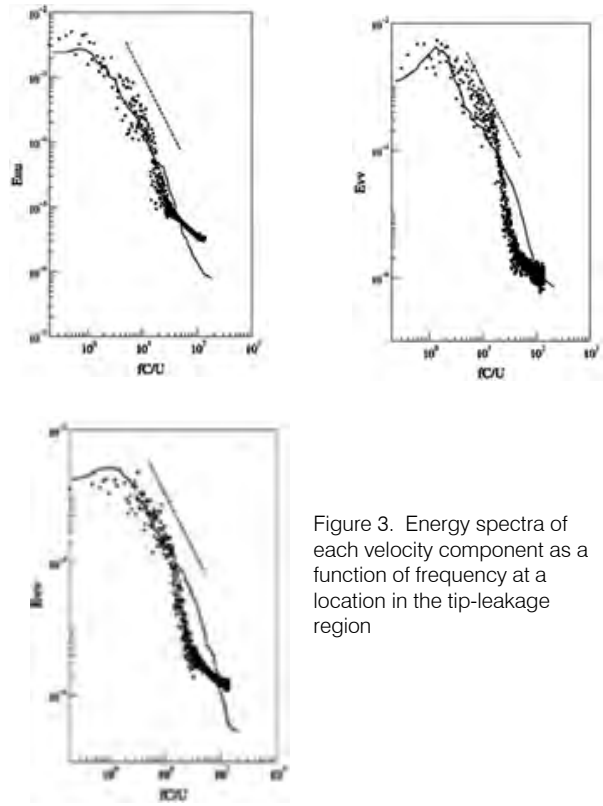

Figure 3. Energy spectra of each velocity component as a function of frequency at a location in the tip-leakage region

of memory on the SGI Origin 3800 and generates over 50 GB of data, rendering these simulations feasible only on large, high performance, parallel platforms. Large-scale simulations of this magnitude would have been impossible without HPCMP resources.

A large-eddy simulation code, which combines an immersed-boundary technique with a generalized curvilinear structured grid, has been employed to carry out the simulations. From the preliminary results, mean velocities, Reynolds stresses and energy spectra show reasonable agreements with experimental measurements (Figure 3). The flowfield exhibits strong circular motions associated with the tip-leakage and tip-separation vortices. These swirling structures convect downstream, expand in size and generate intense turbulent fluctuations in the endwall region. Strong pressure fluctuations that may be responsible for the cavitation and acoustic noise have also been observed. Analysis of the results indicates that further improvement may be obtained by increasing the streamwise resolution in the region where the tip-leakage and trailing edge vortices interact with each other.

Expanding Naval Understanding

The simulations conducted to date have shown encouraging results in terms of predicting both the qualitative and quantitative features of the rotor tip-leakage flow as observed experimentally. Grid-refinement studies are underway, and the solutions will be fully validated. Once this is done, Professor Moin's team will focus on a detailed analysis of the data with emphasis on understanding the turbulence characteristics, vortex dynamics and pressure fluctuations in and downstream of the tip-gap region. In addition, stator-rotor interaction and rotational effects will be included to simulate the flow in a more realistic configuration. The parallel performance of the code will be further enhanced by employing domain decomposition strategies coupled with explicit Message Passing Interface (MPI), instead of the loop level directives (OpenMP) currently in use.

The results of this research will eventually lead to a new generation of quieter weapons systems capable of greater performance at reduced costs.

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CTA: Computational Fluid Dynamics

Computer Resources: SGI Origin 3800 [ARL] and Compaq GS320 [ASC]

Spoil the Strikes

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The Air Force has recently undergone a second round of flight tests to address problems identified on a new refueling pod for the KC-135R aircraft. It is a hose and drogue system called the Multi-Point Refueling System (MPRS) (Figure 1). When the hose and drogue on the KC-135R are retracted, the drogue often strikes and occasionally damages the wing. This can lead to unacceptable downtime to repair the wing trailing edge and tip.

Figure 1. Aircraft view showing installation of MPRS

Conventional Testing Fails to Yield Solutions

Prior to flight test, a team from the Engineering Directorate of the Aeronautical Systems Center (ASC) was called on to perform CFD modeling on the system. Previous wind tunnel and flight tests failed to identify the source of the problem. The wind tunnel measurements were not taken close enough to the wing to discover the flow phenomena responsible for causing the drogue to strike the wing.

High Performance Computing Solutions

The ASC research team used HPCMP computational resources and CFD to solve multiple flight conditions in a reasonable amount of time. The investigating team used CHSSI developed code, Cobalt$_{60}$, for the CFD solutions. They coupled it with an in-house, steady-state catenary solver. The computational solutions provided the entire flowfield, allowing engineers to identify sources of the problem. Solution visualization using Fieldview identified a large upwash in the flowfield just behind the MPRS refueling pod. As Figure 2 illustrates, and as calculated by the catenary solver, the drogue was being pushed up into the wing by the flowfield in proximity to the pod. The design of the back end of the pod allows the flow to remain attached and turn upward. This flow behind the pod contributes to the general upwash flowfield created by the wing tip vortex. HPCMP resources allowed ASC to compute many variations on the geometry including the baseline geometry, the French Air Force variant, the wind tunnel geometry, rotated fins, inboard fins, three spoilers, and the

> "The use of major shared resource center resources is saving program dollars in helping identify causes and potential solutions to a current operational problem that were not identifiable by other methods at hand."

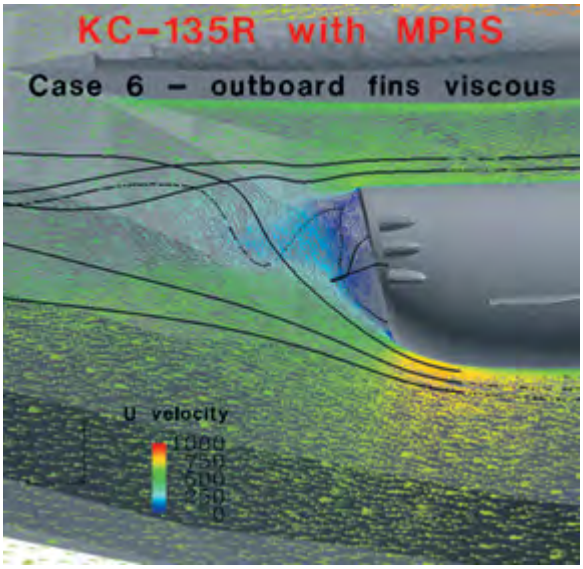

Figure 2. Baseline geometry resulting in local upwash behind pod

entire aircraft in sideslip. Computational grids were generated with the National Aeronautics and Space Administration, Langley and Air Force Research Laboratory codes Gridtool/Vgrid and Blacksmith. The largest grid was 14 million tetrahedral and prismatic cells.

The largest spoiler geometry provided the best flowfield analytically (Figure 3) and was manufactured for flight-testing. The flight test showed the spoiler to be partially successful in reducing the frequency of wing strikes. Follow-on studies are already in progress that identify means to also reduce the impact of the wing tip generated upwash on the retracting drogue. The use of MSRCs is saving program dollars in helping identify causes and potential solutions to a current operational problem that were not identifiable by other methods at hand.

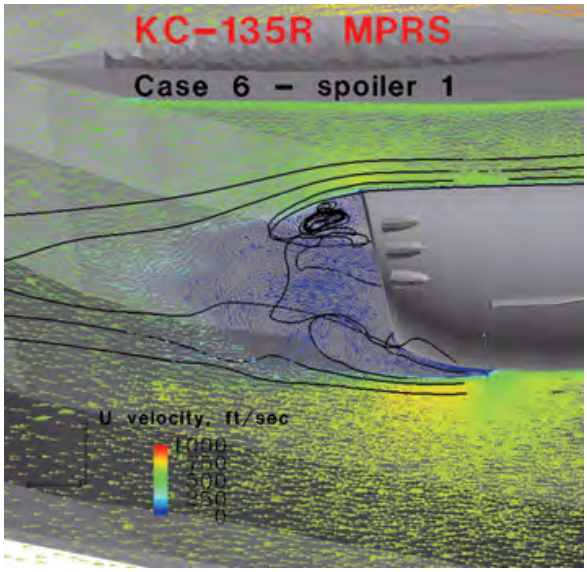

Figure 3. Spoil geometry that removed local upwash behind pod

CTA: Computational Fluid Dynamics

Computer Resources: SGI Origin 3000 [ARL, ERDC], IBM SP3 [MHPCC, ASC], and SGI Origin 2000 [ASC]

CFD Modeling of Antenna Structures Using Cobalt Internal Boundary Conditions

Susan Polsky
Naval Air Warfare Center, Aircraft Division (NAWCAD), Patuxent River, MD

The objective of the Ship Aircraft Airwake Analysis for Enhanced Dynamic Interface (SAFEDI) Program is to develop computational fluid dynamics methods to predict the time-accurate airwake produced by Navy ships for application in manned and unmanned flight simulation. Wind tunnel tests have shown that "small" geometric details on ships can significantly affect the character of the airwake turbulence that aircraft must operate in. These "small" geometric features include the antenna arrays that are placed atop the ships superstructure. These arrays are very complex geometrically and present an extremely difficult gridding problem for both grid construction and required grid density.

Difficulties of Modeling Antenna Structures

Traditionally, geometric details of the scale of the antennas have simply been ignored because of the difficulties in modeling the true geometric detail of the structures. In this work, internal boundary conditions have been developed to model the antenna arrays on a sub-grid scale. The initial approach taken was to modify the momentum equations using a source term to retard the flow by removing momentum, but still allow for a permeable surface. The "porosity" of the structures were specified as a drag coefficients in an input deck. However, it was found that determining the correct drag coefficient to use was more of an art than science. Therefore, the current approach is to tag all the cells within the structures as solid walls. The areas where the antennas exist are specified in an input deck along with the general shape (i.e., cylinder, sphere, etc.).

Modeling Ship Air Wakes

Ship air wakes are inherently unsteady and must be modeled as such. In addition, the ships are very large while details on the order of thousandths of inches must be modeled to properly resolve boundary layers. This requires large amounts of memory and large amounts of computer time.

"The primary impact is significantly improving manned and unmanned flight simulation by providing realistic airwake models. Improved simulations can reduce operating costs by providing an alternative method for pilot training and dynamic interface envelope development."

Visualization of the resulting three-dimensional flow fields is an essential part of the development and analysis tasks related to ship air wake predictions. State-of-the-art visualization software is heavily relied on for all aspects of the program. In particular, animation of the time-varying solutions has provided insight into never before appreciated features of the air wake flow field.

Access to HPC resources has enabled the development of a new method of modeling fine geometric details for the prediction of ship air wake.

Improving Manned and Unmanned Flight Simulation

The primary impact is significantly improving manned and unmanned flight simulation by providing realistic airwake models. Improved simulations can reduce operating costs by providing an alternative method for pilot training and dynamic interface envelope development. In addition, this work provides a unique opportunity to improve the general understanding of ship airwake aerodynamics.

Finally, the analysis techniques developed here can be used to aid in the design of the flight decks and islands on new ships and thereby address flight operations at the very initial stages of ship design.

An internal boundary condition to simulate first order effects of an antenna array on the flow field has been developed, implemented, and tested. The method developed imposes a solid wall boundary condition within the antenna array. This approach avoids the need to determine the porosity (i.e., drag coefficient) of varied geometric shapes.

The several simple test cases that were run prove that the cells within the antenna array box are being found correctly, the orientation of the antenna is the requested orientation and the momentum is being reduced by the presence of the antenna array boundary condition. The remaining challenges are to use the method for an actual antenna geometry (Figure 1) and to validate against both CFD and, if possible, experimental data. For validation against CFD data, the actual antenna geometry will be gridded and run using the same CFD code, Cobalt. This process has already begun and some resulting flow fields are shown in Figures 2 and 3. The method itself is still under development and may be modified based on results from the validation effort.

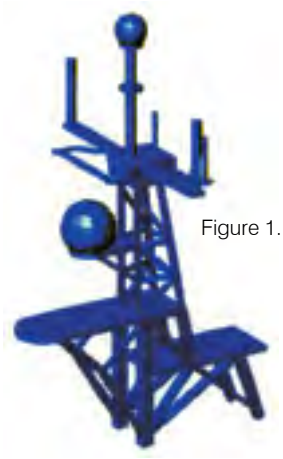

Figure 1. Actual antenna geometry

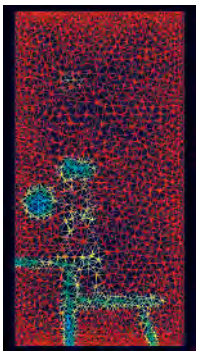

Figure 2. Supporting grid structure and application of subscale boundary condition (colored by speed)

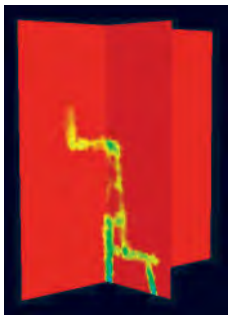

Figure 3. Two planar cuts showing affects of internal boundary condition

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CTA: Computational Fluid Dynamics
Computer Resources: IBM SP3 [ASC]

Flow Control for Aircraft Weapons Bay Enhanced Acoustic Environment

DONALD RIZZETTA
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High-speed flows over open cavities produce complex unsteady interactions, which are characterized by a severe acoustic environment. At flight conditions, such flowfields are both broadband, small-scale fluctuations typical of turbulent shear layers, and discrete resonance whose frequency and amplitude depend upon the cavity geometry and external flow conditions. While these phenomena are of fundamental physical interest, they also represent a number of significant concerns for aerospace applications.

Researchers at AFRL are studying these phenomena, hoping to influence aircraft weapons bay environments (as shown in Figure 1), where aerodynamic performance or stability may be adversely affected, structural loading may become excessive, and sensitive instrumentation may be damaged. Acoustic resonance can also pose a threat to the safe release and accurate delivery of weapons systems stored within the cavity.

"High performance computing resources, particularly large-scale computing platforms, are allowing the investigator to represent, with more accuracy, the fundamental properties of supersonic turbulent aircraft weapons bay cavities."

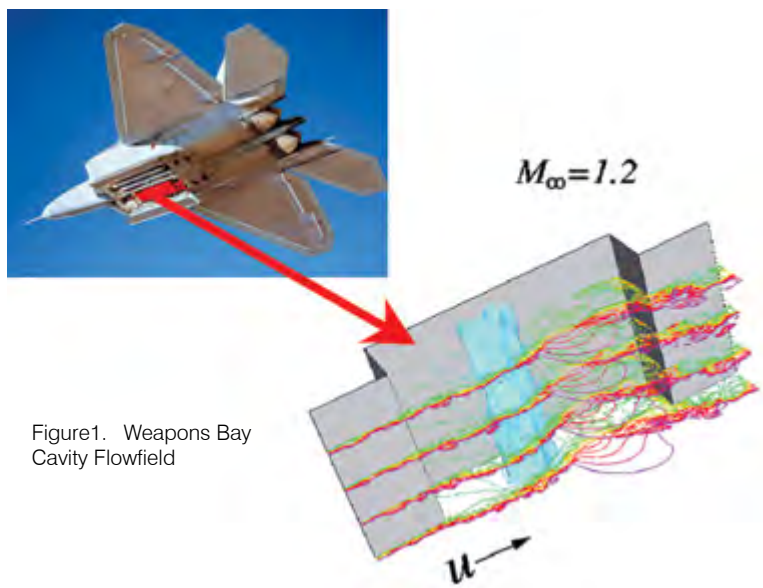

Figure1. Weapons Bay Cavity Flowfield

Shortfalls of the Traditional Approach

Traditionally, solving the RANS equations has allowed simulation of the flow about aircraft weapons bay cavities. This approach precluded a precise description of the turbulent cavity flowfield, which consists of fine-scale fluid structures. The models, which accounted for the effects of turbulence, were unreliable and incapable of representing high-frequency fluctuations of the fluid structures.

HPC resources, particularly large-scale computing platforms, are allowing the investigator to represent, with more accuracy, the fundamental properties of supersonic turbulent aircraft weapons bay cavities (Figures 2 and 3). In particular, the engineers can use large-eddy simulations to overcome deficiencies of the RANS approach and failure of traditional turbulence models.

Using Large-Eddy Simulations to Improve Acoustic Pressure Levels

Large-eddy simulations numerically generated the turbulent flowfields about weapons bay cavities. The ability of high-frequency forced mass injection to suppress cavity resonant acoustic modes was investigated. Scientific visualization was used extensively to clarify the physical characteristics of unsteady three-dimensional turbulent cavity flowfields. The construction of videos made it

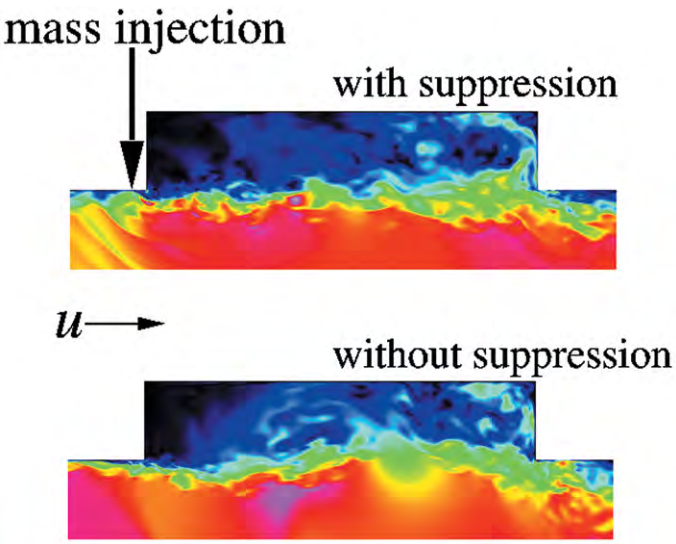

Figure 2. Instantaneous Mach Number Contours

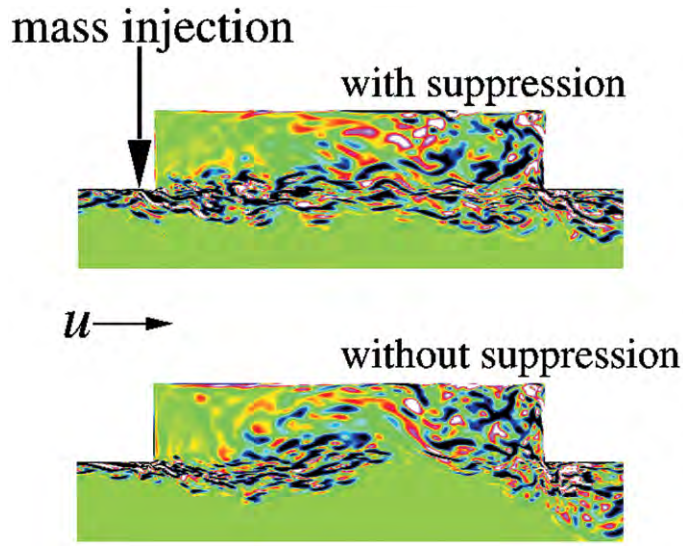

Figure 3. Instantaneous Vorticity Contours

possible to understand the basic mechanisms contributing to the suppression of resonant acoustic modes through forced mass injection. It was found that the use of flow control appreciably reduced amplitudes of acoustic pressure levels within the cavity.

Using HPC resources, the engineers numerically reproduced supersonic turbulent flow about an aircraft weapons bay both with and without flow control. Large-eddy simulations have made it possible to correctly describe the small-scale fluid structures that characterize turbulence. Pulsed mass injection was found to be an effective flow control mechanism for mitigating undesirable resonant acoustic modes. This considerably enhanced the acoustic environment within the weapons bay, thereby reducing the loading and potential damage to weapons systems, surrounding structure, and instrumentation.

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CTA: Computational Fluid Dynamics

Computer Resources: SGI Origin 3000 and Cray SV1 [NAVO] and IBM SP3 [ASC]

Using Strongly Coupled Fluid/Structure Interaction Code to Predict Fighter Aircraft Wing Response to Anti-Aircraft Artillery (AAA) Damage

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Sponsor: Joint Technical Coordinating Group for Aircraft Survivability

It's becoming clear that current static loading techniques for live-fire testing fail to accurately replicate the loads of aircraft that are damaged in flight. Vulnerability assessments based on such loading techniques may also, in turn, fall short of providing accurate and complete results. The good news is that advances in a proposed technique for dynamic live-fire ground testing may remedy the shortcomings of current static ground testing. High performance computers are being used to develop a methodology to predict the in-flight response of manned and unmanned air vehicles to hostile threats they may encounter during wartime operations. The methodology gives DoD a physics-based, high fidelity tool for use in new aircraft design as well as pretest prediction and dynamic test planning of on-going and future live-fire test and evaluation.

Shortfalls of Static Ground Testing

In the past, only static predictions could be made using engineering level tools, which neglected the influence of structural damage to the airflow over the aircraft. The main shortfall with static ground testing is that the quasi-static techniques do not account for changes in structural stiffness and mass that occur from damage. As such, current loading methodologies fail to reconfigure correctly for representing in-flight loads. Ground loading methodologies also fail to consider damage induced changes to the flutter envelope that can lead to premature failure.

Boundary Element Method Models Flow Fields

The methodology of this research was to use HPC resources to model a current fighter aircraft structure using the Lagrangian perspective coupled with a boundary element method for modeling the flow field around the aircraft. The boundary element method used in this work is consistent with several "paneling methods" which are used for inviscid, incompressible flows. The wing model was initially loaded with the airloads and g-loads representing a given flight condition (Figure 1 and Figure 2). Ten seconds into the simulation, a section of structure was instantaneously removed to simulate the damage resulting from a threat detonation or impact. The simulation was allowed to continue for another 10 seconds and resulting stresses and wing displacements were observed (Figure 3).

"The new methodology has led to a new way of thinking about aircraft response to in-flight damage. By moving the simulated damage from one place to another, certain "vulnerable spots" were identified which were not previously anticipated."

Simulations of this type require stepping in time with steps on the order of 0.1 microseconds. Thus a 20 second simulation would require 200 million steps. Without the HPC resources, each simulation would have taken days to perform. With the multi-processor capability that HPC brings to the table, each simulation took hours to complete.

The new methodology has led to a new way of thinking about aircraft response to in-flight damage. By moving the simulated damage from one place to

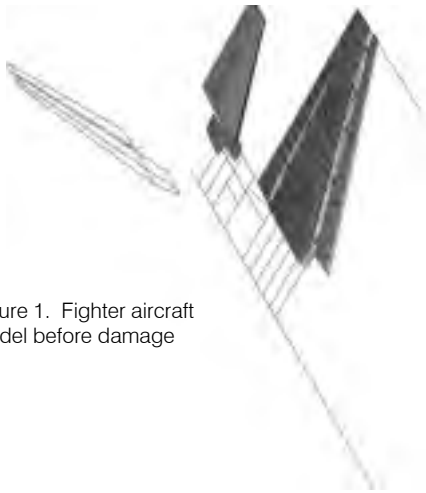

Figure 1. Fighter aircraft model before damage

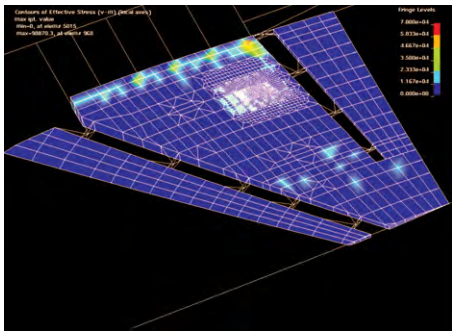

Figure 2. Von Mises stress contours before damage

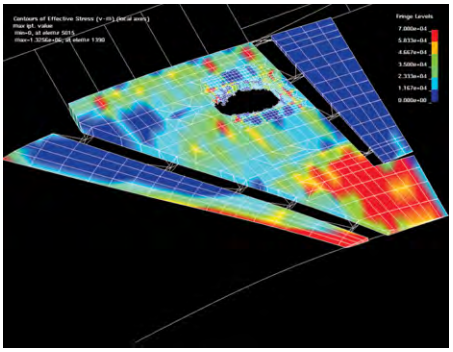

Figure 3. Von Mises stress contours immediately after damage

another, certain "vulnerable spots" were identified which were previously not anticipated. For instance, at some flight conditions and store loading, damage near the wingtip was seen to be more catastrophic than the same damage near the wing root.

New Methods Improve Predicted Structural Response

This research is significant as it points the way to an effective and efficient method for predicting aircraft response resulting from the damage from detonation or impact of a missile or an AAA threat. These results, in turn, will help provide a pathway for test engineers to determine the most appropriate test method. That method could either be static, dynamic, or a combination of the two. Subsequent concept designs of dynamic ground tests may be based on improved predicted structural response. This work will be used in the future to assist live fire test planners in designing and controlling dynamic ground test to more realistically reproduce what actually happens in flight.

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CTA: Computational Structural Mechanics

Computer Resources: Compaq ES40 and Compaq GS320 [ASC]

Modification of the F/A-18C Wing to Determine Effect of Wing Parameters on Abrupt Wing Stall

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During the engineering, manufacturing, and development phase of the F/A-18E/F program, it was discovered that the F/A-18E (Figure 1) was susceptible to abrupt wing stall (AWS). Abrupt wing stall occurs when an aircraft undergoes a rapid, severe upper surface flow separation. If this occurs asymmetrically, large rolling moments can be produced, which result in uncommanded lateral motion. To eliminate AWS on the F/A-18E, the flap schedule was modified and a porous door was added. However, the cause of the F/A-18E's initial encounter with AWS is not well understood. As a result, the AWS program was formed to investigate the causes of AWS and to develop a set of design guidelines to help designers avoid AWS on future aircraft.

Figure 1. The F/A-18E Super Hornet, the Navy's strike-fighter aircraft (DoD photo by Vernon Pugh)

Abrupt wing stall has been traditionally addressed through expensive flight testing, relatively late in an aircraft development program. With advances in CFD, AWS can now be approached using CFD to solve the RANS equations. However, solving these equations for this class of flow requires large memory resources and long computational times.

During the redesign of the F/A-18E from the F/A-18C, the wing camber, thickness, twist, leading-edge radius and leading-edge flap-chord ratio were modified. In addition, a leading-edge snag was added to the wing. Since the F/A-18C does not experience AWS, these wing parameters are likely contributing to the AWS experienced by the F/A 18E. Using CFD, these wing parameters were studied independently and simultaneously to determine their effect on AWS and to develop a set of design guidelines.

> "Current results indicate that the addition of the snag and the reduction of the leading-edge flap-chord ratio could be contributing significantly to AWS on the F/A-18E."

The effects of these six wing parameters on AWS were analyzed using eleven different configurations. These eleven configurations included configurations in which one or more of the wing parameters were modified. For example, to determine the effect of twist on AWS, the twist was removed from the F/A-18C wing to form one of the configurations. In some cases, two wing parameters were modified simultaneously. For example, one of the configurations was obtained by adding a snag to the F/A-18C wing while removing the camber.

The eleven configurations were analyzed at two transonic Mach numbers and six different angles of attack (AoA). This resulted in 132 different cases, which were analyzed. As each case required approximately 6,000 hours of CPU time on an SGI

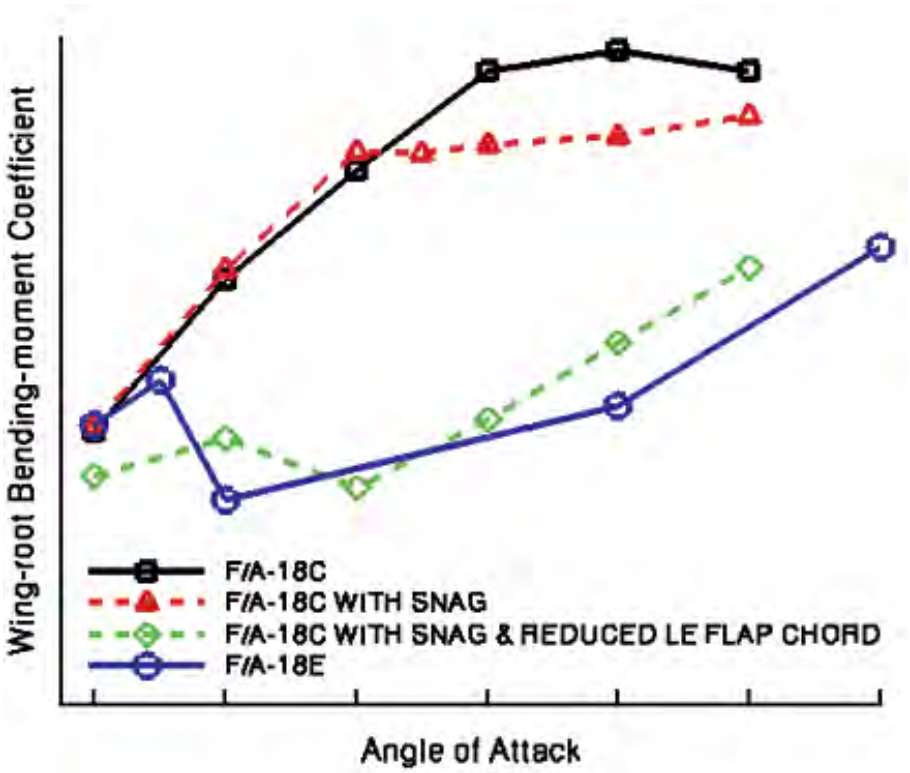

Figure 2. Wing-root bending-moment coefficient as a function of AoA for the F/A-18C, F/A-18C with a snag, F/A-18C with a snag and reduced leading-edge flap-chord ratio and F/A-18E

Origin, extensive CPU time and computer resources were necessary to complete this task. Through using the resources of the HPCMP, it was possible to analyze all 132 configurations.

Although this research is ongoing, meaningful results have been obtained. The current results indicate that the addition of the snag and the reduction of the leading-edge flap-chord ratio could be contributing significantly to AWS on the F/A-18E. In Figure 2, the wing-root bending-moment coefficient is plotted as a function of AoA for the F/A-18C, F/A-18C with a snag, F/A-18C with a snag and reduced leading-edge flap-chord ratio and the F/A-18E. AWS can occur when the slope of this curve changes sign. It can be seen from the figure that the addition of the snag and reduction of the leading-edge flap-chord ratio on the F/A-18C moves the wing-root bending-moment curve toward that of the F/A-18E.

The results of this research also indicate that the camber may be contributing to AWS on the F/A-18E, while the twist, thickness and leading-edge radius do not appear to be impacting AWS. Although this is on-going research, the team expects to finish the remaining cases expeditiously so that they can confirm their current observations and contribute to the elimination of AWS on the F/A-18E and other aircraft.

CTA: Computational Fluid Dynamics
Computer Resources: SGI Origin 2000/3000/3800 [ASC]

Detached-Eddy Simulation of Massively Separated Flows Over Aircraft

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United States Air Force Academy (USAFA), Colorado Springs, CO
Kyle Squires
Arizona State University, Tempe, AZ
Kenneth Wurtzler, William Strang, and Robert Tomaro
Cobalt Solutions, LLC, Dayton OH
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Boeing Commercial Airplanes, Seattle, WA

Currently, fighter development is under close scrutiny due to ever increasing acquisition costs. The Joint Strike Fighter program made low cost a primary requirement in their acquisition strategy. Unfortunately, there is little confidence that CFD modeling for full aircraft is accurate under massive separation, limiting its usefulness.

Reynolds Averaged Navier-Stokes Deficiencies

While advances have taken place in areas such as grid generation and fast algorithms for solution of systems of equations, CFD has remained limited as a reliable tool for predicting inherently unsteady flows at flight Reynolds numbers. Current engineering approaches to predicting unsteady flows are based on solution of the RANS equations. The turbulence models used in RANS methods model the entire spectrum of turbulent motions. While often adequate in steady flows with no regions of reversed flow, or possibly exhibiting shallow separations, it appears that RANS turbulence models are unable to accurately predict phenomena dominating flows characterized by massive separations. Unsteady, massively separated flows are characterized by geometry-dependent and three-dimensional turbulent eddies. These eddies, arguably, are what defeat RANS turbulence models, of any complexity.

To overcome the deficiencies of RANS models for predicting massively separated flows, Detached-Eddy Simulation (DES) was proposed with the objective of developing a numerically feasible and accurate approach combining the most favorable elements of RANS models and LES. The primary advantage of DES is that it can be applied at high Reynolds numbers, as can Reynolds-averaged techniques, but also resolves geometry-dependent, unsteady three-dimensional turbulent motions as in LES.

> "DES applied today using HPC resources is making more "routine" the full-configuration prediction of complex geometries and at flight conditions."

Testing Detached-Eddy Simulation

Two geometrically simple cases were examined to test the method and build confidence for full aircraft simulation — a delta wing at 27° angle-of-attack exhibiting vortex breakdown, and a forebody at 90° angle of attack. Although the geometries are simple, the resulting flows are quite complex. In fact, accurately predicting delta wing vortex breakdown at high Reynolds number has challenged researchers for decades. These applications are then used to build confidence in the full aircraft simulations (F-16, F-15E) that have been performed. The computations were performed using the unstructured-grid solver

Cobalt. Cobalt is the commercial version of the Common High Performance Computing Software Support Initiative code, $Cobalt_{60}$. Grids used in the calculations of all the geometries summarized below are unstructured, comprised of a combination of prisms, pyramids, and tetrahedra.

The forebody modeled is the flow at 90° angle-of-attack around a rectangular ogive, with the main cross-section a round corner square as shown in Figure 1. The Reynolds number based on the width of the body is 2.1×10^6. Grid sizes for the computations performed to date have ranged from 4.2×10^6 to 5.2×10^6 cells. Visualization of the pressure distribution on the surface and the instantaneous vorticity at eight stations along the body are shown in Figure 1. Predictions obtained using both DES and RANS (using the Spalart-Allmaras one-equation model) are shown. Evident in the surface pressure prediction from the RANS computation is that along the forebody, the separated structure is more coherent than that obtained in the DES, with a low-pressure footprint evident along most of the forebody. The DES result is characterized by a more chaotic and three-dimensional structure over most of the body, resulting in a reasonably constant pressure region along the top (aft) surface (c.f., Figure 2). Time-averaged pressure distributions were measured in experiments at eight axial stations, corresponding to the eight locations at which vorticity contours are shown in Figure 1. Compared in Figure 2 is the pressure coefficient at 11% of the forebody length. The angle $\theta = 0°$ is in the symmetry plane on the windward side, with $\theta = 180°$ in the leeward side symmetry plane. As shown in the figure, the strong coherent vortices predicted in the RANS solution give rise to a large variation in pressure on the leeward side that differs markedly from the experimental measurements. The largest differences in the RANS predictions occur closest to the tip of the forebody, resulting in large errors in moment predictions. The DES prediction of the pressure coefficient, on the other hand, is in excellent agreement with the measurements, a result of the more accurate resolution of the unsteady shedding that yields a flat pressure profile on the leeward side.

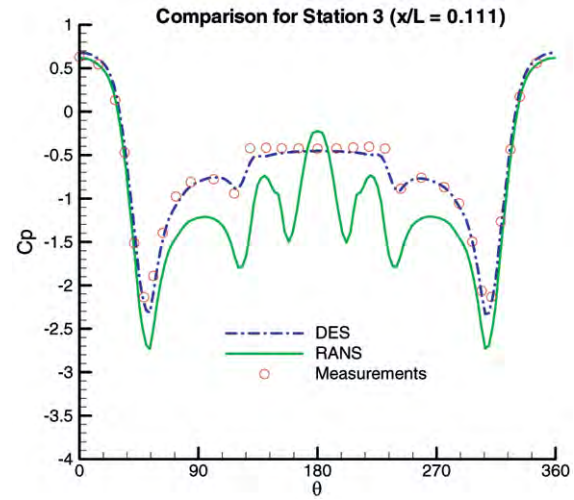

Figure 2: Pressure distribution around the rectangular ogive forebody. Comparison of DES and RANS to experimental measurements at station 3 (c.f., Figure 1).

The 70° delta wing at 27° angle-of-attack has also been calculated. A comprehensive grid refinement study was performed on a half-span model with the number of cells ranging from 1.2×10^6 to 10.5×10^6. The finest grid results are shown in Figure 3. Numerous flow features are clearly resolved including shear layer instabilities prior to vortex breakdown, reverse flow near vortex breakdown, post breakdown windings, and vortex shedding off the blunt trailing edge. Resolved turbulent kinetic energy in a line along the vortex core is plotted in Figure 4. DES possesses the same characteristics as LES, in that a wider range of turbulent length scales is resolved as the grid density is increased. The finest grid matches the peak turbulent kinetic energy measured experimentally. Other parameters such as velocity in the core of the vortex and breakdown location were in excellent agreement with experiments. Accurately predicting turbulent kinetic energy levels provides increased confidence that DES will be able to predict the unsteady loads on an aircraft due to vortex breakdown (e.g., the F-18 with tail buffet).

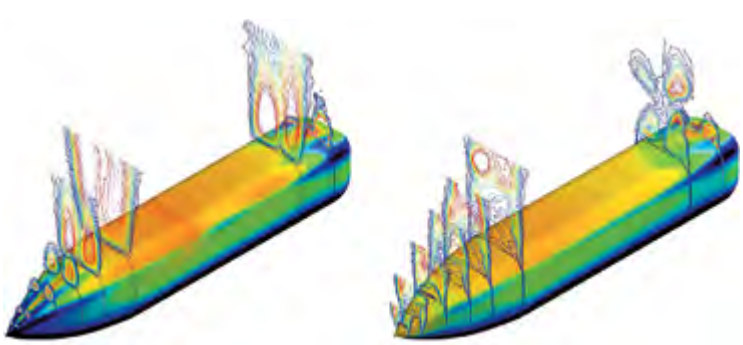

Figure 1. RANS (left) and DES (right) predictions of the flow around the rectangular–ogive forebody. The freestream flow is at 90° angle-of-attack (from top to bottom in the visualizations). Surface colored by pressure and vorticity contours at eight stations. The location of the eight stations is the same at which experimental measurements of the pressure distribution were available.

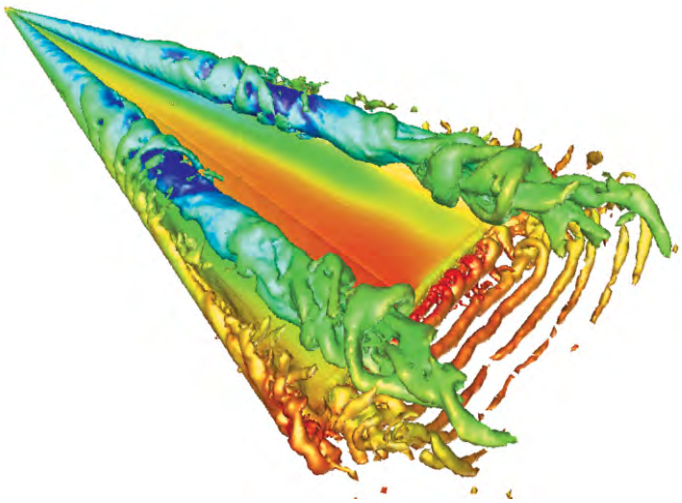

Figure 3. Flow over the delta wing at 27° angle of attack. Isosurface of vorticity.

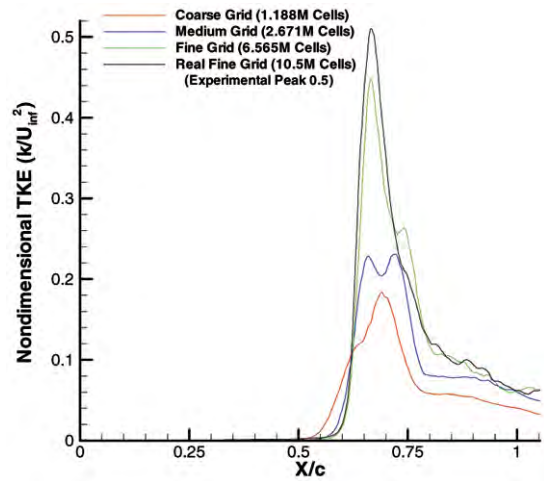

Figure 4. Resolved turbulent kinetic energy in the core of the vortex on the delta wing

Key Advances in DES

Work to date has provided key advances in application, assessment, and improvement of DES. Computation of building block flows such as two- and three-dimensional forebodies and delta wings has established a foundation for resolution of several issues important to using DES to predict the flow field around full aircraft, helping to provide guidance in grid-generation aspects, turbulence treatments, and numerical parameters. The subsequent application of DES to the F-16 and F-15E has further enhanced the confidence level with lift and drag predictions that are accurate compared to flight test data. These developments will soon provide aircraft designers with a powerful tool for the prediction of massively separated flows over complex configurations and at flight conditions. The availability of high performance computing continues to accelerate the development of this powerful technique. DES applied today using HPC resources is making more "routine" the full-configuration prediction of complex geometries and at flight conditions. Accuracy in lift, drag, and moment predictions around the F-15E, for example, are within 5% of flight test data. While already relatively accurate, increases in HPC capacity will enable efficient simulation using substantially larger grids. DES flow fields will offer richer detail on denser grids, with associated increases anticipated in overall accuracy. Increases in HPC capacity coupled with the emergence of more efficient and accurate algorithms will soon enable prediction of additional physical effects such as fluid-structure interactions.

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CTA: Computational Fluid Dynamics

Computer Resources: Cray T3E [AHPCRC]

Radar Signature Database for Low Observable Engine Duct Designs

Kueichien Hill
Air Force Research Laboratory (AFRL), Wright-Patterson AFB, OH
Sunil Navale and Maurice Sancer
Northrop Grumman Corporation, Wright-Patterson AFB, OH

Modern and future aircraft, such as the F-117 (Figure 1), B-2, F-22, and Joint Strike Fighter (JSF), all require low observability (LO) to gain air superiority and increase survivability. This significantly increases the development costs of advanced aircraft. Fortunately, the use of HPC enabled Computational Electromagnetics (CEM) tools is reducing LO vehicle design costs.

Figure 1. US Air Force ground crew members do a final inspection of an F-117A Nighthawk aircraft before it departs for Kuwait from Holloman Air Force Base, NM. (DoD photo by Senior Airman Roberta McDonald, US Air Force)

A team of scientists and engineers led by Dr. Kueichien Hill of AFRL, other DoD agencies, and Drs. Navele and Sancer of Northrop Grumman Integrated Systems are developing new methods to compute accurate radar signatures for a large class of inlet and exhaust ducts with LO features. Engine inlet and exhaust ducts are contributors to the overall air vehicle signature. In addition to real world geometries for explicit aircraft, ducts with generic material treatments and shapes were used to generate a radar signature database.

Lowering the Costs of Modeling and Testing

Until very recently, the designs of low radar cross-section vehicles relied almost exclusively on costly experiments with some support of computational electromagnetics. While first-principle computer codes satisfy all LO requirements, they involve the solution of large linear systems of equations, the order of which increases at the cubic power of the radar frequency being studied and with the complexity of the modeled target. The increasing complexity of modern LO weapon systems coupled with higher frequencies of interest has meant that such simulations are too computationally intensive for even the most advanced desktop or serial computers. Massively parallel supercomputers such as those provided by the HPCMP must be used to accurately predict the radar cross section of real targets at higher frequencies. With the use of HPC resources, several large test models (many of which cost about 10 million dollars) could be eliminated. Not only could model cost be reduced, but the associated test cost (on the order of $15,000 per measurement shift) could also be reduced.

"Massively parallel supercomputers such as those provided by the HPCMP must be used to accurately predict the radar cross section of real targets at higher frequencies. With the use of HPC resources, several large test models (many of which cost about 10 million dollars) could be eliminated."

CEM Tools Considerations

In order to be useful for LO designs, CEM tools have to satisfy three LO imposed CEM requirements: accuracy, material modeling, and scalability. Many CEM codes do not satisfy all three LO requirements. CEM codes, based on approximate asymptotic high

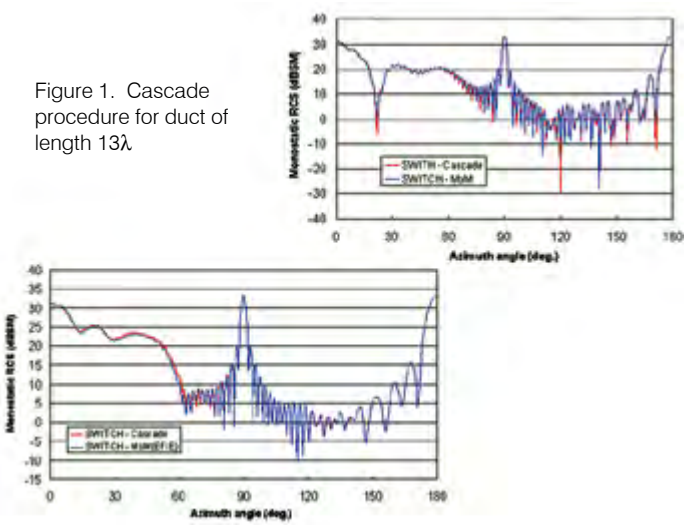

Figure 1. Cascade procedure for duct of length 13λ

frequency techniques such as the XPATCH code (developed by the Automatic Target Recognition [ATR] community) cannot satisfy the LO accuracy and material modeling requirements. The presence of LO material treatments and the close coupling of scattering features violate the fundamental assumptions of the asymptotic techniques. CEM codes based on the finite volume/difference time domain techniques also cannot satisfy the LO accuracy requirement. They employ an approximate radiation boundary condition, which causes a non-physical reflection that contaminates the solution.

Developing a Novel Approach

To satisfy all three LO requirements, Northrop Grumman developed a first principle-based (solving Maxwell's equations exactly without making limiting assumptions) hybrid finite element/method of moments (FEM/MoM) code. The finite element portion of the code allows flexibility in material modeling and the moment method portion of the code generates accurate solutions using an exact radiation boundary condition. Under the support of the HPCMP's CHSSI CEA-3 project (Maturation of a LO Component Design Code), this code evolved into a robust, portable, and scalable code that was used to generate the radar signature database for engine inlet and exhaust ducts.

A new modular duct cascading technique was employed to efficiently generate the radar signature database, especially for higher frequency bands. This technique allowed the doubling of the duct length without repeated computations. This level of problem size and accuracy had never been demonstrated before and was only possible because of HPC resources. Simulations were performed with and without the newly discovered technique to corroborate the accuracy of the new technique and to demonstrate the several orders of magnitude savings in run time and memory requirement.

"Radar cross-section computations for the Defense Advanced Research Projects Agency's (DARPA) future strike aircraft were accomplished in 3.5 days on 121 processors of the Origin 3000 at ARL. Such a computation would have been impossible without the use of HPCMP resources."

Influencing the Design of Engine Ducts

Dr. Hill's team's work has influenced the design of engine ducts in three different areas.

First, the modular duct cascading technique reduced the simulation time by several orders of magnitude and produced a more accurate solution by reducing the size of the finite element system. Such a reduction is of paramount importance when modeling very large targets as the finite element technique is susceptible to accumulation of numerical errors. Figures 1, 2, and 3 illustrate the impact of the modular cascading technique on duct design. Figure 1 shows the radar cross section computed using the cascading technique for a duct of 13 wavelengths. The excellent agreement between the cascading technique and the standard FEM/MoM technique in Figure 1 is lost in Figure 2, which illustrates the same

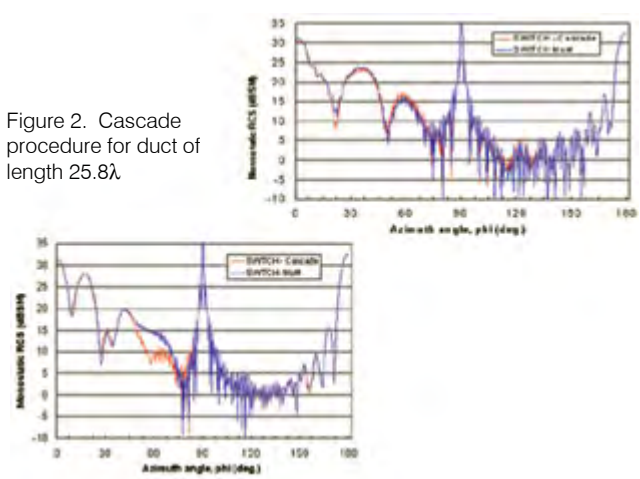

Figure 2. Cascade procedure for duct of length 25.8λ

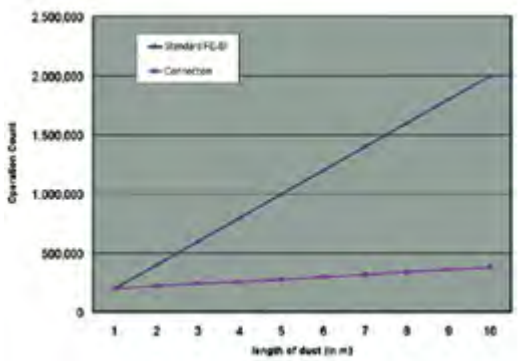

Figure 3. Reduced computational requirement of innovative "cascading" technique. Computational requirement comparison of standard FEM-MoM and cascading techniques.

computations but for a longer duct of 25.8 wavelengths. This disagreement is due to the numerical errors that accumulate in the standard FEM/MoM, which are resolved in the cascading technique by modeling only a small section of the duct, performing computations on the small section, and cascading such computations to produce the actual target. Such a cascading procedure yields greater accuracy and saves computation time as seen in Figure 3.

The second major impact was in the generation of radar images for duct configurations. Such radar images are crucial in understanding the phenomenology of radar scattering from engine and exhaust ducts. Figure 4 shows typical radar images that were generated on the ARL's Origin 3000.

Thirdly, the work influenced the simulation of future air vehicles including the engine and exhaust ducts. Radar cross-section computations for the Defense Advanced Research Projects Agency's (DARPA) future strike aircraft were accomplished in 3.5 days on 121 processors of the Origin 3000 at ARL. Such a computation would have been impossible without the use of HPCMP resources.

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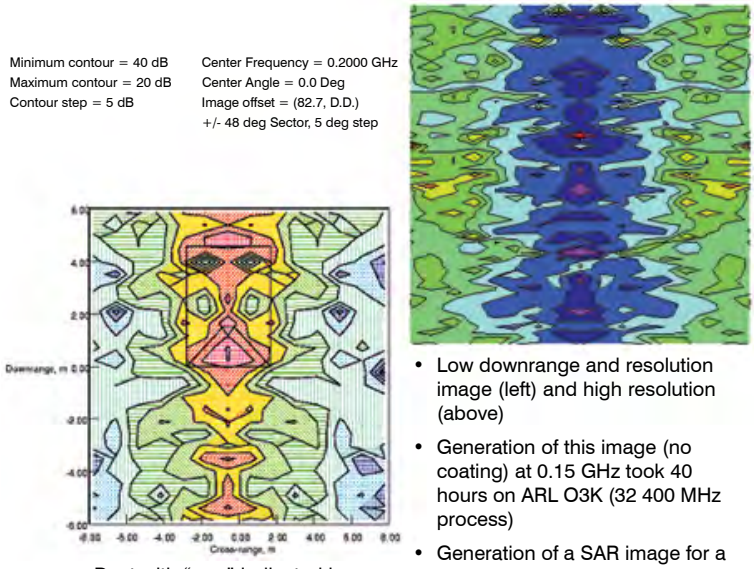
CTA: Computational Electromagnetics and Acoustics

Computer Resources: SGI Origin 3000 [ARL] and IBM SP P3 [ASC]



Duct with "pug" indicated in outline

- Low downrange and resolution image (left) and high resolution (above)
- Generation of this image (no coating) at 0.15 GHz took 40 hours on ARL O3K (32 400 MHz process)
- Generation of a SAR image for a realistic Duct at X-Band will require resources of an order of magnitude

Figure 4. Downrange and cross-range image of generic duct at very high frequencies (center - 0.15 GHz)

Scalable Pre- and Post-Processing Approaches for Large Scale Computational Electromagnetic Simulations

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John Neherbass
Ohio State University, Columbus, OH

The overall objective of this research is to develop and demonstrate a scalable computational electromagnetic software environment to address accurate prediction of radar cross sections (RCS) for full range armored vehicles with realistic material treatments and complex geometric configurations. A software environment consisting of scalable pre-processing, post-processing, and accurate finite-difference time-domain software was developed which demonstrated a significant reduction in overall simulation time for large-scale military applications. Computational electromagnetic simulations of full range military vehicles play a critical role in enhancing the design and performance of combat systems including the Army's FCS. This high fidelity software environment can also address wide band communications applications for DoD.

Developing Scalable Software Tools

Traditional serial pre- and post-processing approaches cannot generate the desired meshes. They are also inefficient when used to visualize very large-scale, high fidelity electromagnetic simulations. To overcome this problem, a team of scientists at the ARL developed a suite of scalable software tools using the Interdisciplinary Computing Environment (ICE). ICE was developed at ARL for generating desirable meshes from the available computer aided design (CAD) geometries and/or surface models. For computational approaches such as Method of Moments (MoM) and Finite Difference Time Domain (FDTD) codes, simple surface model information is not sufficient. These approaches require volumetric information or at least appropriate thickness. In addition to generating desirable meshes on scalable systems, this technique automatically decomposes the domain for efficient load balancing. In addition, these software tools provide run time visualization of very large-scale data from multiple processors.

"Computational electromagnetic simulations of full range military vehicles play a critical role in enhancing the design and performance of combat systems including the Army's Future Combat Systems".

Applicability of the approach was demonstrated for simulating a full-scale ground vehicle in free space at X-band using scalable finite difference time domain software. Simulations at X-band using a finite difference time domain approach require 2.56 billion cells and 480 processors of IBM SP3. Numerical simulations show good qualitative agreement with experimental results. Figure 1 illustrates the capability of modeling a very large-scale application.

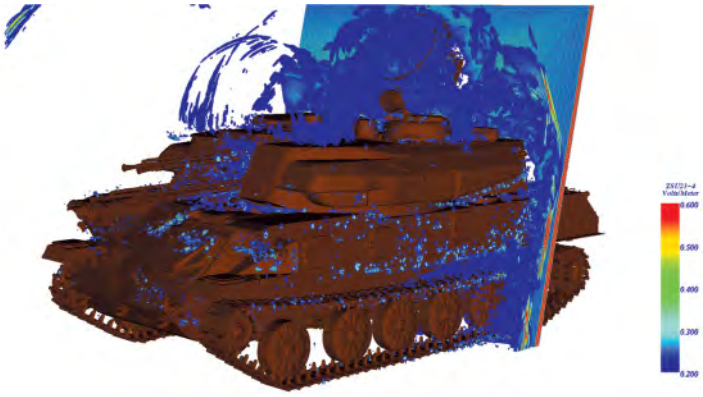

Figure 1. ZSU 23-4 combat vehicle subjected to an electromagnetic pulse at X-band

Software tools developed under this research along with different scalable applications software create a virtual design tool for addressing large-scale practical applications. This technology will assist not only in optimizing systems performance but also in performing trade-off studies for the competing requirements in the design of FCS.

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CTA: Computational Electromagnetics and Acoustics

Computer Resources: IBM SP3 and SGI Origin 3000 [ARL]

Unsteady RANS Simulation for Surface Ship Maneuvering and Seakeeping

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The Chief of Naval Operations noted in his Top Five Priorities: Future Readiness:

> "The DD(X) program literally outlines what the ship-borne Navy is going to be like in the next 30 years. It's not just a destroyer that's going to support the United States Marine Corps with a precision gun that is going to fire a round from 75 to 100 miles… It is about spiraling that technology off into the missile defense cruiser of the future. And it is about creating what I believe is one of our most pressing requirements, a littoral combatant ship that is going to operate in the near-land areas and address real threats in the future in near-land anti-submarine warfare and in mine warfare …"

As today's Navy continues its transformation, the Naval ships of the future will be fundamentally different from those currently in the fleet in order to meet evolving missions and related operational requirements and to accommodate emerging technologies such as electric drive as the main propulsion system. Such missions include increased littoral operations that require unprecedented ship signature reduction. Because these ships will be radically different from existing designs, there is no historical database to benchmark new designs against. Additionally, seakeeping and maneuvering behavior of these new ships is significantly different from conventional naval ships. The US Navy needs a way to analyze these new hull forms, their flow physics, and associated operating behavior to properly design the next generation of naval combatants.

Surface ship design has traditionally been developed by the build-and-test approach. Stealth has not been part of the major performance requirements. Maneuvering and seakeeping have largely been addressed using extensive experiments. Historically, simple analysis methods are used to evaluate a given ship under a large range of operating conditions, but these existing codes rely heavily on experimental empiricism. Consequently, the simple analysis methods often used are suspect when applied to an unconventional shape without an existing experimental database. This limits the applicability of such techniques for future designs.

> "HPC resources enabled the team to perform the first nonlinear free surface simulation with a surface tracking approach for a fully-appended conventional combatant hull form."

Through HPC resources it is becoming possible to predict flow phenomena that are related to hydrodynamic seakeeping and maneuvering analysis by solving the RANS equations rather than by simple strip theory approaches. For example, the computation of Model 5415, a conventional surface combatant, with rudders, propeller shafts, support struts and rotating propellers at 436 rates per minute

(RPM), required over 5.7 million nodes, 7.7 million prisms, and 9.6 million tetrahedra for its unstructured mesh. This calculation took 48 hours on 75 IBM SP3/512 Mb processors (3600 processor hours) for each propeller revolution. Using HPC environments, the engineers and scientists can model more realistic physics as part of the computation, as shown in Figure 1. The Navy can now use a computational-based approach to address new designs. It is only with the large parallel HPC resources available in the last several years that such computations could be done with sufficient accuracy that a computational-based approach is feasible.

Enabling the First Nonlinear Free Surface Simulation for a Fully-Appended Combatant Hull Form

HPC resources enabled the team to perform the first nonlinear free surface simulation with a surface tracking approach for a fully-appended conventional combatant hull form. The hull form was similar to DDG-51, with rudders, propeller shafts, support struts, and rotating propellers. The simulation was performed at model-scale for steady ahead motion in calm water. Such calculations allow the whole flow field to be studied, unlike traditional experimental data, which supplies limited amounts of information. This can lead to better understanding of the flow physics affecting maneuvering and seakeeping. Additionally, because simpler empirical-based methods will continue to be needed for a considerable time, the community is evaluating using the more complicated physics-based calculations, where new hull forms can be analyzed for a limited number of highly complex computations. This can provide the necessary empirical database, such as for roll damping models, for the simpler codes. This, in turn, will reduce the need for building and testing new models.

The Navy team has had promising successes using the physics based calculations in their research. Computations have been done for increasingly complex bodies. Bilge-keel forces on a three-dimensional rolling cylinder were accurately predicted. Detailed flow and force characteristics were calculated for an unappended naval combatant hull in prescribed roll motions. Initial calculations for a fully-appended combatant hull gave good qualitative predictions for surface pressure and free-surface elevation (Figure 2). Calculations for a rudder-induced turn led to evaluation of improved methods for representing a free surface.

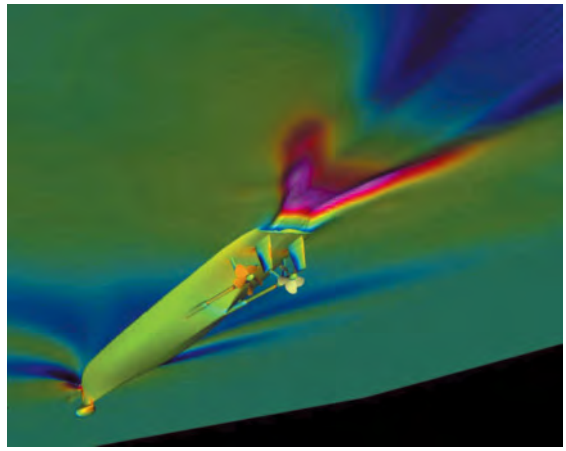

Figure 1. Wave elevation and surface pressure distribution on Naval surface combatant Model 5415

Future Challenges to Increase Insight

Future work in this area, while challenging, will vastly expand the Navy's insight into the transformational technologies Admiral Clark envisioned. A surface-capturing technique appears very promising in terms of robustness. A rudder-induced maneuver with the surface-capturing method will be computed for the fully appended Model 5415. Integration of the computed viscous stresses and pressure distribution on this configuration will provide the hydrodynamic forces and moments acting on the ship. Integration of the 6-Degrees of Freedom (DOF) equations using these forces and moments will yield the time evolution of the ship's velocity and rotation rate. The sensitivity of the computed trajectory with respect to the free surface will also be examined by comparing this maneuvering solution to the one obtained at Fr=0. Future efforts will also include unsteady simulations of Model 5415 in incident waves with both forced and free roll motions. Initial free roll simulations will include prediction of roll decay after

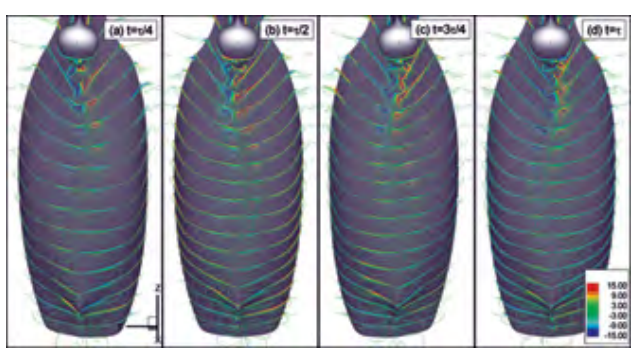

Figure 2. Time sequence of axial vorticity contours for surface combatant simulations with prescribed roll motion using CFDSHIP-IOWA

the model is released from some initial angular displacement at $t=0$ and will allow for comparison with experimental measurements. Planned simulations for Model 5415 with forced and free roll motions will be considerably more complex and computationally demanding. The most difficult challenge to address is computing the complexity of the air/water interface that is necessary for accurately predicting ship motions. This will require the ability to handle breaking waves and other complexities such as water on deck.

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CTA: Computational Fluid Dynamics

Computer Resources: Cray T3E [ARSC, NAVO], IBM SP3 [MHPCC], and SGI Origin 3000 [ARL, NAVO]

Computational Structural Mechanics Provides a New Way to "Test" Behind-Armor Debris

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Army Research Laboratory (ARL), Aberdeen Proving Ground, MD

The Survivability/Lethality Analysis Directorate of the ARL notes, "In survivability analysis, the ability to prevent or mitigate personnel casualties and component or system destruction is directly related to the ability to understand and analyze the process of how damage occurs.

Behind-armor debris (BAD) effects are the result of a combination of stochastic events: fragment masses, shapes, and velocities, as well as the shape and dispersion of the debris cone depend upon:

(1) armor composition
(2) munition type
(3) attack angle (obliquity)

Significant reductions in debris amount and effects will increase crew survivability chances and preserve the system and its subcomponents. By doing this, we better the chance of system survivability and afford it the opportunity to complete its intended mission."[1]

"This is an important new result, as there is at present no practical way to obtain the velocity distribution of fragments by direct experimental measurement."

BAD plays a critical role in the evaluation of both the survivability of crew and components in combat vehicles and of the lethality of such weapon systems. The US ARL generates BAD data at its experimental research facilities to determine the debris characteristics for input into survivability analysis codes. Thus, BAD data is a critical input to an analysis that plays a central role in every major Army acquisition program, including the FCS, the Interim Armored Vehicle, and the "Stryker" (Figure 1), a highly deployable-wheeled armored vehicle which will be the combat vehicle of choice for the Army's Interim Brigade Combat Teams (IBCTs).

[1] http://www.arl.army.mil/slad/Services/BAD.html

Figure 1. A Stryker Infantry Carrier Vehicle rolls of a C-130 at Fort Irwin, CA, after being transported there for a National Training Center exercise (Photo from US Army)

Using Physics Based Modeling to Collect BAD Data

Supplementing this experimental capability for armor testing is an important goal. Dr. Anand Prakash of the US Army Research Laboratory is developing a new capability to obtain BAD characteristics by using physics-based modeling to conduct 3-D computer simulations. The expected advantage of this approach is three fold. First, it will reduce costs by reducing the number of experiments. Second, it will provide a means to conduct survivability analyses involving new armors before they are actually manufactured. Third, it is capable of providing physical details of BAD (e.g., velocity vectors of fragments and the ability to distinguish the trajectories of penetrator debris from armor debris) that are difficult to obtain experimentally. Three-dimensional simulations of BAD were conducted with the CTH code on the supercomputers at the ARL MSRC. CTH is an Eulerian wave code that solves the equations of continuum mechanics over a spatial mesh in small time steps. The material properties are provided as an input. Dr. Prakash used the Johnson-Cooke model of plasticity and obtained BAD patterns

for Kinetic Energy (KE) long rods at normal impact on rolled homogenous armor (RHA) of finite thickness. Wave codes like CTH are suitable to obtain the net result of complex wave propagation, reflection, and interference phenomena. However, the high resolution necessary to keep track of behind armor debris in three dimensions required a mesh with 6 million cells and 96 nodes, with 200 CPU hours per node for complete simulation. Without the modern HPC resources of the MSRC, it would not have been feasible to conduct such a simulation. These simulations have provided new information on the spatial and velocity distribution of BAD fragments.

Capturing the Results

Figure 2 shows the cross-sectional view of an early stage of a 3-D simulation in which a rod of 12.45 cm in length and a diameter of 0.4 cm strikes a steel armor plate 11.45 cm thick with a velocity of 1.6 km/s normal to the plate. A thin witness plate is placed 11.45 cm behind the armor plate. After the rod perforates the armor plate, the behind armor debris strikes the witness plate. Figure 3 shows the BAD distribution on the witness plate obtained by simulation. The spatial and time distributions of various physical quantities associated with BAD were also obtained. For example, Figure 4 shows the distribution of fragment velocities as a function of radial distance from the point of intersection of the line of impact with the back surface of the target

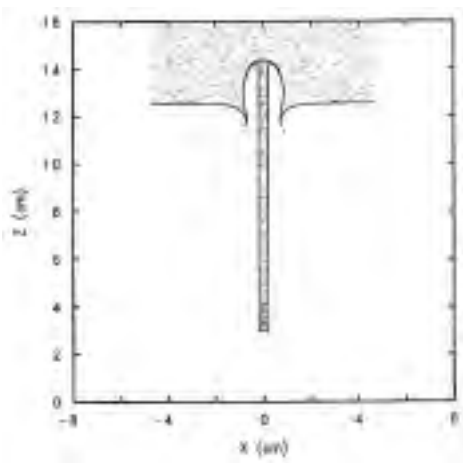

Figure 2. The simulated impact of a long rod on a thick armor plate to determine the characteristics of behind armor debris (BAD)

plate. This is an important new result, as there is at present no practical way to obtain the velocity distribution of fragments by direct experimental measurement. Until now, survivability analyses simply made assumptions regarding this distribution.

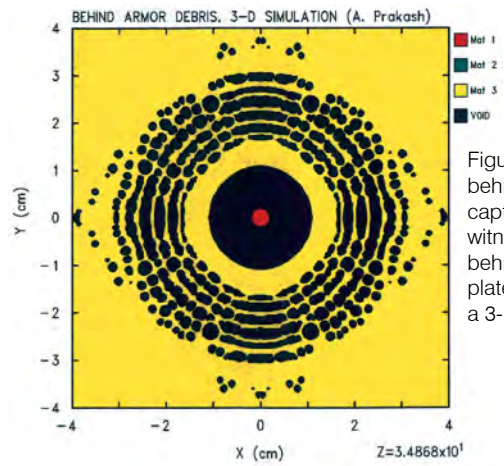

Figure 3. Pattern of behind armor debris captured on a thin witness plate placed behind the target plate, as obtained by a 3-D simulation

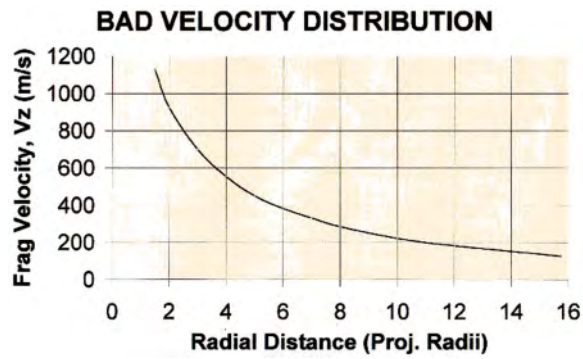

Figure 4. Fragment velocity (component in the direction of initial rod velocity) as a function of radial distance of origination from the impact axis

Impacting the Future

The team is now performing a validation study, comparing the results of this simulation approach to actual experimental data. When this is completed, together with application of the approach to further weapon/target conditions, the Department will have a powerful and flexible new capability to improve the timeliness, cost, and accuracy of vulnerability/lethality analysis products for system developers and the Army's independent evaluators and decision makers.

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CTA: Computational Fluid Dynamics
Computer Resources: SGI Origin 3000 [ARL]

Airdrop Systems Modeling: Fluid-Structure Interaction Applications

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Airdrop technology is a vital DoD capability for the rapid deployment of warfighters, ammunition, equipment, and supplies. In addition, the demand for airdrop of food, medical supplies, and shelters for humanitarian relief efforts has increased significantly in recent years. Airdrop systems development, which traditionally relies heavily on time-consuming and costly full-scale testing, is leaning increasingly on modeling and simulation. Government and academic researchers, who have teamed to make computational modeling a valuable tool for a broad range of airdrop applications, are addressing a variety of challenges. HPC capabilities are being used to numerically model parachutes and airdrop system performance. These capabilities are reducing the time and cost of full-scale testing, minimizing the life cycle costs of airdrop systems, assisting in the optimization of new airdrop capabilities, and providing an airdrop virtual proving ground environment.

Modeling Fluid Structure Interaction Behaviors

HPC modeling methods are being developed that can be applied to many airdrop systems problems including aerodynamics, structural dynamics, and fluid-structure interaction (FSI) behaviors. These methods are based on the Deforming-Spatial-Domain/Stabilized Space-Time (DSD/SST) method for the fluid and a semi-discrete finite element formulation based on the principle of virtual work for the cable-membrane parachute structure. An iterative coupling procedure couples the fluid and structure along the parachute canopy surface. Recent applications simulations have focused on the aerodynamic interaction between two separate parachutes and between different canopies in a parachute cluster, FSI between two separate parachutes and four parachute clusters, FSI for steerable round parachutes with riser control inputs, and the FSI experienced by parachute soft-landing payload retraction systems. In addition to these application simulations, FSI validation simulations are being carried out and numerical results are being compared with water tunnel experiments for scale model parachutes. In one set of simulations, the dynamics of a small-scale round parachute canopy

"High performance computing capabilities are being used to numerically model parachutes and airdrop system performance. These capabilities are reducing the time and cost of full-scale testing, minimizing the life cycle costs of airdrop systems, assisting in the optimization of new airdrop capabilities, and providing an airdrop virtual proving ground environment."

are compared against the experimental data from a similarly scaled canopy for validation purposes. The experiments, which were carried out under ARO sponsorship and using AHPCRC and White Sands Missile Range (WSMR) resources, have sufficient spatial and temporal resolution to permit detailed comparison with the simulation results. In Figure 1, the three snapshots show the vorticity field surrounding two parachutes predicted by the FSI software. In this simulation, the lower canopy is kept rigid while the upper parachute deforms due to its interaction with the surrounding flow field. Deformation of the upper canopy is evident as it is drawn into the wake of the lower canopy and approaches canopy collapse. The frames correspond to physical times of 0.00, 1.75, and 3.50 seconds.

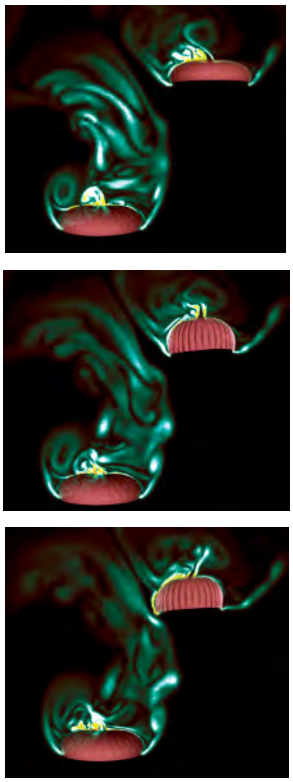

Figure 1. The three snapshots show vorticity field surrounding two parachutes predicted by the FSI software. In this simulation, the lower canopy is kept rigid while the upper parachute deforms due to its interaction with the surrounding flow field. Deformation of the upper canopy is evident as it is drawn into the wake of the lower canopy and approaches canopy collapse. The frames correspond to physical times of 0.00, 1.75, and 3.50 seconds.

Figure 2 shows the structural response of the upper canopy as it deforms and interacts with the surrounding flow field. The colors on the canopy correspond to the differential pressures, which are a part of the fluid dynamics solution.

Summary

New computational technologies based on state-of-the-art methods are being developed to advance airdrop systems modeling capabilities. These technologies are necessary to address a variety of

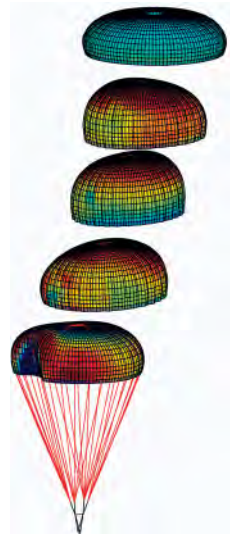

Figure 2. This figure shows the structural response of the upper canopy as it deforms and interacts with the surrounding flow field. The colors on the canopy correspond to the differential pressures, which are a part of the fluid dynamics solution.

challenges associated with airdrop systems modeling. With these new capabilities, numerical simulations are being carried out for the fluid dynamics, structural dynamics, and FSI interactions experienced by airdrop systems. It is expected that further development of this capability will result in significant reduction of life-cycle costs for future airdrop systems.

CTA: Computational Fluid Dynamics

Computer Resources: Cray T3E [AHPCRC] and SGI Origin 2000 [WSMR]

3-D Bomb Effects Simulations for Obstacle Clearance

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The Navy needs a system capable of simultaneously breaching obstacles and clearing mines during an amphibious assault. The rapid creation of transit lanes through shoreline defenses allows landing craft to deposit troops and equipment directly onto and beyond the beaches. The Navy and Marine Corps needs the capability to conduct an efficient amphibious assault, minimizing the number of sorties required to conduct mine and obstacle clearance, and to minimize amphibious lift requirements. In the past few years, PMS-490 and the ONR have sponsored brainstorming sessions and Broad Area Announcements to generate concepts for obstacle clearance. In response to the obstacle-breaching concern, the ONR started the Bomb Effects for Obstacle Clearance Program, along with several other alternative mine/obstacle-breaching programs. The Bomb Effects Program is a potentially effective means of defeating obstacles and mines in the surf zone and beach zone.

This is a highly visible, high priority problem that supports the Navy's investment in organic mine countermeasures (MCM), and is part of the Navy's Future Naval Capabilities (FNC) investments in organic mine countermeasures. This weapon system is part of the Analysis of Alternatives (AoA) for rapid, organic, standoff technologies for breaching surf zone and beach zone mines and obstacles. This effort will provide important input into that analysis for comparing Bomb Effects to other alternatives.

The Bomb Effects Program

The Bomb Effects Program is based on using standard general-purpose bombs as an existing, rapidly deployable, building block for developing an effective system against obstacles. Two components in this program are a testing component and an analytic component. The goal of the testing component is to study, identify, and verify the damage mechanisms of obstacles, both on land and in water, subjected to multiple bomb detonations. However, only limited experimental and full-scale testing of bomb effects has been and can be performed. The goal of the analytic component is to generate semi-analytic/empirical models that, when incorporated in system effectiveness studies, will determine the lethality of general-purpose bombs against obstacles in the beach zone and surf zone. In order to generate these analytic models, experimental data or hydrocode data is required. Prior modeling and simulation techniques generated a flow field due to a bomb detonation and then applied the loads to determine the response of the obstacle. This decoupled method was the only feasible method since the applicable hydrocodes were either not well advanced or were not parallelized at the time.

"This is a highly visible, high priority problem that supports the Navy's investment in organic mine countermeasures (MCM), and is part of the Navy's Future Naval Capabilities (FNC) investments in organic mine countermeasures."

This 3-D modeling and simulation effort complements both the experimental and analytic efforts in providing data that would otherwise be difficult to obtain experimentally. These "live-fire" simulations are effectively an operational test of the real-life scenario of multiple bombs detonated in the beach and surf zone.

Applying High Performance Computing Resources to Live-Fire Simulations

The parallel hydrocode Alegra is being used for these simulations. In Alegra, a problem is divided into blocks; each block can then be run as Eulerian, Lagrangrian, or Arbitrary Lagrangian Eulerian (ALE).

The flexibility to blend Eulerian, Lagrangian, and ALE methods is appealing for modeling these types of surf zone simulations since an Eulerian solver can accurately capture the shocks in water and/or air, the Lagrangian elements most accurately model the tetrahedons and the Eluerian or ALE solver can be used to model the sand. The complex shock interactions of multiple bombs in water and sand strongly influence the loads experienced on these obstacles. The goal is to model the full-scale tests to determine the impact of bomb detonations on tetrahedron obstacles as a function of time. Simulations include modeling subsets of the full-scale tests as well as the full domain.

Due to advances in parallel hydrocodes and the availability of HPC resources, this effort is now able to model scenarios that can not be tested experimentally, solved analytically, or modeled using earlier computational methods. Specifically, the ability to model a single bomb detonation impacting multiple obstacles was lacking. This project has demonstrated a single bomb detonation impacting multiple objects for both a detonation in air and for a detonation in water. More complex scenarios including multiple bombs detonated simultaneously or a bomb sequentially impacting multiple obstacles can now be performed.

A general methodology was developed for mesh generation, flow solver execution, and post-processing on DoD HPC platforms. This methodology included linking Patran© to multiple Sandia National Laboratory software packages and then linking to post-processing software including Ensight© and CTHPLT. The development of a general, efficient methodology allows for rapid model generation, on the order of hours rather than days.

Simulations were typically run to several milliseconds (1–6 ms). These times were based on either time history data from full-scale tests or the computational domain size. Simulations performed included (1) Mk 82 and Mk 83 bombs detonated in air and in water on a sand surface, (2) two Mk 83 bombs 8 feet apart detonated simultaneously in air on a sand bottom, (3) five Mk 83 bombs 32 feet apart detonated simultaneously in air on a sand bottom (typical separation distance for air detonations) and 8 feet apart (typical separation distance for underwater detonations), (4) Mk 83 bomb detonated in air near a "leg" of tetrahedron on a sand bottom (smaller physical domain, simulation used for debugging and analysis), (5) Mk 83 bomb detonated in air near a tetrahedron on a sand bottom at 4 foot and 8 foot stand-off (separation distance for full-scale tests in air), and (6) Mk 82 bomb detonated in air and in water near 4 tetrahedrons on a sand bottom with 8 foot, 12 foot, 16 foot, and 20 foot standoffs.

The following is a highlight resulting from a Mk 83 bomb detonated in air near a single tetrahedron. Modeling and simulation of the impact of a bomb detonation near a full tetrahedron is difficult due to the large mesh size required to accurately mesh the geometry of the tetrahedron as well as the large physical domain surrounding the bomb and tetrahedron. Each leg of the tetrahedron is a 5 foot long by 4 inches wide angle iron by 5/8 inch thick steel. A tabular Sesame EOS with an elastic-plastic model was used to model the steel tetrahedron leg. Figure 1, in which the tetrahedron is 4 feet from the bomb, shows an isocontour of the high explosives (HE) gas as it impinges on the tetrahedron at t = 275 ms. The isocontour and a centerline slice are colored by pressure. The pressure on the forward leg of the tetrahedron is increasing as well as beginning to deform the tetrahedron.

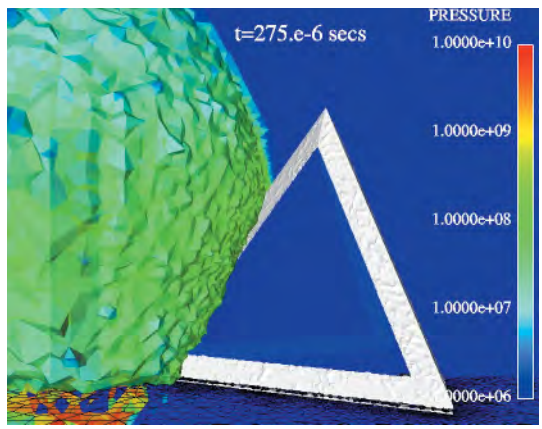

Figure 1. Mk 83 detonated in air near a single tetrahedron. Isocontour of HE gases colored by pressure.

In addition, simulation of a Mk 82 bomb detonated in air and in water near four tetrahedrons was performed. One of the successes of this effort has been the modeling and simulation of a bomb detonation impacting multiple tetrahedrons in air and in water. Figure 2 is the detonation in air at t=1ms. This figure shows an isocontour of HE gas colored by velocity magnitude. These simulations would not be possible without HPC resources.

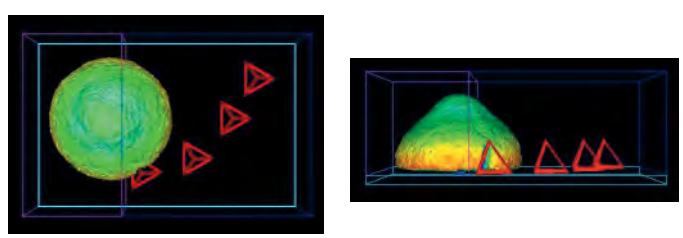

Figure 2. Mk 82 detonated in air near four tetrahedrons. Isocontour of HE gases colored by velocity magnitude.

Future Efforts

To date, the simulations have been run in pure Eulerian mode. One of the key remaining challenges is to run these simulations with Eulerian, Lagrangian, and ALE blocks. The interfaces between these blocks has been problematic. These issues are being addressed both in-house and through consulting with Sandia National Laboratories, the developers of Alegra, and the staff of the ARL, who also use the Alegra hydrocode.

CTA: Computational Structural Mechanics
Computer Resources: SGI Origin 3800 [ARL, SMDC]

Providing the Warfighter Information Superiority in Littoral Waters

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The littorals of the world are areas of great strategic importance. Approximately 95% of the world's population lives within 600 miles of sea, 80% of all countries border the coast, and 80% of the world's capitals lie within 300 nautical miles of shore. With the end of the cold war, DoD's focus has shifted from a large land/sea battle scenario with a monolithic global adversary to dealing with low-intensity conflicts in the near-coastal or littoral regions. In wartime, forces that dominate the littoral, including the undersea environment, operate with impunity in the face of area denial threats while taking initial action to defeat those threats and prepare the battlespace for follow-on forces.

Information superiority—understanding and exploitation of the natural environment—is critical to the safe and effective operation of joint forces engaged in littoral expeditionary warfare. The tactical advantage will depend on who can most fully exploit the natural advantages gained by a thorough understanding of the physical environment. Every aspect of the littoral environment is critical to conducting military operations, a huge challenge to both the warfighters and the Meteorology and Oceanography (METOC) community that supports them.

"The HFSOLE models have been shown in literature to provide a realistic depiction of the complex physical processes that occur in the littoral battlespace, from rivers and estuaries to oceanic waters. CHSSI has given DoD an opportunity to make these large numerical codes scalable on a host of HPC computational platforms and greatly reduce the wallclock time needed to perform a simulation, hindcast, or forecast. "

Characterizing the Battlespace Environment

Characterization of the battlespace environment to ensure optimal employment of personnel, systems and platforms depends on continuous improvement in science and technology. Key and essential elements in that characterization are effective, relocatable, high-resolution, dynamically linked mesoscale, meteorological, coastal oceanographic, surface water/groundwater, riverine/estuarine, and sediment transport models. The linkages between these models, coupled with the complexity and the scale of the environment, require the implementation of focused sets of these models on DoD HPC architectures in support of real time operations, scenario (operational and/or training) planning, and course of action analysis.

The High Fidelity Simulations of Littoral Environments (HFSOLE) Portfolio is funded by CHSSI. The HFSOLE effort encompasses four projects; 1) the System Integration and Simulation Framework Project is developing the interface algorithms for the atmospheric, riverine, estuarine, wave, tidal, and ocean models; 2) the Near-shore and Estuarine Environments Project is coupling and enhancing nearshore process models to efficiently simulate interactions between winds, waves, currents, water levels, and sediment transport; 3) the Surface Water/Groundwater, Riverine

and Tidal Environments Project is enhancing the capabilities of the Adaptive Hydraulics (ADH) model. This project will provide DoD the tools to generate fast and accurate estimates of water depths and velocity distributions for use in ingress/egress assessments for rivers and streams. They will also support flow rate and sediment loading as input for coastal simulation, and ground-surface inundation and moisture content predictions for use in local atmospheric simulations. The fourth project, the System Applications Project, is improving the fidelity and execution speed of DoD maritime operation simulation systems dependent on data from ocean surface behavior models. Such simulations include amphibious assault, mine clearing, and sea keeping operations. This project provides for the development, implementation, and testing of an environmental server to support Modeling and Simulation (M&S).

Modeling the Littoral Waters

Previously, these models ran independently, without any coupling or linkages, and typically in serial fashion on one processor. The HFSOLE Portfolio includes eight numerical ocean, wave, and riverine models. They use HPC resources to solve for a host of equations including the shallow-water equations, primitive continuity and momentum equations, and the spectral action balance equation. For example, the evolution of the wave spectrum in the Simulating WAves Nearshore (SWAN) (Booij et al. 1999) wave model is described by the spectral action balance equation, which for Cartesian coordinates is:

$$\frac{\partial}{\partial t}N + \frac{\partial}{\partial x}c_x N + \frac{\partial}{\partial y}c_y N + \frac{\partial}{\partial \sigma}c_\sigma N + \frac{\partial}{\partial \theta}c_\theta N = \frac{S}{\sigma} \qquad (1)$$

The first term in the left-hand side of this equation represents the local rate of change of action density in time. The second and third terms represent propagation of action in geographical space (with propagation velocities c_x and c_y in *x*- and *y*-space, respectively). The fourth term represents shifting of the relative frequency due to variations in depths and currents (with propagation velocity c_σ in σ-space). The fifth term represents depth-induced and current-induced refraction (with propagation velocity c_θ in θ-space). The expressions for these propagation speeds are taken from linear wave theory. The term S ($= S(\sigma,\theta)$) at the right hand side of the action balance equation is the source term in terms of energy density representing the effects of generation, dissipation, and nonlinear wave-wave interactions.

The HFSOLE models have been shown in literature to provide a realistic depiction of the complex physical processes that occur in the littoral battlespace, from rivers and estuaries to oceanic waters. CHSSI has given DoD an opportunity to make these large numerical codes scalable on a host of HPC computational platforms and greatly reduce the wallclock time needed to perform a simulation, hindcast, or forecast. Additionally, the Model Coupling Environmental Library (MCEL) being developed in HFSOLE allows for the coupling of these numerical models running on distributed HPC platforms. The distributed model-coupling infrastructure uses a data flow approach where coupling information is stored in a centralized server and flows through processing routines or filters to the numerical models. The resulting software is expected to provide substantial improvements over existing technologies by including inter-model interactions. The models are used by a DoD Challenge Project that allows for more experimentation and the ability to perform simulations at higher resolutions.

Japan/East Sea Circulation Simulations

Using HPC resources, HFSOLE researchers are performing complex computations in a timely manner. This will greatly impact providing the warfighter with a tactical advantage. An example of this time savings is illustrated with the coastal ocean model ADvanced CIRCulation Model (ADCIRC) that was applied to the simulation of rip currents generated by breaking waves. As shown in Figure 1, barred beaches with channels often produce rip currents (at the channels) when incident waves break in the vicinity of the bars. The laboratory wave-driven experiments of Haller and Dalrymple (1999) were simulated. The dimensions of the beach are 20 m by 18.2 m with a water depth variation from 0.37 m

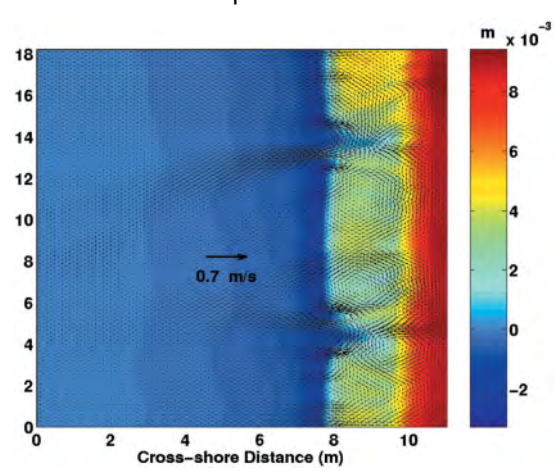

Figure 1. ADCIRC model computed circulation of the steady state sea surface height and current velocity over a laboratory barred beach. Note the presence of rip currents in the two channels.

offshore to -0.01 m at the shoreline. The computational domain is discretized to a spacing of 0.1 m using 40,040 elements and 20,313 nodes. The simulation extends 0.6 days to a steady state with computations made every 0.025 seconds, producing a rip current in the upper channel. Computational times dropped from 123 hours using one CPU to 2 hours using 128 CPUs.

A series of ocean circulation simulations in the Japan/East Sea have been performed on the NAVO Cray T3E. The model used is a Hybrid Coordinate Ocean Model (HYCOM), a next generation circulation model under development at the Naval Research Laboratory (NRL), the University of Miami, and Los Alamos National Laboratory. Ideally, an ocean general circulation model should (a) retain its water mass characteristics for centuries (a characteristic of isopycnal coordinates), (b) have high vertical resolution in the surface mixed layer (a characteristic of z-level coordinates), and (c) have high vertical resolution in surface and bottom boundary layers in coastal regions (a characteristic of terrain-following coordinates).

The Japan/East Sea has been used to test the robustness of HYCOM because it contains many circulation features found in the global ocean, such as a western boundary current, subpolar gyre, and rich eddy field, and it is small enough to allow simulations with very high grid resolution. Under this HPC DoD Challenge Project, several simulations with 3.5 km resolution were performed for several years each. Scalability was via MPI/SHared MEMory (SHMEM), or OpenMP, or both, although SHMEM was used exclusively for the simulations performed on the T3E. The mesh size for the high-resolution configuration is 394x618x15, and a one-year simulation requires about 12,000 CPU hrs/model year. The HYCOM simulations have shown (Figure 2) that high horizontal grid resolutions are needed to adequately resolve the mesoscale features as well as the coastline and bottom topography, especially over the shelf.

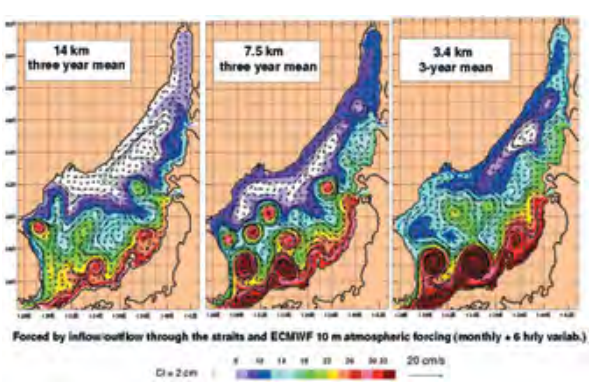

Figure 2. Impact of progressively increasing the horizontal grid resolution using HYCOM. At 14 km resolution, unrealistic overshoot of the East Korea Warm Current (130°E, 39°N) is evident. This overshoot is diminished at 7.5 km, and at 3.5 km the current separates from the coast at the observed latitude. The strength of the subpolar gyre strengthens as the horizontal resolution is increased.

Software Testing to Begin

Ongoing work in HFSOLE includes preparation for individual Alpha and Beta software tests for each of the models included in the portfolio. A portfolio wide Alpha test using the MCEL software took place in January 2003. Inputs to these models include topographically controlled mesoscale atmospheric forcing such as wind stress, sensible and latent heat fluxes, incoming solar radiation and sea level pressure, high-resolution bathymetry and tidal constituents. The final results of this effort will be a scalable suite of dynamic models for real-time operational applications and high-fidelity simulations for modeling and simulation scenarios.

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Haller, Merrick C., and Robert A. Dalrymple, "Rip Current Dynamics and Nearshore Circulation", Res. Report CACR-99-05, Center for Applied Coastal Research, Univ. of Delaware, 1999.

CTA: Climate/Weather/Ocean Modeling and Simulation and Environmental Quality Modeling and Simulation

Computer Resources: Cray T3E [ERDC, NAVO], SGI Origin 3000 [ERDC], and IBM SP, Cray SV1, and SUN E10000 [NAVO]

Getting the Waves Right

Jane McKee Smith

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Ocean waves near the coast have a huge impact on military activities aimed at getting soldiers, sailors, marines, and equipment on the shore. Although waves are generated in the open ocean and propagate over long distances, the last kilometer or less near the shore is the critical region for landing and docking. Nearshore wave transformation is solved in the model STeady-state WAVE (STWAVE) using the wave action balance equation. The model includes the processes of shoaling and refraction (increases in wave height and changes in wave direction in shallow water), wave-current interaction (changes in wave properties caused by tidal or nearshore currents), wave growth due to the wind, and wave breaking. The model is based on linear wave theory and does not include reflection or bottom friction. By linking the nearshore wave transformation model STWAVE with deepwater wave forecasts or hindcasts (at large spatial scales), nearshore waves can be estimated on beaches and at harbor and inlet entrances. Forecasts are used for short-term planning of operations, and hindcasts are used to garner climatological information for longer-term planning (typical and extreme conditions, seasonal variation, storm probability).

Using STWAVE to Model Nearshore Waves

In the past, nearshore wave transformation modeling has been run on HPC platforms to make forecasts to support warfighters. To meet stringent time requirements for producing the forecasts, the model was run with very coarse spatial resolution and less frequency in time than is optimal. Under the CHSSI High Fidelity Simulations of Littoral Environments project, STWAVE was parallelized to exploit HPC capabilities. Tests earlier this year demonstrated that the parallel version of STWAVE was over 90 percent efficient using 32 processors on both the Cray T3E and SGI Origin 3000. This translates into increasing the model throughput by a factor of 28. The highly efficient parallelization allows improved resolution of the nearshore domain (which improves model accuracy) and more frequent model runs (more resolution in time), while still meeting or beating required forecast time constraints. Improved nearshore modeling times also allows more time for other modeling components and for decision making. Figure 1 shows verification of the parallel version of STWAVE at Duck, NC, for the year 1997. Full-year simulations were not run prior to the parallel capability.

"Tests earlier this year demonstrated that the parallel version of STWAVE was over 90 percent efficient using 32 processors on both the Cray T3E and SGI Origin 3000. This translates into increasing the model throughput by a factor of 28."

Continuing challenges include expanding to more HPC platforms and a larger number of processors, implementing additional improvements to model efficiency, and upgrading model physics. The CHSSI work will focus on interfacing STWAVE with circulation and sediment transport models to provide a greater understanding of the physical processes that impact directly on operations, equipment, and training.

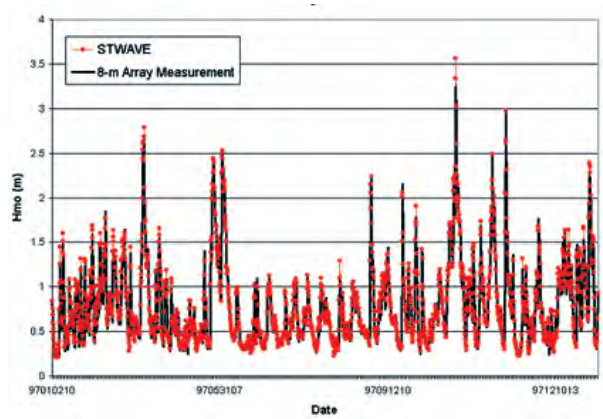

Figure 1. Parallel version of STWAVE at Duck, NC, 1997

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http://chl.wes.army.mil/research/wave/wavesprg/numeric/wtrasformation/downld/erdc-chl-sr-01-11.pdfl

CTA: Climate/Weather/Ocean Modeling and Simulation

Computer Resources: Cray T3E and SGI Origin 3000 [ERDC]

Rapid Transition to Operations: Numerical Weather Modeling

William Burnett
Naval Meteorology and Oceanography Command (NAVMETOCCOM), Stennis Space Center, MS

The Primary Oceanographic Prediction System (POPS) produces and provides critical, classified and unclassified atmospheric and oceanographic guidance to Navy and DoD activities worldwide on a fixed schedule, 24 hours a day. POPS covers the entire Fleet Numerical Meteorology and Oceanography Center (FNMOC) enterprise including the supercomputing, communications (including receipt of hundreds of thousands of observations and transmission of model products), databases, data assimilation and distribution, and systems control/monitoring. It is the engine that operates all the Navy's global/regional/tactical atmospheric, oceanographic, wave, ice, and tropical cyclone models, and DoD's only coupled air/ocean model. The POPS is the only national system that assimilates classified and unclassified data, and produces and disseminates classified and unclassified global/regional atmospheric guidance.

Meteorological Data Assimilation

Keeping operational numerical weather models "state-of-the-art" while transitioning to future, scalable computing architectures is a difficult but necessary task. The computing industry is evolving into a new state in which the preferred mode of large-scale computers is a hybrid system composed of hundreds of nodes, each using tens of processors. Memory is distributed among the nodes, meaning that explicit communications are needed for synchronization of data during computations across the nodes. The industry standard for performing this communication is known as the Message Passing Interface (MPI). Within each node, the individual processors share memory in a manner similar to today's multi-processor, shared memory computers, such as the Cray C90. Communications among the individual processors is accomplished through the emerging standard OpenMP. However, the shared memory in the newer systems is cache-based with a relatively small bandwidth, and the processors are scalar, rather than vector processors. These differences, and the use of distributed memory across the nodes, requires a significantly different programming system than what has been used in the past in order to realize the full potential of this newer architecture.

The Navy Operational Global Atmospheric Prediction System (NOGAPS) and the Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS) are complete numerical weather prediction (NWP) systems. Each receives raw meteorological observation data from myriad sources around the world, and with a variety of data processing and computational steps, produces numerical, gridded "products" to satisfy DoD requirements for meteorological support. This process is known as meteorological data assimilation and is typically performed by marching forward in 6-hour steps known as "update cycles."

"The POPS is the only national system that assimilates classified and unclassified data, and produces and disseminates classified and unclassified global/regional atmospheric guidance."

HPC Resources Crucial

The Oceanographer of the NAVMETOCCOM and FNMOC agreed to a very aggressive schedule to completely upgrade the Navy's and DoD's POPS supercomputer from vector to scalable architectures in 1997. This schedule could not have been successfully accomplished without DoD's HPC resources. MSRC, CHSSI, and PET are invaluable assets. They ensured that the distributed memory systems purchased by the Oceanographer of the Navy in 1999 were efficient and that the modeling codes were optimized for the new architecture. CHSSI funds were leveraged with the Oceanographer's research and development (R&D)

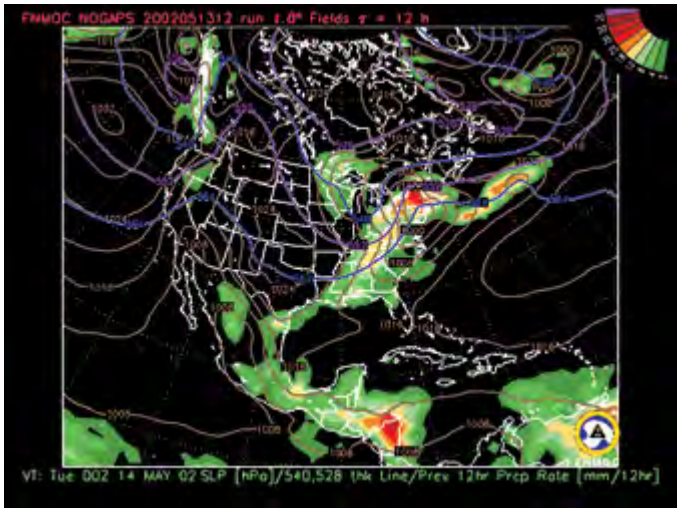

Figure 1. Navy Operational Global Atmospheric Prediction System (NOGAPS) previous 12-hr forecast of precipitation rate[mm/12hr filled areas in color], 540 and 564 thickness lines [dm - blue contours], and sea level pressure [hPa - orange contours] valid 14 May 2002 at 00 Zulu

funds to rapidly upgrade and rewrite the NOGAPS and the COAMPS codes. These funds were crucial to ensuring that the updated codes were ready for the new systems. The CHSSI code conversion effort ensured that the Naval Meteorology and Oceanography community could provide higher-resolution and more accurate numerical weather products, in a faster amount of time, for less costs. Second, MSRC resources (both DoD Challenge Projects and CHSSI) were used to test and benchmark the codes on various machines to help determine which machines could efficiently and effectively operate the code. This was crucial to ensuring that the codes were ready for rapid transitions to operations. Third, PET resources were used to train both the researchers and operators on the new types of HPC architectures, and help them understand how to develop and operate scalable systems.

Visualization of atmospheric data (both global and regional) is crucial to the scientist and the warfighter. Both NOGAPS and COAMPS outputs contain millions of bits of information. Visualization techniques helps the user understand the information and the impact of the environment on exercises/operations.

The HPC resources allowed the operational community to continue to provide seamless operational weather products and information to the warfighters during a crucial time. The conversion from the Cray C90 supercomputers to the SGI Origin 3800s was an enormous and highly successful undertaking. During this extraordinarily complex effort, HPC resources ensured that FNMOC continued to provide exceptional service to the Fleet and DoD other customers.

New Codes Work Heterogeneously

The new NOGAPS and COAMPS codes work in a heterogeneous computing environment that is a significant departure from previous generations. Historically, these systems have run in a homogeneous computing environment with all modules running on the same platform, e.g., a Cray C90. This was possible because supercomputers such as the C90 delivered considerable computational power for codes ranging from serial to parallel vector applications. The new generation of scalable architecture supercomputers, with distributed memories and cache-based processors, are not general-purpose machines and require code that works in a heterogeneous environment.

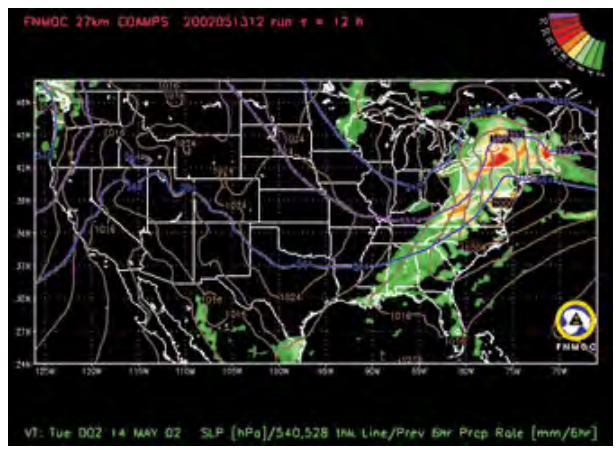

Figure 2. Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS) previous 12-hr forecast of precipitation rate [mm/12hr filled areas in color], 540 and 564 thickness lines [dm - blue contours], and sea level pressure [hPa - orange contours] valid 14 May 2002 at 00 Zulu

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CTA: Climate/Weather/Ocean Modeling and Simulation

Computer Resources: IBM SP3, SGI Origin 2000, SGI Origin 3000, and Cray T3E [NAVO]

3DVAR — AFWA's New Forecast Model Ties Research to Operations

Paige Hughes
Air Force Weather Agency (AFWA), Offutt AFB, NE

The Air Force Weather Agency (AFWA) implemented an advanced observation integration method September 26, 2002, that significantly improves weather forecast model accuracy.

The three-dimensional variational data assimilation (3DVAR) processes nearly four times the amount of weather observations than the previous method. Additionally, 3DVAR ingests a wider spectrum of observations, as many as 21 various data types. Developers contend that all of the forecasts produced using 3DVAR show significantly enhanced resolution.

3DVAR is capable of running on 45, 15, and 5 kilometer grids further enhancing the analysis on initial conditions. Real-time verification of the data shows improved cloud and precipitation locations of the initial forecast time of the model.

"It's a more sophisticated way of determining the initial conditions, ultimately leading to a better forecast," said Dr. Jerry Wegiel, chief of Fine Scale Models team at AFWA and the principle investigator for 3DVAR. "This is a significant milestone for the operational and research community," he added.

AFWA is the first in the country to use this method operationally and with the increased capability, AFWA is producing weather forecast products with greater accuracy for the warfighter. AFWA maximizes the nation's aerospace and ground combat effectiveness by providing accurate, relevant and timely air and space weather information to the DoD, coalition, and national users.

3DVAR is one facet of a larger initiative to replace the current fine scale modeling process used operationally. As part of this initiative, developers are working on the Weather Research and Forecast (WRF) model slated to replace the Mesoscale Model Five.

WRF is the object of major interest for meteorologists because it provides a common framework for research and operational modeling. WRF incorporates a portable modeling infrastructure with the latest atmospheric science allowing researchers to develop new numerical methods while incorporating real-time operations. The WRF initiative teams the nation's top weather scientists from AFWA, the National Center for Environmental Prediction, National Center for Atmospheric Research, and various universities; in fact, more than 700 scientists are involved in this effort.

AFWA has long been the DoD's center of excellence for cloud analysis using high-resolution satellite data, and now, with the implementation of WRF-3DVAR, AFWA is being touted as a leader in forecast mode R&DI.

"AFWA is the first in the country to use this method operationally and with the increased capability, AFWA is producing weather forecast products with greater accuracy for the warfighter. AFWA maximizes the nation's aerospace and ground combat effectiveness by providing accurate, relevant and timely air and space weather information to the Department of Defense, coalition, and national users."

Funding for the WRF-3DVAR initiative comes from the HPCMP. The HPCMP provides the supercomputer services, high-speed network communications, and computational science expertise that enables the Defense laboratories and test centers to conduct a wide range of focused research, development, and test activities. This partnership puts advanced technology in the hands of US forces more quickly, less expensively, and with greater certainty of success.

AFWA's fine scale models team is looking farther down the research road and has unveiled a concept

called four-dimensional variational data assimilation (4DVAR). With funding, 4DVAR, the program could be implemented operationally as early as 2006.

CTA: Climate/Weather/Ocean Modeling and Simulation
Computer Resources: IBM SP3 [ASC,NCAR, AWFA], SGI Origin 3000 [ERDC], and IBM SP PWR PC [AWFA]

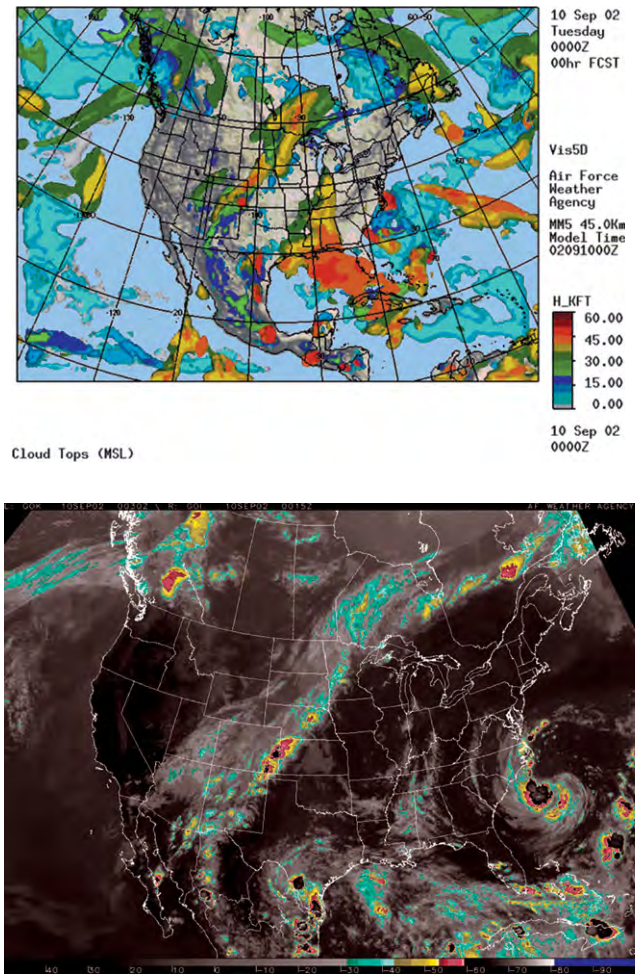

Figure 1. The first panel shows cloud top heights from an operational MM5 run using WRF-3DVAR as the data assimilation scheme. The bottom panel is verifying MB enhanced IR imagery. (JAAWIN)

Forecasting the Weather Under the Sea: NAVO MSRC Scientific Visualization Center Allows Navy to See the Ocean Environment for Undersea Recovery Operations

PETE GRUZINSKAS

Naval Oceanographic Office (NAVO), Scientific Visualization Center, Stennis Space Center, MS

The ability to accurately predict environmental conditions is paramount to operational consideration within the Navy and the DoD. The recent Navy salvage operation (SALVOPS) of the Japanese fishing trawler Ehime Maru provides an excellent example of the need for these accurate predictions. Through the application of state of the art software analysis tools designed for the analysis of R&D ocean circulation models to the SALVOPS, the Navy was able to successfully complete its mission.

On February 9, 2002, a collision between a US Navy submarine and the Ehime Maru sent the fishing vessel to the bottom of the Pacific Ocean about 10 miles south of Diamond Head, Oahu, Hawaii. The decision was made to retrieve the vessel, which lay in approximately 1800 feet of water. A Crisis Action Team was formed, and the NAVO MSRC Visualization Center was asked to provide visualization support for the Ehime Maru retrieval operation. The first challenge was to visualize the high-resolution model output generated by the Shallow-Water Analysis and Forecast System (SWAFS), running on the MSRC's IBM-SP. SWAFS, as shown in Figure 1, is a 3-D ocean circulation model that produces time-series data containing ocean current speed and direction, temperature, and salinity fields. Initially, a 2-kilometer grid that covered the entire Hawaiian Islands was generated and used to provide input to a higher resolution (500-meter) nest, which bounded the operation area.

> "With the Navy's ever evolving 3-D ocean modeling capabilities and the matching HPCMP hardware advances, it is now possible to place model results on the desktop of the DoD user and, in the case of the Ehime Maru SALVOPS, on the laptop of analysts in the field."

Development of Analytical Software Environments

Part of the NAVO MSRC Visualization Center's mission is the development of analytical software environments for the DoD research community. Some of these tools, designed to analyze ocean model output, were modified to analyze the Navy's operational model output for the Ehime Maru SALVOPS. These software tools provided significant diagnostic capability, which assisted in the validation of the model output in a very complex environment.

While virtual environments may not provide all of the answers to data analysts, the fact of the matter is the real world environment is 3-D. Features within the environment have a 3-D structure that can be difficult, if not impossible, to realize in two-dimensional (2-D)

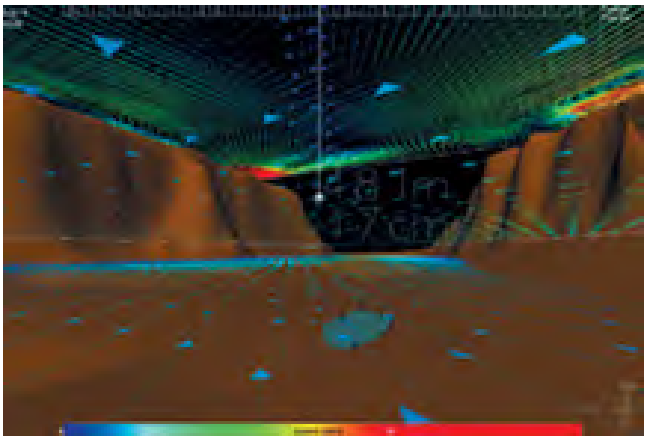

Figure 1. SWAFS surface currents in the operational area

space. The same technology that was built to help research and development modelers scrutinize their model output was applied to this operational scenario where the speed and direction of the ocean currents were critical factors.

An additional feature added to the application, unique to the Ehime Maru retrieval operation, was the display of an Acoustic Doppler Current Profiler (ADCP) buoy. The display of the ADCP data provided analysts a direct comparison between model output and in-situ current measurements in near real-time. Another significant feature of the virtual environments built for ocean model analysis is portability — the ability to run on a variety of hardware architectures, including laptop computers — which proved to be critical in this operation.

Portability is accomplished by savvy application of graphics techniques, as well as smart Input/Output and memory management. This ability was critical to the provision of an analysis environment and data to forward-deployed personnel on-scene at the Ehime Maru recovery site. Other support products were developed to render the recovery area in 3-D from high-resolution bathymetry (water depth) data to delineate critical areas (Figure 2). Conceptual animations were built to demonstrate the mechanics of an extremely difficult recovery operation.

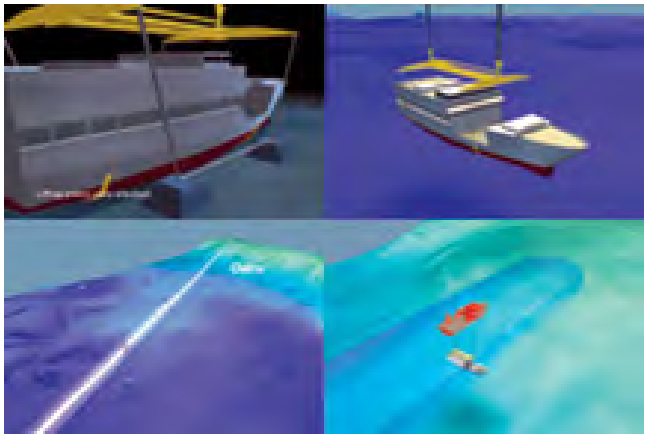

Figure 2. Still image showing Ehime Maru retrieval over real bathymetry data. The animation was designed to conceptualize/visualize what the recovery would look like in the context of the real data collected by the USNS SUMNER.

Using Virtual Environments to Analyze Results

3-D ocean circulation models, like those supported by the HPCMP, represent 3-D grids with output that varies over time (four-dimensional). To analyze the output of these models the computational space is reconstructed into a virtual environment where a variety of analytical techniques can be applied and subsequently visualized.

The NAVO MSRC Visualization staff was approached before this recovery operation to assist in the analysis of the current fields in the vicinity of the Ehime Maru, which lay at a depth of approximately 1800 feet. The work accomplished in the R&D analysis arena was directly applied to this naval operation. Techniques, such as colorized vectors and advected particles, were employed to ensure that critical thresholds of current speed were not exceeded in and around the salvage area. On scene (in situ) sensors provided near real-time measurements, which were displayed along with the model output. This was all packaged and automated, to provide daily results to analysts' on-scene in Oahu.

A level of confidence was established, based on model output and in situ measurements, that the ocean currents in and around the salvage area would not represent a threat to the salvage operation. The virtual environments created by the staff at the NAVO MSRC Visualization Center provided a critical look into the environment around this operation, with regard to the undersea terrain (bathymetry), ocean current speed, direction, and temperature. This was a successful SALVOPS and the tools brought to bear before and during this operation will serve both the R&D and operational ocean modeling communities.

Future 3-D Ocean Models

Advances in hardware and software technology have helped close the gap between computational technology and the technology required to manipulate and display the results of the 3-D ocean model output. With the Navy's ever evolving 3-D ocean modeling capabilities and the matching HPCMP hardware advances, it is now possible to place model results on the desktop of the DoD user and, in the case of the Ehime Maru SALVOPS, on the laptop of analysts in the field.

The operation was successful, and all mission objectives were accomplished. This recovery operation demonstrates the excellent synergy that has developed between the operational Navy and the DoD research infrastructure built by the HPCMP.

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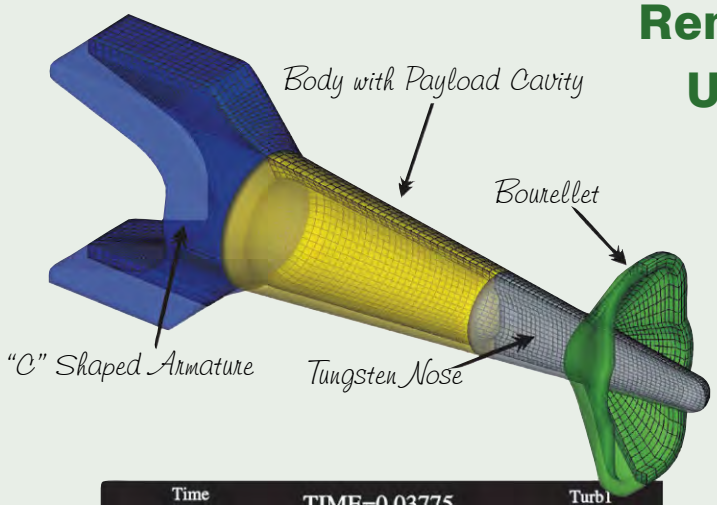
CTA: Climate/Weather/Ocean Modeling and Simulation
Computer Resources: RS/6000 SP3 [NAVO]

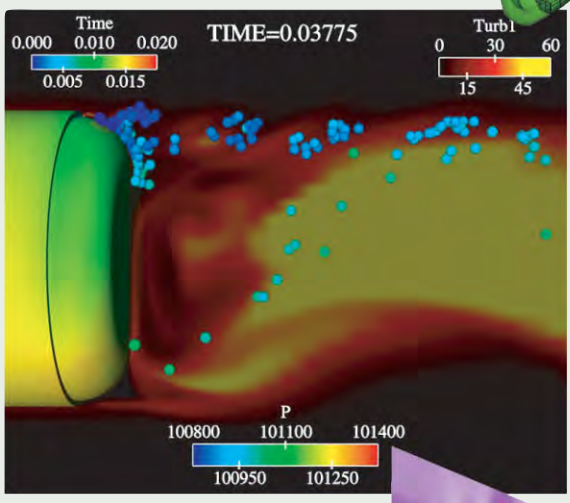
Deny Enemies Sanctuary

Remote Sensing

Unmanned Aerial Vehicles

Long-Range Precision Strike

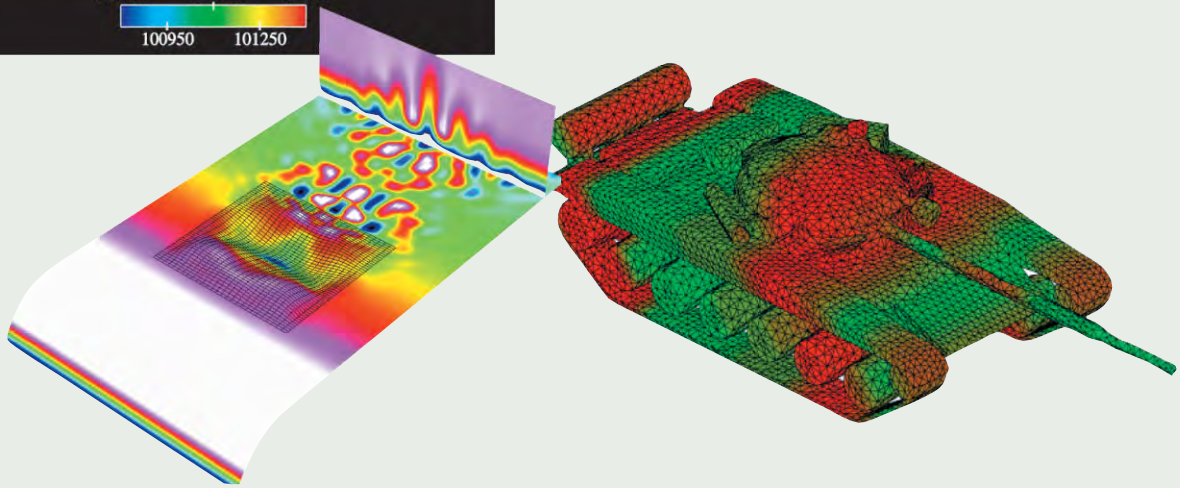




Small-Diameter Munitions

Deep Mobile Target Attack in Denied Areas

Defeating Hard and Deeply Buried Targets



References (from top to bottom):

Accuracy Modeling for Electro-Magnetic Launched Anti-Armor Projectile by James Newill
Typical electromagnetic projectile

Time-Accurate Aerodynamics Modeling of Synthetic Jets for Projectile Control by Jubaraj Sahu
Computed time-coded particle traces show the interaction of the unsteady synthetic jet with the projectile wake flow at Mach = 0.11 and zero degree angle of attack

Development of a High-Fidelity Nonlinear Aeroelastic Solver by Raymond Gordnier
Three-dimensional panel flutter due to interaction with a transitional boundary layer

Identification of "Hot-Spots" on Tactical Vehicles at UHF Frequencies by Anders Sullivan
Impulse response mapped on T-72

Deny Enemies Sanctuary

"Deny enemies sanctuary — so they know no corner of the world is remote enough, no mountain high enough, no cave or bunker deep enough, no SUV fast enough, to protect them from our reach… To achieve this objective, we must have the capability to locate, track and attack both mobile and fixed targets—any where, any time, and under all weather conditions… To achieve this, we must develop new data links for connecting ground forces with air support; new long-range precision strike capabilities; new, long-range, deep penetrating weapons that can reach our adversaries in the caves and hardened bunkers where they hide…" — from testimony of US Secretary of Defense, Donald Rumsfeld, prepared for the House Armed Services Committee 2003 Defense Budget Request, February 6, 2002.

These words ring true. Recent events in our nation only underscore their importance. As scientists and engineers the message is clear. All our efforts must be directed towards satisfying the Secretary's transformational goal. The following success stories highlight the outstanding accomplishments of DoD scientists and engineers in striving towards this goal. The transformational goal is actually a continuously evolving process that requires constant innovation by the scientific community. The ability to solve very complex problems from quantum physics to high-speed fluid flow is a hallmark of these success stories. By applying state-of-the-art algorithms, coupled with high performance computing resources, problems that could not be solved as little as 5 years ago can now be solved routinely. A selection of these stories illustrate the practical application of modeling and simulation in the design process — with the goal of producing better and cheaper weapon systems for the warfighter. Other stories reflect basic research efforts in materials modeling and device development. Overall, the stories span many of the HPCMP computational technology areas including computational fluid dynamics (CFD), computational structural mechanics (CSM), computational chemistry and material science (CSM), and computational electromagnetics and acoustics (CEA).

The first group of stories in this section highlights the use of high performance computing in the design process for air, sea, and ground weapon systems applications. These stories include using high-fidelity simulations for the design of an advanced submarine sail, end-to-end simulation capabilities for projectile-target interactions, and advanced modeling and simulation of revolutionary unmanned air vehicles (UAV). These stories are examples of the paradigm shift taking place within the DoD as part of the transformation. That is, developing cost effective weapons in a "virtual" design environment. The next group of stories discuss materials and chemistry modeling. The first in this set is a story on atomistic modeling techniques for the development of new energetic materials. This is followed by a story on materials modeling for device development. Next is a story on quantum mechanical molecular modeling for the design of advanced resins used in gun testing. Finally there is a related story on nanoparticles used in the design of high energy density materials. In the next group, there are two stories on modeling and simulation of weapons of mass destruction. In both stories, the authors study the effects of the non-ideal airblast on the environment. The next group of stories illustrates the application of modeling and simulation in advanced sensor technology and advanced radio frequency (RF) weapon technology. The first in this group discusses modeling the performance of unattended ground sensors in the modern complex battlefield environment. It is shown that high-fidelity simulations are essential to assess the performance limitations of next-generation sensor technology. The next story is on modeling and simulation of foliage penetrating radar and how electromagnetic models can be used in the development of advanced detection algorithms. The last story in this group discusses the use of electromagnetic particle-in-cell methods to design high power microwave devices. These devices are designed to defeat enemy battlefield electronics using non-lethal means. This capability will be very important in future conflicts where over-matched enemy forces may seclude themselves into the civilian population. The last group in this section shows examples of the outstanding progress that has been made in reactive flow modeling. The first in this set discusses

multi-phase CFD simulations used for next generation gun propulsion systems. The next is a related story on the interaction between high temperature gas and solid propellant in tank and artillery gun rounds. The final story in this group, and in this section, discusses the production of nanoenergetic particles in turbulent reacting flows, which are expected to be employed in next-generation Army gun systems. In summary, each of these stories can relate to the Secretary's transformational goal on denying enemies sanctuary — whether it is in unmanned surveillance and tracking technology (sensors, UAV) or improved lethality technology (weapon platforms, materials).

As the DoD leadership continues to transform military training and doctrine, it is incumbent upon the scientific community to continue to develop and deliver the best technologies to the warfighter. In the end, these stories are just a small sampling of the outstanding contributions made by scientists and engineers across the country in government service, academia, and industry. The common thread running throughout this national fabric is high performance computing. In large measure, the work represented by these stories could not have been accomplished without the significant investments made in high performance computing hardware, software, and networking. These stories are a tribute, and in some sense a validation, of this investment.

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Design of an Advanced Submarine Sail

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With submarine operations shifting to littoral missions, there is an increased desire for new systems that improve littoral warfare effectiveness, and designs that will allow flexibility for mission-specific reconfiguration and rapid insertion of new technologies. Candidate systems under consideration include countermeasure enhancements, high data rate antennas, unmanned underwater vehicles, littoral warfare weapons, advanced buoyant cable antennas, and Special Operating Forces stowage, among others. Conventional sails with their low drag and low volumes cannot accommodate these systems. A new sail shape, with up to four times the volume, is necessary to enclose such new systems. This new sail, which has a dual curved canopy-like shape, has already been tested on the US Navy's Large Scale Vehicle (Figure 1) with plans for eventual insertion on the Virginia Class submarine.

Limited Experimental Data

This sail shape is a radical new design for the US Navy. There is no historical database to use as a reference for its design. Traditionally, designing such a new shape requires a whole series of tests. Large numbers of variants are built, tested, and evaluated encompassing both large and small changes. A variety of concepts are also explored. Additionally, design decisions are frequently based on limited amounts of experimental data of a large number of geometries.

Impacting Design Decisions

HPC environments bring a computational-based approach to addressing such designs. Many shapes can be evaluated computationally so that only a few candidate shapes are actually built and tested, saving money. Computational studies can be conducted in a timely manner, saving time in the design cycle over the traditional build and test procedure. It is only with the large, parallel, HPC resources available in the last several years that such computations can be done to sufficient accuracy and speed to impact design decisions in both the preliminary and final stages.

Unlike traditional experimental data, which supplies limited amounts of data and information, the whole flow field can be studied using HPC resources and a computational based approach. This analysis showed that large vortical flow structures were being developed from the early sail designs, causing a large impact on the propulsor inflow. It was possible to modify the sail shapes to reduce this impact on the propulsor inflow once the vortical structures phenomena was better understood.

> "High performance computing allows many shapes to be evaluated computationally so that only a few candidate shapes are actually built and tested, saving money. Another aspect of this is the timely manner in which it is now possible to do computational studies saving time in the design cycle over the traditional build and test procedure."

Figure 1. Advanced sail installed on the US Navy's large scale vehicle

Scientific visualization has been used to help understand the vortical flow created by the large sails. The visualization was used to help identify how the vortices are formed around the sail and then flow downstream into the propulsor. A better understanding of how these vortices are formed has led to better ideas of how to minimize them in the redesign effort.

Better Designs in Shorter Time

Over the last decade, there has been an increased emphasis on the use of computational tools to evaluate submarine flows and guide their design. With the advent of parallel computational capabilities, viscous simulations have seen a larger role in predicting these flow fields. The shift to a more computational based design and analysis approach leads to the possibility of better designs in a shorter amount of time. Such computations allow for the rank ordering of designs as well as providing the entire flow field, which can lead to better understanding of the flow physics. In the current effort, modifications to candidate sail shapes were evaluated computationally providing drag differences as well as propulsor inflow. This allowed for the development of a new sail shape, which was built and tested on the US Navy's Large Scale Vehicle—with plans for future implementation on the Virginia class of submarines. Such computations provide a cost effective way to evaluate various shapes that may improve a design. In this way, computations are reducing many design-oriented tests. Future efforts need to include full propulsor modeling as part of the calculations. As requirements become stricter, future design efforts will be more sophisticated involving maneuvering as well as more complicated operating scenarios. This will require large computer resources, as it will be extremely difficult if not impossible to perform such evaluations experimentally.

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CTA: Computational Fluid Dynamics
Computer Resources: Cray T3E [ARSC]

Penetration into Deeply Buried Structures: A Coupled Computational Methodology

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The ARL scientists, working through the CHSSI, are developing an end-to-end simulation capability to simulate complex projectile-target interaction applications. This work will accelerate the fielding of new weapon systems, improve armor technologies, and enhance protective structures technology. Simulation of penetration into deeply buried structures is the primary targeted application area.

"These preliminary results and coupled computational environment show promise for applicability to a wide class of penetration-target applications and practical applications for fielding new weapon systems, improving armor technologies, and enhancing protective structures technologies."

Solving Individual Discipline Areas

Typically, penetration into deeply buried structures involves solving two coupled physics applications: one application is associated with addressing the modeling and simulation of the penetrator; the other application is associated with the modeling and simulation of deeply buried structures. Most of the earlier efforts were confined to solving the individual discipline areas because of the application's complexity and computer resource limitations. Simulating the complex projectile-target interaction in a seamless, coupled, or interdisciplinary environment requires increased use of HPC resources.

Fully Coupling the Discipline Areas

Penetration into deeply buried structures addresses development of a scalable-coupled Eulerian-Lagrangian approach for a wide class of penetration-target applications in the areas of weapon performance, weapons effects, and performance and defeat of targets. This class is represented by problems involving high-pressure, high-strain, and/or high-strain-rate material interactions, where one or more of the material regions undergoes relatively small deformations, while the other materials in the problem undergo arbitrarily large deformations. The penetration into earth problem is a good example of this, where the penetrator remains essentially elastic, while the target can undergo very large strains and deformations in the region of interaction with the penetrator (Figure 1). Nevertheless, deformation of the penetrator can often have a strong influence on the loading exerted on it by the target. Thus, a fully coupled treatment of the penetrator/target interactions and deformations is required for these applications.

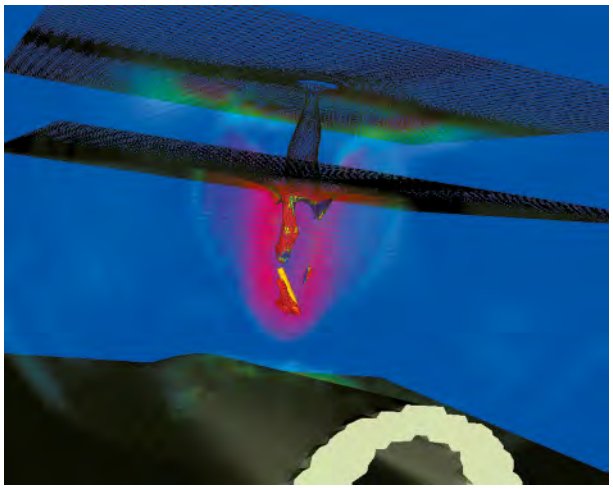

Figure 1. Penetrator traveling through two different layers of soil material towards a deeply buried structure

Simulations were performed of the large deformation response of a complex buried structure to the penetrator. A buried structure using two different layers of clay and concrete was modeled using shock physics software. The penetrator was modeled with all the details using large deformation

finite element structural analysis software. The coupled simulations showed good scalability and the results showed good qualitative agreement. These preliminary results and coupled computational environment show promise for applicability to a wide class of penetration-target applications and practical applications for fielding new weapon systems, improving armor technologies, and enhancing protective structures technologies.

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CTA: Computational Structural Mechanics
Computer Resources: SGI Origin 3000 [ARL]

Development of a High-Fidelity Nonlinear Aeroelastic Solver

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Correct prediction of the aeroelastic behavior of current and future air vehicles remains a challenge for the Air Force. The revolutionary concepts being proposed for a new UAV that will be required to operate under extreme flight conditions magnify the problem. These new systems may also incorporate new lightweight composites or have wing designs that are routinely subjected to large deflections during their operation. A high-fidelity simulation capability is required to accurately model the complex, nonlinear physical phenomena involved in these types of aircraft. New generations of multidisciplinary computational tools that couple highly accurate CFD solvers with computational structural dynamics modules are required. The incorporation of these types of computational techniques into DoD weapons programs promises cost and development time savings as well as improved operational performance.

Linear Aerodynamic Techniques

Traditional aeroelastic analysis has coupled linear aerodynamic techniques such as vortex lattice and panel methods with linear modal techniques for the structural model. These techniques have been preferred due to their ease in implementation and rapid solution times. While these simplified analysis tools have been used extensively, they often fail to predict detrimental aeroelastic phenomena since they ignore important nonlinear physical features of the problem. The simplified aerodynamic models cannot address such critical issues as transition, turbulence, separation, buffet, and transonic shocks. The linear modal structural models are limited to small amplitude responses and linear material properties.

New Nonlinear Aeroelastic Solver

The computational power available through the HPCMP now allows higher fidelity modeling to be brought to bear on the problem of simulating aeroelastic response. Specifically, CFD solvers may replace linear aerodynamic models for the nonlinear Euler and Navier-Stokes equations. Nonlinear structural models employing finite difference and finite element techniques may be used to represent the structural response. Coupling of these enhanced techniques provides a powerful new nonlinear, aeroelastic simulation tool that can address challenging fluid-structure interaction problems such as limit-cycle oscillations, tail buffet, and transition delay and drag reduction via compliant surfaces.

By exploiting the computer power available through the HPCMP, the present work seeks to overcome the deficiencies in current aeroelastic methods by developing a new fully nonlinear aeroelastic solver. In this new procedure, a higher order (2 to 3 times more accurate than many existing CFD codes), unsteady, 3-D Navier-Stokes code is used to simulate the aerodynamics of the problem. The structural dynamics are simulated using nonlinear finite difference and finite element models. These independent solvers are coupled in a synchronized fashion to provide a powerful new nonlinear aeroelastic tool, which has been applied to several problems that could not previously be simulated with classical linear techniques.

> "The revolutionary concepts being proposed for a new UAV that will be required to operate under extreme flight conditions magnify the problem."

One problem considered is the direct numerical simulation of the interaction of a transitional boundary layer flow with a flexible panel for both subsonic and transonic flow speeds (Figure 1). At the higher flow

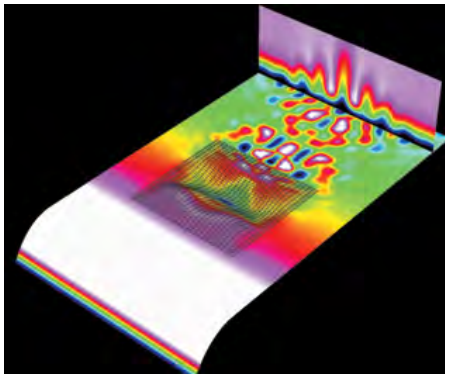

Figure 1. 3-D panel flutter due to interaction with a transitional boundary layer

speed, a traveling wave flutter phenomena occurs that originates from the coupling of the transitional Tollmien-Schlichting waves in the boundary layer with higher-mode flexural waves in the elastic panel. This results in significant acoustic radiation above the fluttering panel (Figure 2). The highly refined meshes (up to 15 million grid points) and long time histories (500,000 time steps) required to accurately compute this problem demand the use of the most powerful computing platforms available to successfully complete this simulation.

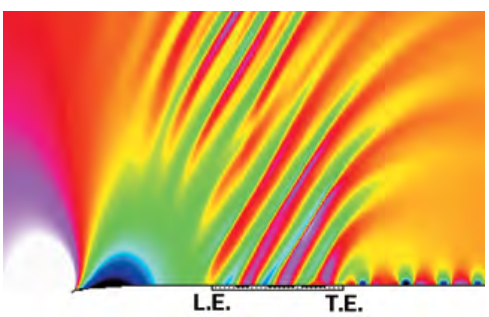

Figure 2. Acoustic radiation due to travelling wave flutter of a flexible panel

This unique nonlinear aeroelastic tool has also successfully captured the proper limit cycle behavior of a delta wing. Previous computations using linear structural models over predicted by four to five times the amplitude of the experimentally measured limit cycle response of the delta wing. The inability of the linear structural models to simulate the actual nonlinear structural mechanisms in the problem was identified as the cause of this discrepancy. The present nonlinear structural techniques accurately capture the correct amplitude and frequency of the delta wing limit-cycle oscillation (Figure 3).

A novel, fully nonlinear, aeroelastic solver has been developed, which exploits the extensive computing capacity of the HPCMP. The ability of this new tool to address fluid-structure interaction problems that cannot be computed with current linear aeroelastic techniques has been demonstrated. This high-fidelity simulation capability may now be exploited to enhance the development of current and future manned and unmanned air vehicles.

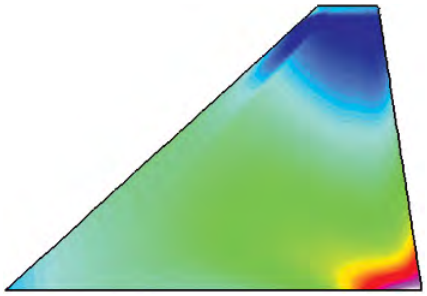

Figure 3. Stress developed in a delta wing at the point of maximum deflection in the limit cycle response

Detecting and Explaining Relevant Flow Features

The ability to effectively visualize the computed results for the complex physical problems considered in this work is essential in order to develop a complete understanding of the problem being simulated. The massive amounts of information produced by these high-fidelity computations may not be exploited without resorting extensively to scientific visualization. Three-dimensional visualizations of the resulting flowfields have been used to detect and explain relevant flow features critical to the analysis of the physical phenomena being investigated. Furthermore, the dynamic nature of these problems could not be discerned without the production of animations of the unsteady computed results. Without the ability to produce these types of scientific visualizations, a complete interpretation of these costly simulations would not be possible and much of the computational effort would be wasted.

Developing a New Nonlinear Aeroelastic Computational Capability

Present computational capabilities employed to analyze and predict the aeroelastic behavior of current and future Air Force vehicles rely almost exclusively on linear aerodynamic and structural models. These simplified models fail to predict many detrimental aeroelastic phenomena since they ignore important nonlinear physical features inherent to the problem. The present research focuses on developing a new, nonlinear aeroelastic computational capability to overcome these

deficiencies. Exploitation of this new computational capability earlier in vehicle design and development will provide a means to predict adverse fluid/structure interaction problems before the flight test and manufacture phase when redesign of the vehicle is costly. This can provide significant cost and development-time savings to an air vehicle program. This type of computational tool will also allow for a more rational design of future UAVs, which will be required to operate in extreme flight conditions where nonlinear aeroelastic phenomena will be prevalent.

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CTA: Computational Fluid Dynamics
Computer Resources: Cray SV1 [ARSC, NAVO]

Novel Energetic Material Development Using Molecular Simulation

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Advances in defense weaponry often require the development of new energetic materials. These technological advances often outpace the energetic material development process, however, not allowing for the complete utilization of the new weapons platforms. It is critical that the process of developing high-performance energetic materials be optimized to meet the needs of these innovative applications. Modeling and simulation must be used in the development process where possible, eliminating the traditional costly and time-consuming approaches of formulation and experimentation. With this goal in mind, researchers at ARL have recently developed a computational tool for assessing the detonation performance of new energetic materials.

Early Models Lacked Predictive Capabilities

Historically, theoretical models parameterized to experimental data were used in simulations to aid in analyses of experiments. The models were heavily dependent on measurements before high performance computing. For such models, predictive capabilities were extremely limited. They lacked the means of discerning whether discrepancies between the theoretical predictions and the experimental measurements were a result of an inadequate model or an inaccurate theory.

The Role of the New Computational Tool

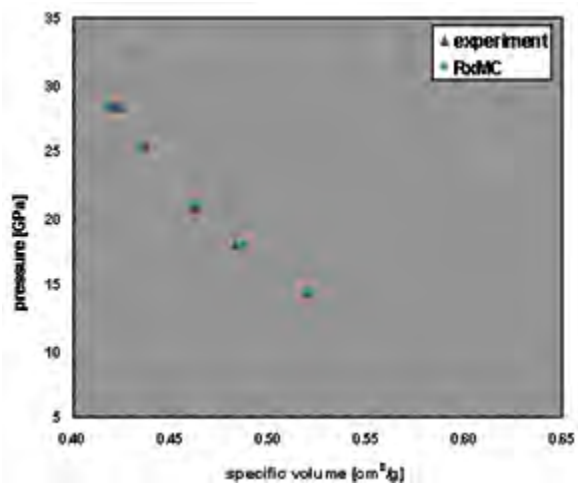
The role of this method in the development process is two-fold. First, the method can be used to provide the fundamental understanding of energetic materials necessary for exploitation in the weapons system. Second, the method can be used to screen candidate notional materials immediately, substantially impacting time and financial considerations. This computational tool can also be used to meet the demands of advancing weapons technology that requires nano-structured energetic materials. As defense weapons technology and engineering continues to grow past the current understanding of the microscopic-level phenomena, the implementation of this tool will continue to fill in existing knowledge gaps.

To date the computational tool, exercised using the resources of the ARL MSRC, has allowed successful prediction of the detonation properties for several simple systems. With the advances in modern theoretical chemical modeling methods, highly scalable software, and parallel computer architectures, more elaborate, accurate, and predictive atomistic simulations are being performed that provide information about energetic materials that is not amenable to direct experimental observation.

"This computational tool can also be used to meet the demands of advancing weapons technology that requires nano-structured energetic materials. As defense weapons technology and engineering continues to grow past the current understanding of the microscopic-level phenomena, the implementation of this tool will continue to fill in existing knowledge gaps."

More Realistic and Complex Systems Simulated

Future research objectives are to simulate more realistic and complex systems, which can only be implemented through the use of resources supplied through the HPCMP. The calculation of detonation properties requires a multitude of simulations at a variety of temperatures and pressures, with each simulation requiring millions of computations for systems containing tens of thousands of atoms. As a result, the calculation of the detonation properties of



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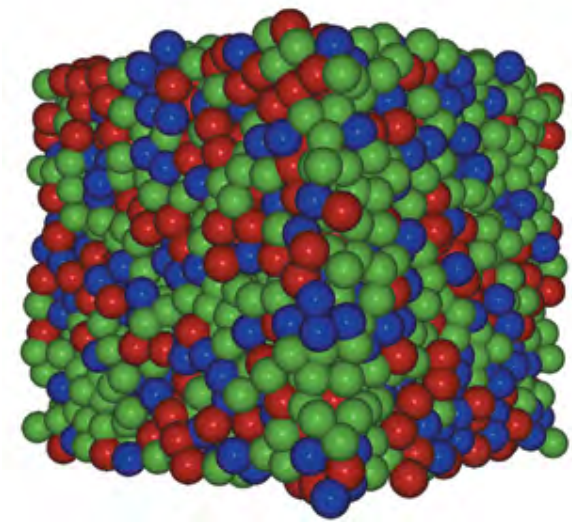

(b)

Figure 1. Application of the Reactive Monte Carlo (RxMC) method to the detonation of nitric oxide ($2NO <=> N_2 + O_2$): (a) Detonation properties of NO; (b) Molecular configuration snapshot of reacting system at P=28.47 GPa (blue: N_2 molecules; red: O_2 molecules; green: NO molecules)

a single energetic material might require several CPU weeks. The resources available through the HPCMP have enabled the evaluation of detonation properties using the atomistic modeling technique.

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CTA: Computational Chemistry and Materials Science
Computer Resources: SGI Origin 2000, SGI Origin 3000, and IBM SP3 [ARL]

Relationship Between Local Structure and Phase Transitions of a Disordered Solid Solution

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Sponsor: Office of Naval Research (ONR), Arlington, VA

Ferroelectric (FE) materials have a wide range of applications, from the nonvolatile memory modules in computers to piezoelectric transducers. In particular, lead zirconate titanate (PZT) exhibits a large piezoelectric effect, making PZT the primary active material in naval Sound Navigation and Ranging (SONAR) devices, medical ultrasound systems, and many other important applications. PZT is piezoelectric — this means that it converts tiny underwater pressure waves to electrical signals, or vice versa. The Navy needs to understand PZT so that it can develop new materials with even better properties. The next-generation piezoelectric materials need to be more sensitive to small signals, more durable, and lighter.

Due to its technological importance, PZT has been extensively studied both theoretically with quantum mechanical studies of small supercells and experimentally with methods such as neutron scattering and X-ray diffraction. PZT assumes the ABO_3 perovskite structure, (Figure 1). However, the disorder in the B-cation arrangement makes small, density functional theory (DFT)-accessible supercells only an approximate model of the real material. Experimental methods only probe the ensemble average properties of the material. All phases of PZT have extremely similar experimental pair distribution functions (PDFs), indicating similar local structure despite different macroscopic properties.

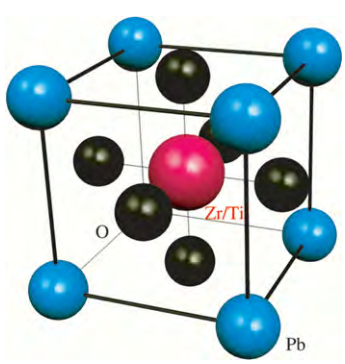

Figure 1. ABO_3 perovskite structure

Thus the relationship between the local structure of the material and its superior properties is not clear.

Using Supercell Calculations to Study Chemical Composition

The focus of the work has been the use of large, many atom supercell calculations to study the relationships between chemical composition, disorder, and piezoelectricity in complex oxide $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) solid solutions not accessed with previous small quantum mechanical calculations. Supercells of PZT that are four to eight times larger than previous calculations were investigated. The large size and the variety of the supercells studied allowed probing of the effect of various atomic arrangements on the structure of the material, something impossible to do with the ordered cells used in previous studies.

"The properties which make PZT effective also make it complicated to model. The extensive resources of the HPCMP enable us to model large enough regions of the PZT so that we can understand how disorder affects the SONAR capabilities of PZT."

Although there are differences in the macroscopic phases and polarization of various compositions of PZT, there are many similarities within the local structure of each composition. The direction of lead atom distortions in PZT governs the orientation of the polarization and therefore the high piezoelectric response, which gives PZT its excellent SONAR properties.

In the calculations, lead atoms mostly make tetragonal (aligned with the x-axis) and orthorhombic (with non-zero components along x and y, or x and z axis) displacements. The distortions are toward titanium (Ti) neighbors and away from zirconium (Zr) neighbors, conforming to the overall polarization as

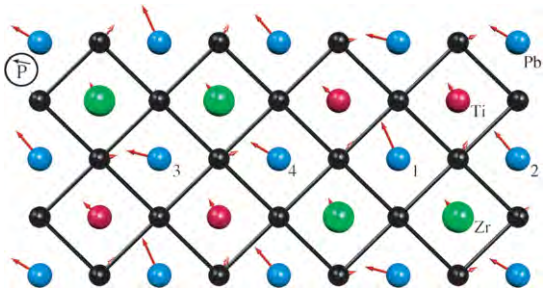

Figure 2. Projection of the 4 × 2 × 1 50/50 supercell DFT PZT structure on the xy plane. The oxygen octahedra are depicted by diamonds, and distortions from the ideal cubic perovskite positions are shown by arrows. Black for O, blue for Pb, green for Zr and red for Ti. Pb atoms are 1/2 unit cell above the plane and apical O atoms are left out.

much as possible. Both preferences are understandable. Zr is a larger ion than Ti, which means that the purely repulsive interaction between Pb and B cations will be stronger for Pb-Zr than for Pb-Ti. The conformity to overall direction of polarization is due to simple electrostatics, which make dipole alignment favorable. In the case of Pb atoms 1 and 2 in Figure 2, both driving forces can be satisfied. However, in the case of Pb atoms 3 and 4, the local preference to move toward Ti conflicts with the desire to align with the overall polarization. This competition results in a compromise, with distortions predominantly along the x-direction for these Pb atoms.

The dependence of Pb distortion direction on the local environment and overall polarization is particularly important, as it is responsible for the compositional transitions in PZT. In the Ti-rich phase, due to the abundance of Ti ions, a tetragonal displacement satisfies the local repulsion energy preferences for the majority of Pb atoms. This can be seen from the angular distribution of the Pb distortions (Figure 3). The Ti-rich composition of PZT has no Pb distortions with more than a 15-degree deviation away from the tetragonal ferroelectric direction. The small scatter in the direction of Pb off centering gives rise to a fairly ordered phase with large overall polarization along the x-axis. On the other hand, in the Zr-rich phase, Ti ion scarcity means that no single direction can satisfy the local energy preferences of all or even most of the Pb atoms. Consequently, the Pb displacement angles are more broadly distributed between 30 and 80 degrees away from the x-axis.

As a result of the disorder in the direction of Pb displacements, the magnitude of the overall polarization is smaller for the rhombohedral phase than that of the tetragonal phase. The monoclinic phase is the bridge between the rhombohedral and the tetragonal phases. While many Pb ions can satisfy their local energy preferences by making a tetragonal distortion, other Pb ions cannot. The displacement of the latter Pb ions will therefore contain significant y-axis and z-axis components, producing the overall polarization of the monoclinic phase.

Development of a Model That Will Allow Study of Disordered Systems

Crystal chemistry (where atoms are regarded as possessing properties transferable between various environments) provides an intuitive understanding of how the atomic composition affects the structure and the material behavior, closing the gap between the small unit cells available to first-principles theorists and real disordered materials with complex B-cation arrangements. The results of the DFT calculations firmly establish the validity and the accuracy of the crystal chemistry approach by revealing the distinction between intrinsic and the environment-dependent behavioral motifs in the material and correlating the structural motifs with the local environment for each of the constituent atoms.

The existence of intrinsic atomic behaviors makes it possible to extract a simple intuitive framework, which explains both the DFT results and the macroscopic compositional phase transitions. This framework can then be made quantitative by encapsulating the chemical interactions in a phenomenological, crystal chemistry type model using well-known formalisms to characterize electrostatic and bonding interactions. This model would contain only physically intuitive interactions, could be applied to any perovskite material, and would lend itself naturally to materials design.

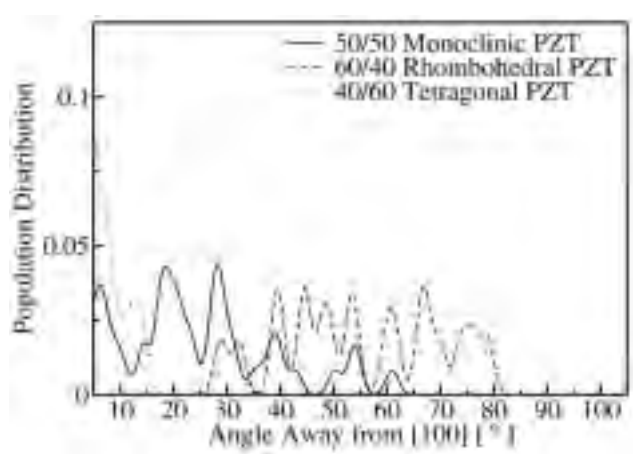

Figure 3. Distribution of Pb distortion angle away from tetragonal direction for the rhombohedral, monoclinic and tetragonal phases of PZT

Such first-principles based, crystal-chemical modeling will enable the design of materials with desired macroscopic properties by relating the variations in atomic composition of the material to its macroscopic behavior.

The properties which make PZT effective also make it complicated to model. PZT is $Pb(Zr_{1-x}Ti_x)O_3$, and the disordered positions of the Ti and Zr atoms are directly related to the piezoelectricity. The extensive resources of the HPCMP enable researchers to model large enough regions of the PZT so that we can understand how disorder affects the SONAR capabilities of PZT. The plan is to extend this development to the design of the new piezoelectric materials for future Naval SONAR needs.

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CTA: Computational Chemistry and Materials Science
Computer Resources: SGI Origin 3000 [ERDC]

Polymer Modeling for Smart Munitions Electronics

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Novel materials to aid and promote the adhesion and survivability of aerodynamic measurement apparatus in the extreme operating conditions of gun launched munitions would be beneficial for improved munitions performance and ultimately improved weapon lethality. The goal of this project was to employ quantum mechanical molecular modeling and quantitative structure-property relationships methods and to design and guide the synthesis of novel epoxy resins with enhanced shock absorption properties for use as adhesives in smart munitions electronics.

Predicting Bulk Polymer Properties

Quantitative Structure-Property Relationships (QSPRs), based on molecular properties calculated using the AM1 semiempirical quantum mechanical method, have been developed to predict bulk polymer properties without the need for costly and time-consuming experimentation. A QSPR model was generated for complex cross-linked copolymers, using the regression analysis program, COmprehensive DEscriptors for Structural and Statistical Analysis (CODESSA). By applying an ad hoc treatment based on elementary probability theory to the QSPR analysis, the ARL scientists developed a method for computing bulk polymer glass transition temperatures for stoichiometric and non-stoichiometric monomeric formulations. A model polymer — that represents potentially ideal properties that can be achieved experimentally — was synthesized and found to validate the specific initial model predictions and in general the computational approach.

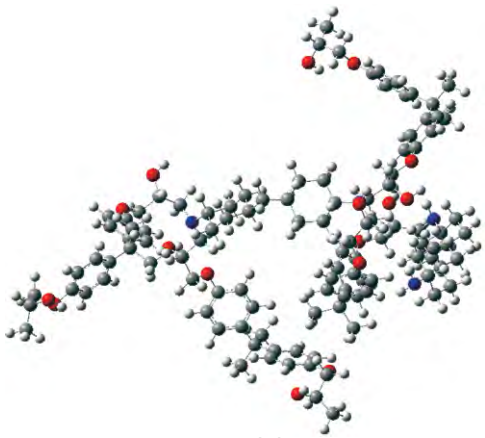
Glass Transition Temperature for Polymers

The model was used to predict the glass transition temperature for a series of polymers composed of the widely used epoxide, diglycidyl ether of bisphenol A, cured with an aliphatic or aromatic amine curing agent, all having a stoichiometric formulation of reactive functional groups. The experimental data for the glass transition temperature QSPR analysis was obtained from published literature sources. The experimental data used to validate the non-stoichiometric glass transition temperature predictions was obtained at ARL. For 13 polymers, a designer correlation equation having a coefficient of determination (R^2) of 0.9977 was obtained using four computed molecular properties. The molecular properties describe the propensity for intermolecular attractions and stiffness of backbone atoms of the model polymer systems. Fundamentally, it is known that stoichiometric formulations of amine-cured epoxy resins give maximal glass transition temperature values and that for non-stoichiometric formulations the glass transition temperature decreases in a manner dependent on the extent of cross-linking in the polymer, which in turn, is dependent on the stoichiometric ratio of amine and epoxide functional groups. By applying a treatment based on elementary probability theory to molecular models, each representing a different level of cross-linking, the trend in experimental glass transition temperatures for non-stoichiometric formulations was accurately predicted (Figure 1).

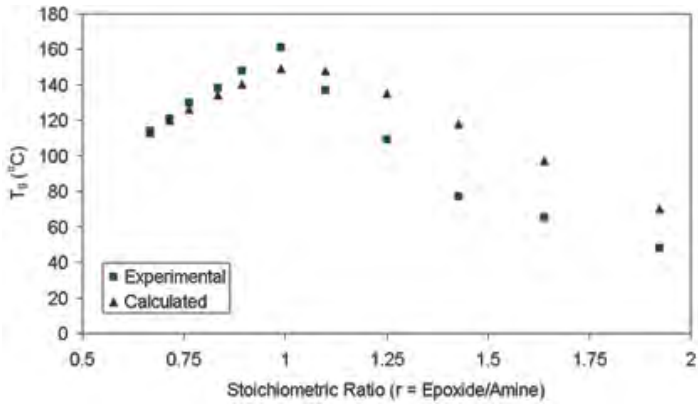
> "Quantitative Structure-Property Relationships (QSPRs) have been developed to predict bulk polymer properties without the need for costly and time-consuming experimentation."

Benefits of the Quantitative Structure-Property Relationships

Two principle benefits are envisioned. First is a revolutionary tool to rapidly design and develop polymer materials using robust computational methods to keep pace with the timeline requirements dictated by the FCS and the Objective Force Warrior by avoiding the need for extensive synthesis and



(a)



(b)

Figure 1. a) Sample polymer structure used in prediction of glass transition temperatures for non-stoichiometric formulations. b) Plot of experimental and predicted glass transition temperatures vs. stoichiometric ratio for non-stoichiometric polymer formulations.

testing. The second benefit is significantly enhanced survivability and reliability of electronic components for smart munitions that will be enabled by the newly developed polymer packaging materials.

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CTA: Computational Chemistry and Materials Science

Computer Resources: SGI Origin 2000 and SGI Origin 3000[ARL]

Dynamics of Oxidation of Metallic Nanoparticles

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DoD researchers are reducing the size of reactant particles such as aluminum (Al) to accelerate the burn rates of propellant and explosives. Microscopic understanding of the structure and mechanical properties of encapsulated Al nanoparticles will have significant impacts on the design of high energy density materials.

In recent years, there has been a great deal of interest in the synthesis of nanostructured composites consisting of metallic nanoparticles coated with a protective layer. Such nanocomposites have mixed metallic and ceramic properties such as high electric conductivity and high-temperature stability. The objective of this research is to investigate the oxidation, structure, thermodynamics, and mechanical properties of these encapsulated nanoparticles at high temperatures under high pressures.

Studying the Chemical Bonding between Dissimilar Materials

Interfaces between soft/ductile materials (metals or polymers) and hard surfaces (metal oxides or ceramics) dominate many properties of composite materials and coatings. The present variable-charge molecular dynamics (VCMD) study of the oxidation of metallic nanoparticles paves a way to atomistic investigations of how chemical bonding between dissimilar materials at the atomic level determines macroscopic properties such as structure, adhesion, friction, stiffness, and fracture toughness.

New Algorithm Developed for VCMD Scheme

To describe chemical reactions such as oxidation, the VCMD scheme developed by Streitz and Mintmire was employed in which atomic charges are determined at every time step to equalize electronegativity. This variable N-charge problem amounts to solving a dense linear system, and its solution typically requires $O(N_3)$ operations.

"Recent advances in parallel computing have made it possible for scientists to perform atomistic simulations of materials involving billions of atoms."

To perform multimillion-atom VCMD simulations on massively parallel computers, an O(N) algorithm was developed in which the fast multipole method by Greengard and Rokhlin was used to operate matrix-vector multiplications in O(N) time and the temporal locality was used by initializing the iterative solution with the previous time step's charges. To further accelerate the convergence, a multilevel preconditioning scheme was developed by splitting the Coulomb interaction matrix into short- and long-range components and using the sparse short-range matrix as a preconditioner. This algorithm was incorporated into a suite of scalable parallel molecular dynamics algorithms.

VCMD Provides Detailed Picture

The VCMD scheme was successfully used to study the oxidation dynamics of an aluminum nanoparticle (diameter 200 angstrom). The VCMD simulations provide a detailed picture of the rapid evolution and culmination of the surface oxide thickness, local stresses, and atomic diffusivities. The VCMD simulations reveal that an aluminum nanoparticle in an oxygen-rich environment goes through a rapid three-step process culminating in a stable oxide scale: i) Dissociation of oxygen molecules and the diffusion of oxygen atoms into octahedral and subsequently into tetrahedral sites in the nanoparticle; ii) radial diffusion of aluminum and oxygen atoms and the formation of isolated clusters of corner-sharing and edge-sharing OAl_4 tetrahedra; and iii) coalescence of OAl_4 clusters to form a neutral, percolating tetrahedral network that impedes further intrusion of oxygen atoms into and of Al atoms out of the nanoparticle. Structural analysis reveals a 40

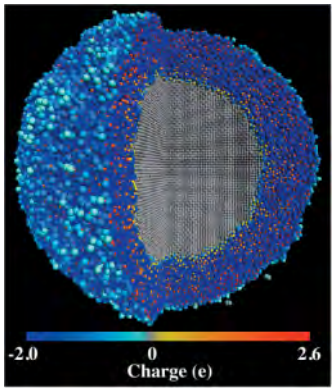

Figure 1. Snapshot of an Al nanoparticle after 466ps of simulation time. (A quarter of the system is cut out to show the aluminum/aluminum-oxide interface.) The larger spheres correspond to oxygen and smaller spheres to aluminum; color represents the sign and magnitude of the charge on an atom.

angstrom thick amorphous oxide scale on the Al nanoparticle (see Figure 1).

Recent advances in parallel computing have made it possible for scientists to perform atomistic simulations of materials involving billions of atoms. However rendering such large datasets with an interactive speed is a major challenge. To solve this problem, a visualization system incorporating parallel and distributed computing paradigms has been developed. This system named Atomsviewer uses a parallelized, fast visibility-culling algorithm based on the octree data structure to reduce the number of atoms sent to the graphics pipeline.

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CTA: Computational Chemistry and Materials Science
Computer Resources: IBM SP3 and Cray T3E [NAVO]

SHAMRC Environment and Vehicle Loads Calculations in Non-Ideal Flow

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High performance computing resources have enabled scientists and engineers to perform high fidelity computational fluid dynamics calculations in support of the DTRA Non-Ideal Air Blast (NIAB) program. The NIAB program seeks to quantify the effects of NIAB on military vehicles over a wide range of geographical areas and scenarios. Of particular interest is the ability to simulate computationally the environment and vehicle loads from the exit jet produced by the DTRA Large Blast and Thermal Simulator (LB/TS).

The goal of this project is the simulation of environment and vehicle loads caused by non-ideal airblasts. The ERDC scientific visualization team was presented with the challenge of providing a visualization methodology and toolset. The visualization needs of this project had outstripped the capabilities of the commercial-off-the-shelf tools originally used as the size and sophistication of the computational simulations grew. The Scientific Visualization Center (SVC) team studied the alternatives in view of the growing requirements, and developed a new approach that leveraged the research team's existing investment in a previously developed OpenGL-based visualization application. After collaborating with the research team on enhancements to the visualization code, the SVC team was able to deliver a tool that enabled analysis of the team's data in terms of vehicle and environment loads and the dust entrainment resulting from a blast.

The Code

Second-order Hydrodynamic Automatic Mesh Refinement Code (SHAMRC) — pronounced shamrock — is a two- and three-dimensional, finite difference, hydrodynamic computer code. SHAMRC is a descendant of SHARC (Second-order Hydrodynamic Advanced Research Code). It is used to solve a variety of airblast related problems which include high explosive (HE) detonations, nuclear explosive (NE) detonations, structure loading, thermal effects on airblast, cloud rise, conventional munitions blast and fragmentation, shock tube phenomenology, dust and debris dispersion, and atmospheric shock propagation.

> "SHAMRC is used to solve a variety of airblast related problems which include high explosive (HE) detonations, nuclear explosive (NE) detonations, structure loading, thermal effects on airblast, cloud rise, conventional munitions blast and fragmentation, shock tube phenomenology, dust and debris dispersion, and atmospheric shock propagation."

SHAMRC's capabilities and attributes include multiple geometries, non-responsive structures, non-interactive and interactive particles, several atmosphere models, multi-materials, a large material library, HE detonations, a K-ε turbulence model, and water and dust vaporization. SHAMRC is second-order accurate in both space and time and is fully conservative of mass, momentum, and energy. It is fast because it employs a structured Eulerian grid and it is efficient due to the use of the pre-processor source library. SHAMRC is a production research code that currently has the capability to run in single-grid mode or with an adaptive mesh refinement (AMR), both of which have been parallelized to take advantage of the rapidly developing hardware improvements, and ensure the viability of the code. The AMR capability of SHAMRC allows the efficient calculation of certain classes of problems that are otherwise intractable using the conventional single-grid method.

SHAMRC has been parallelized to run on large scalable parallel platforms. It uses the Message Passing Interface library to achieve parallelism. Initial versions of the code were parallelized in 3-D only and the Eulerian grid was decomposed in only one

dimension. The calculations used this parallel model. Since that time, the code has been modified to perform automatic domain decomposition on the Eulerian grid in up to three dimensions for both the 2-D and 3-D versions of the code. The parallel version of SHAMRC has been tested on several parallel platforms

There are several examples of the effects of using these new codes. Figure 1 shows airblast loads on an M110-A2 self-propelled howitzer located in the test section exterior to the LB/TS. The surface is colored by the pressure from the blast wave. Figure 2 is a close-up of the howitzer. Figure 3 is a wider view of the howitzer on the test platform at the same calculational time. Both images show the interaction of the dust with the vehicle. The presence of the dust significantly modifies the airblast environment and the loads on the vehicle.

CTA: Computational Fluid Dynamics
Computer Resources: SGI Origin 3000 [ERDC]

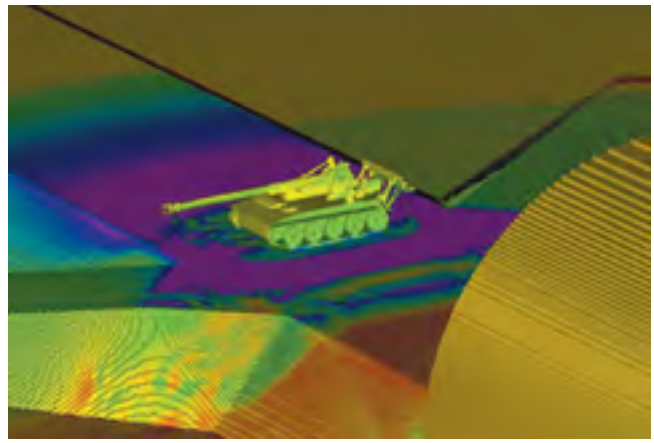

Figure 1. Isosurface of dust density interaction with the M110-A2 self-propelled howitzer

Figure 2. Isosurface of energy interacting with M110-A2 self-propelled howitzer

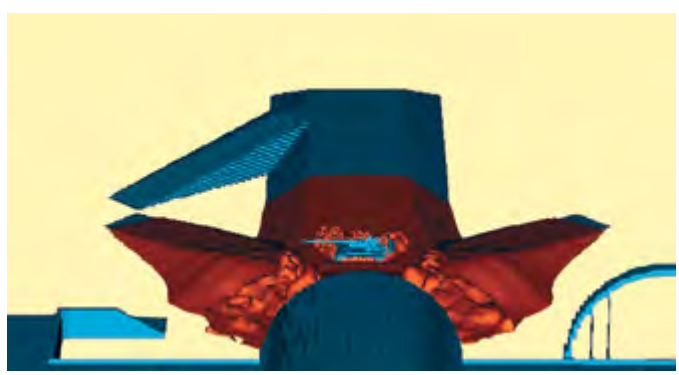

Figure 3. Wide-angle view of isosurface of dust denisty interacting with M110-A2 self-propelled howitzer

Modeling Explosions in Buried Chambers and Tunnel Systems

John Bell, Marc Day, Allen Kuhl, and Charles Rendleman
Defense Threat Reduction Agency (DTRA), Alexandria, VA

Countering the proliferation of weapons of mass destruction (i.e., chemical, biological or nuclear weapons) is a critical mission area for DTRA. Assessment of explosion effects related to military scenarios provides important inputs to military strategy. For example, if an underground bunker filled with chemical/biological (C/B) weapons is attacked, DTRA must predict the consequences. Scientists must address issues like the evolution in space and time of the energy released during the explosion, the risk that the energy released will destroy the structure, the likelihood of C/B weapons breaching containment, and the possibility of destroying the agent from the high-temperature environment of the explosion. Other questions such as how much of the agent will be ejected from the bunker and how the agent is dispersed in the atmosphere (at what risk to civilians) must also be addressed.

> "HPC overcomes the traditional limitations by permitting the scientist to make predictions on the fate of chemical/biological agents using computational models rather than the more costly physical model experiments. The use of HPC allows DTRA researchers to assess different scenarios based on physics-based predictive modeling rather than relying on heuristic scaling laws and phenomenological models."

Scientists at DTRA are developing the computational tools required for detailed assessment of such explosions. By using the advanced computer architectures available in the DoD HPCMP, combined with sophisticated adaptive numerical methodology, it is now possible to perform detailed, end-to-end numerical simulations of the 3-D time-dependent explosion field.

Physical Modeling Time is Consuming

Traditionally, physical modeling, either in reduced scale laboratory settings or in full-scale field experiments, has been used to answer the questions. Such experiments are time consuming and expensive compared to the results that could be obtained using numerical simulations. Furthermore, experiments are difficult to instrument so high quality data is hard to obtain.

Computational Models Overcome Traditional Limitations

HPC is an enabling technology for the simulations that have been undertaken. Chemically reacting compressible flows are basically intractable in three dimensions without the capabilities provided by HPC systems. Typical models considered in the calculations involved 6 chemical species with 10–20 million computational zones.

HPC overcomes the traditional limitations by permitting the scientist to make predictions on the fate of C/B agents using computational models rather than the more costly physical model experiments. The use of HPC allows DTRA researchers to assess different scenarios based on physics-based predictive modeling rather than relying on heuristic scaling laws and phenomenological models.

HPC, as applied with high-order numerically accurate AMR simulations, has made it possible to provide predictions of the rate of combustion of C/B agents in a closed chamber (Figure 1). The results of the numerical simulations have been validated against physical scale model experiments. It is possible for the weapons effects specialist to evaluate numerically the influence of the size of the explosive charge, explosive placement, and C/B agent configuration.

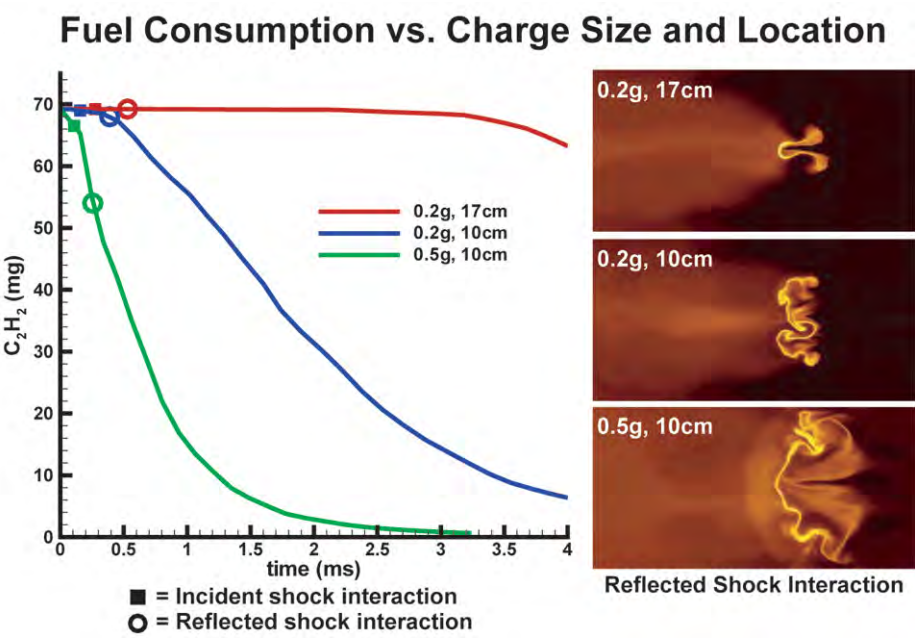

Figure 1. Simulated fuel consumption and temperature profiles for a series of small-scale (1:75) experiments used to model a single bay of the Dipole Jewel Test Field. In the experiments, a small explosive charge detonated inside a closed container induces turbulent mixing and shock-induced combustion of a surrogate for a biological agent. The resulting combustion characteristics depend strongly on the size of the explosion charge, and its proximity to the combustible material. The figure depicts typical time histories for three cases of varying charge size (0.2–0.5g) and separation distance (10–17mm). To the right, the temperature field is shown for the vertical midplane for the side of the vessel containing the combustible; at the instant that reflected blast waves interact with the fuel. When the detonation is far from the initial fuel, very little combustion is observed, even over long times. If the charge is closer, the incident blast wave induces sufficient turbulent mixing of the fuel and air and the waves reflected from the rear wall ignite the mixture. For stronger explosions, the incident shock initiates more vigorous volumetric combustion.

Scientific visualization is an important part of the work. The simulations result in large data sets containing the details of chemical and explosive reactions in complex, turbulent flow-fields. The only effective way to understand and extract information from this data is to use visualization tools.

Extending the Adaptive Mesh Refinement Modeling Software

The computations performed to date provide a compelling qualitative picture to explain the observations obtained during field experiments. Based on the successes achieved with the AMR modeling of confined explosions and the initial work with the simulation of thermobaric explosives, the DTRA scientists intend to extend the capabilities supported by the software. The extended version of the software will provide end-to-end simulation capabilities for the modeling of thermobaric explosive devices in chambers and tunnel complexes by adding the AMR solid-mechanics and low-Mach number reactive Navier-Stokes modeling capability to the present reactive Navier-Stokes software.

Future enhancements to the modeling package are intended to remove some of the limitations in the physical assumptions made in the simulations, for example, by including the effects of radiation in coupled equations of motion. Another improvement will provide for venting of the combustion and explosion products into the background environment in order to track and quantify the release of C/B materials. Finally, DTRA scientists will improve the simulations by examining other explosive agents, such as the new classes of thermobaric explosives.

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CTA: Computational Fluid Dynamics

Computer Resources: IBM SP3 [ARL] and Compaq Cluster [ERDC]

Seismic Propagation Modeling for Army Sensor Networks

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Comprehensive, reliable, situational information is imperative for the success of light-armor, maneuver dominated Future Combat System operations. Tactically significant terrain includes large-scale physiographic features such as forests, hills, passes, narrow valleys, or rivers. These complex battlefield environments are extremely difficult sensor settings. Opposing forces will adapt their counter operations to exploit poor sensor coverage circumstances. In these complex settings/contexts, passive seismic and acoustic Unattended Ground Sensors (UGSs) will provide unique non-line-of-sight (NLOS) and beyond-line-of-sight (BLOS) information under conditions that are poorly covered by air breathing or spaced based sensor platforms. The NLOS attribute is a result of readily "bending" signal wavefronts as they propagate through geologic and atmospheric media. Unfortunately, the inherent variability of terrain and meteorology also leads to large fluctuations in signal characteristics and consequently severe degradations in information accuracy and reliability. These environmental and terrain induced information degradations can be mitigated by deploying high population sensor networks, by calibrating each UGS node to its specific setting, and by fusing diverse sensor information with optimized algorithms.

In recent field trials, seismic sensors have demonstrated their applicability to target bearing, range, and classification problems at target ranges well over 1000 m. However, seismic sensors have, historically, not been heavily relied upon in practical tactical systems. This is largely due to the strong effects of geology on the character of seismic data and the highly variable, unknown geological characteristics of each deployment setting. Before seismic sensors can reach their full potential in fielded systems, methods must be developed that address the geologic variability issues. Geologic adaptation is the central demonstration for this project. The team also addressed the more general problem of how target-track data fusion for a large number (greater than 6) of spatially distributed UGS sensors can be done and the consequent improvement of tracking accuracy. Field demonstrations with comparable numbers of physical hardware are not anticipated for several more years and as a consequence, optimized UGS data-fusion methods have not been previously given. It is only through the use of high fidelity simulations that we are able to develop these new adaptation and tracking methods.

> "This capability supports the advanced sensor network systems envisioned for the Objective Force by demonstrating the target tracking and classification capabilities of seismic sensor networks for non-line-of-sight and beyond-line-of-sight situational awareness and by providing developers of tactical systems with a database of seismic signatures for a wide variety of geologic conditions."

Current Focus

The current focus of the modeling effort includes (1) simulations of armored tracked vehicles moving over open terrain with realistic topography and subsurface geology, (2) the effects of topography and geology on the vehicle signatures, (3) high-fidelity modeling of tracked vehicle dynamics and their track pad forces so that these forces can be used as inputs to seismic simulations, and (4) accuracy validation by comparisons with field test data. Because tracked vehicles generate target-specific seismic signatures at ranges of roughly 1 km, models on the scale of 1

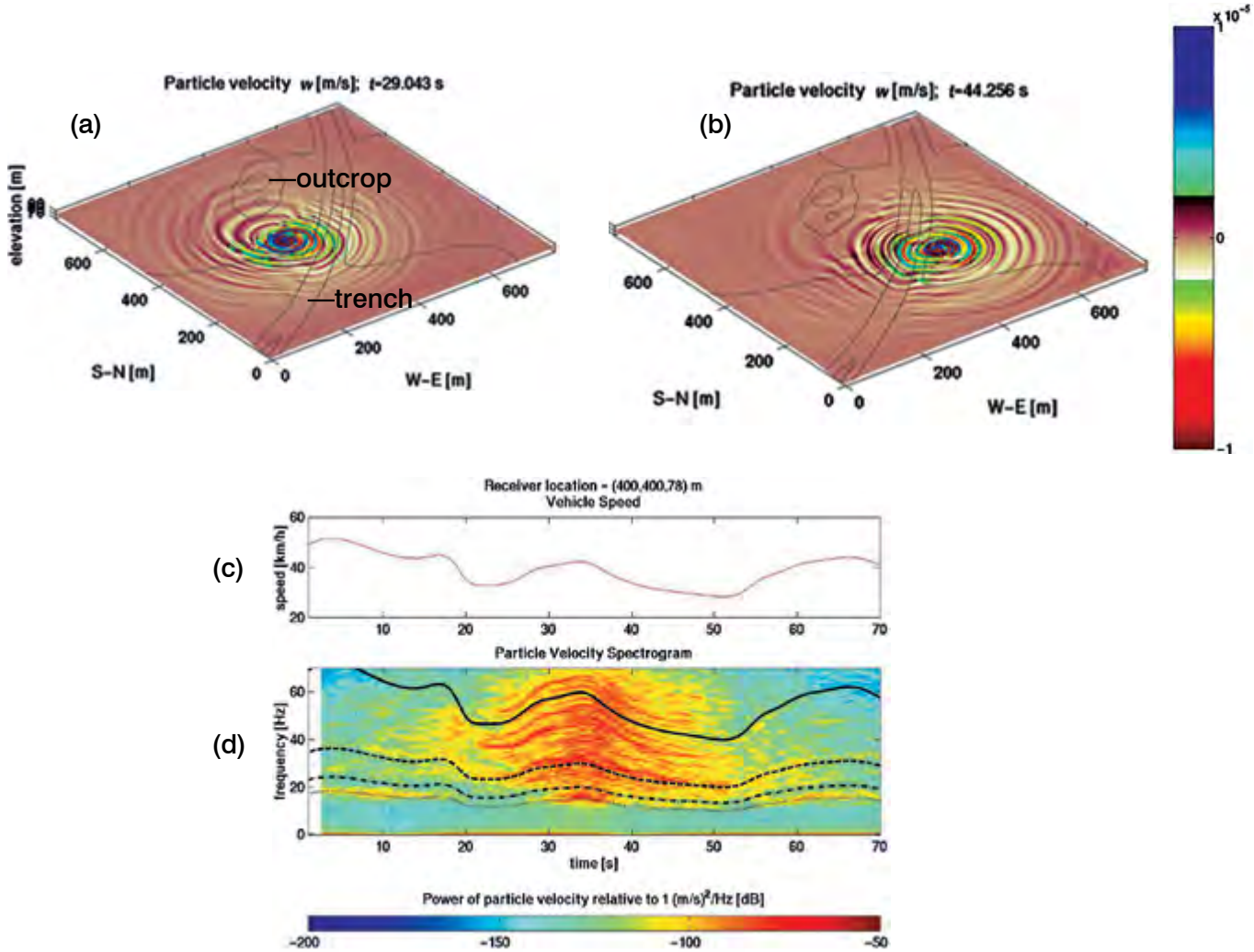

Figure 1. Results from a seismic simulation of a tank moving over complex open terrain

km² in surface area were simulated. The resulting synthetic signatures allow development of sensor system algorithms that fully exploit seismic signals. Furthermore, this capability supports the advanced sensor network systems envisioned for the Objective Force by demonstrating the target tracking and classification capabilities of seismic sensor networks for NLOS and BLOS situational awareness and by providing developers of tactical systems with a database of seismic signatures for a wide variety of geologic conditions.

The ability to simulate high fidelity, time-varying, seismic wavefields that include realistic signal complexity is central to the team's demonstration of seismic sensor geologic adaptation and to the development of optimized track-location information fusion methods. It is particularly important that the signal complexity include the dynamic harmonic energy shifts characteristic of moving targets, and the effects of strong geologic contrasts (large variations in amplitude, coherence, and wavefront curvature).

Geologic Variations

Geology can be highly variable across geographic regions and within a specific location. These variations have first order effects on the character of seismic signals and must be compensated for before seismic sensors can be employed in battlefield systems. For basic seismic system operation, only two geologic parameters are required. These include the propagation speed of the incoming seismic surface waves, and the rate of decay of surface

waves. Using simulated data shows that these basic properties are easily derived from simple calibration methods. It further demonstrates that target tracking information can be corrected allowing compensation for very complex signal effects resulting from strong geologic contrasts. This demonstrates that target tracks to moving vehicles are substantively improved by application of the correction functions and geology parameters derived from the calibration events.

Figure 1 (a-d) shows an example resulting from a simulation of a tank moving over complex open terrain. Seismic sources were taken from a vehicle-dynamics simulation of the tank. Figure 1a and figure 1b show snapshots of ground vibration amplitudes as the tank moves toward and away from a wide trench. Figure 1c shows the speed of the tank, and figure 1d shows a synthetic seismic signature spectrogram of the ground vibration near the middle of the model surface. The signature contains realistic features apparent in field measurements, such as multiple harmonics and evolution of the spectral content with vehicle speed. The series of overlaying black lines show expected harmonics from tank wheels rolling over track blocks.

Fusing Network Nodes

We fuse line-of-bearing (LOB) and range information from each node in the network with two methods. The simplest is an outlier rejection method based on the mean and standard deviation of each individual nodes location estimate. The second approach uses an optimum non-linear, weighted, least-squares error minimization (WLS) with weights determined from the information (LOB and range) variance. Both these approaches are shown to give comparable performance. The WLS approach is expected to be more appropriate with higher network node populations and when considering more diverse sensor inputs.

Seismic UGSs networks can be adapted to specific geologic context by using a sparse sequence of calibrated events. All that is required in the suggested calibration method is a consistent source excitation mechanism and meter scale source position accuracy. These simple criteria can be easily met in a wide variety of ways, including monitoring the seismic signals generated by the network deployment vehicle. The geologic adaptation functions, derived from the calibration data, are then applied to the moving target LOB and range estimates for each UGS node in the network. The results show that the adapted and fused moving vehicle network track results smoothly converge to errors as small as 2 m. The surprising correlation between the location calibration errors and the vehicle tracking error indicate that the network performance might be quantifiable at the time of deployment. This would have broad practical utility in designating target engagement points and weapons systems.

CTA: Computational Electromagnetics and Acoustics
Computer Resources: Cray T3E[AHPCRC, ERDC] and SGI Origin 3000 [ERDC]

Identification of "Hot-Spots" on Tactical Vehicles at UHF Frequencies

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Within the DoD, there is considerable interest in evaluating the use of low frequency, ultra-wideband (UWB) imaging radar to detect tactical vehicles concealed by foliage and targets buried in the ground. At low frequencies, the tree canopy is essentially transparent. Likewise, low-frequency radar can efficiently propagate through the ground for subsurface target detection. Despite these advantages, the development of robust target detection algorithms has been hampered by the complexity of the scattering physics due, in part, to the large number of physical parameters involved and the frequency diversity inherent in UWB systems. The objective of the CHSSI CEA-9 project is to develop high performance software for predicting electromagnetic scattering from general 3-D surface and subsurface targets. In particular, attention was directed toward radar-based, wide-area surveillance of buried mines, unexploded ordnance (UXO), bunkers, tunnels, and large ground vehicles. Validated electromagnetic models will permit the analysis of many target scenarios at a fraction of the cost of a measurements program.

Multi-level Fast Multipole Algorithm Developed

The software developed in this project is based on the fast multipole method (FMM). The FMM constitutes a recently developed extension to the MoM technique. In the MoM, the unknown constituents in an integral equation (*e.g.*, surface currents) are represented in terms of a set of known expansion functions with unknown coefficients. The MoM results in the matrix equation $\boldsymbol{Zi} = \boldsymbol{v}$, where $\boldsymbol{Z}$ is an N x N "impedance" matrix, $\boldsymbol{v}$ is an N x 1 vector representing the incident fields, and $\boldsymbol{i}$ is an N x 1 vector representing the N unknown expansion-function coefficients. While the MoM is a very powerful and general technique, it has limitations that constrain its use. In particular, one must store the matrix $\boldsymbol{Z}$, and therefore, computer memory limits the number of N unknowns that can be considered. Consequently, the need to store the N x N matrix $\boldsymbol{Z}$ translates to a limitation on the electrical size of the target that can be considered with a given computer memory. To mitigate this problem, the ARL team has developed a fully scalable, multi-level fast multipole algorithm (MLFMA), which can be applied to surface (tanks, trucks, etc.) or subsurface (mines, bunkers, etc.) targets. The MLFMA is a technique in which the expansion functions are grouped into M clusters and the interactions are treated globally, cluster by cluster. The MLFMA generally requires $O(N\log N)$ in runtime and memory, while the MoM requires $O(N^2)$ in runtime and memory. To model these large targets where the number of unknowns may approach one million, high-performance computing resources are required. The parallel MLFMA software was developed to run on the MSRC SGI and IBM HPC platforms.

"Validated electromagnetic models will permit the analysis of many target scenarios at a fraction of the cost of a measurements program."

Validating Electromagnetic Models

The ARL has been developing low frequency UWB radar technology for detection of foliage-concealed targets for many years. Based on recent field test data, researchers know that the UWB radar has the

potential to "see" foliage-concealed targets. The question remains, however, on whether they can develop an understanding of the underlying signature and whether it is robust and reliable enough to be militarily significant. Rigorous electromagnetic models such as the MLFMA can help answer this question. As an example, the ARL team computed the vertical transmit-vertical receive (VV) envelope response from a T-72 for nose-on incidence ($\theta = 55°$, $\varphi = 0°$) using a UHF impulse. The UHF pulse spectrum had a bandwidth of 246–434 MHz. This bandwidth corresponded to a range resolution of 0.8 m. As shown in Figure 1, the time-domain response was then transformed into the space domain and mapped onto the surface of the tank. This was done in order to correlate the peak returns in the time waveform impulse response to specific physical features on the target — in this case, the front fender area, cupola, and rear gas tank. These highlighted (red) areas are the local scattering centers (or "hot spots") on the T-72 for this particular angle of incidence. This analysis shows that the response from the target is directly linked to the shape and orientation of the vehicle. This aspect of target scattering may be useful for ATR algorithm development. In the end, it may be the key to discriminating targets of interest such as tanks, trucks, missile launchers, etc., from the large clutter sources (trees).

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CTA: Computational Electromagnetics and Acoustics
Computer Resources: SGI Origin 2000 [ARL]

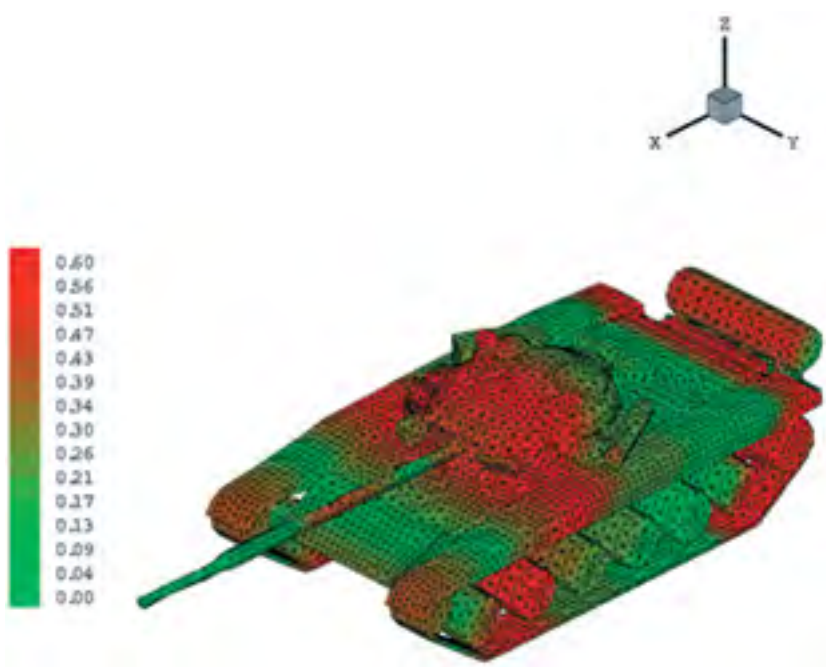

Figure 1. Impulse response mapped on T-72

Simulation and Redesign of the Compact A6 Magnetron

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Radio frequency (RF) weapons will be designed to work against hostile battlefield electronics. Given the importance of electronics in the modern battlefield, the ability to target these electronics will give the US a distinct advantage against technically advanced adversaries. The effect of RF radiation on the electronics can vary from transient disruption to destruction of hardware, depending on the power and frequency of the radiation. Furthermore, since only electronic equipment is affected, RF radiation can be applied in a non-lethal manner, giving the warfighter a broader range of options for dealing with opponents of varying sophistication and strength. This generation of electromagnetic radiation is critical to the DoD's advanced RF weapon effort.

Predicting High Power Microwave Performance Using ICEPIC

Improved Concurrent Electromagnetic Particle-in-Cell (ICEPIC) predicts the performance of several high power microwave (HPM) devices in current development for the US Air Force. With an accurate simulation tool, devices such as the relativistic klystron oscillator (RKO), the magnetically insulated line oscillator (MILO), the relativistic magnetron, and high frequency gyrotrons can be improved. ICEPIC simulates the electrodynamics (Maxwell's equations) and charged particle dynamics (relativistic Lorenz's force law) with second-order time and space accuracy in HPM sources. These simulations accurately predict RF-production and antenna gain compared with experimental testing. In general, ICEPIC development has been driven by the desire to achieve high power in a compact RF device. This implies that the device is operated at high current and high space charge. Consequently, these devices are highly non-linear and have complex three-dimensional geometries with small features. ICEPIC may be used both for fine-tuning well-understood devices and for testing new designs.

Virtual Prototyping with ICEPIC

Researchers at the AFRL are performing virtual prototyping of RF systems, from pulse power drivers to beam sources through the antennas, with the ICEPIC HPC software. They have developed ICEPIC over the past several years with AFSOR funding. This code simulates the electrodynamics (Maxwell's equations) and charged particle dynamics (relativistic Lorenz's force law) from first principles. Such simulations require major computational resources and are scalable to hundreds of nodes.

"ICEPIC development has been driven by the desire to achieve high power in a compact RF device."

The team successfully applied ICEPIC to simulate the University of Michigan's relativistic magnetron by reproducing the RF power level, growth rate, and operating frequency. ICEPIC predicts 300 MW (mega-watt) of total extracted instantaneous power, 150 MW RMS (Root Mean Square), compared with 200 MW RMS measured in the experiment. ICEPIC also predicts the experimental 100 nanosecond (ns) delay in the onset of RF after the diode voltage reaches its peak. The operating frequency observed in the ICEPIC results agrees to within a few percent of the 1.03 GHz measured in the experiment. The ICEPIC results also show that the University of Michigan's A6 does not operate in the desired pi mode (a pi phase shift in the electric field from cavity to cavity). In addition, the ICEPIC results show a large upstream and downstream DC loss current, similar to experimental observation.

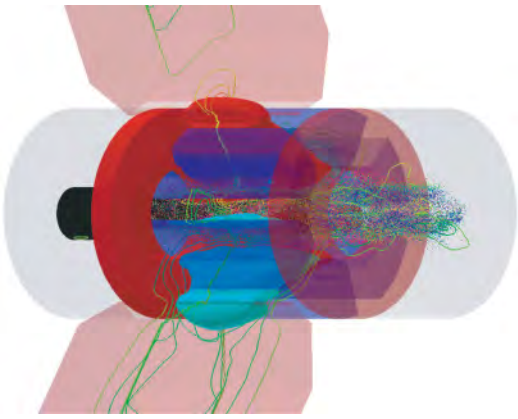


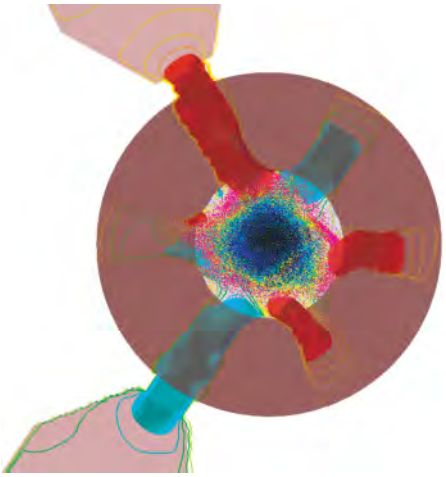
Figure 1. This shows the Titian/PSI A6 magnetron simulated in ICEPIC. This snap shot shows the electric field and particles 50 ns after the start of the applied voltage. The iso-surfaces in this figure are the electric field pointing around the cathode (theta direction). Red is in the clockwise direction when facing upstream (left in this graphic) green is in the counter clockwise direction. The power extracted from the magnetron into the wave-guides shows a pi phase advance between the two cavities. The desired mode has a 2pi phase advance for the extractors, this magnetron is operating in the wrong mode.

In addition to simulating the University of Michigan device, ICEPIC is applied to the Titan/PSI A6 magnetron designed for AFRL (Figure 1). The results verify the 1-GW (gigawatt) capability of the design, but find severe mode competition that hampers the axial extraction concept needed to meet the compact size goal. The current program provides for an evolutionary step by extracting power radially through two waveguides. The simulations show roughly 1-GW of instantaneous power extracted into each arm (for a total of 1-GW RMS power) when the entire cathode region under the anode block is allowed to emit. However, there is severe mode competition between the pi and 2pi/3 modes (Figure 2). The phase advance from cavity to cavity is not constant in this design. The phase advance for the extracting cavities and the cavity between is pi/2. The rest of the cavities have a 3pi/4 advance, which makes the average phase advance 2pi/3. Clearly, the extractors are having a profound effect on the overall electrodynamics of the device. This shows the importance of using 3-D simulation tools and including all the geometry of the source. This issue will not be a problem for the initial proof of principle radial extraction experiments, but limits the output power for the compact axial extraction concepts to about half of the required value. In addition, the peak electric field for these modes is not in the center of the anode block as expected, but downstream of the center (Figure 3). Details of the field and particle structure inside the magnetron is difficult to obtain from experiment because of the high electric field stresses and electron bombardment. Thus, the simulation results are extremely insightful.

Developing Compact, Multi-Gigawatt Microwave Sources

The task is to develop compact, multi-gigawatt microwave sources. The next step is now being taken in AFRL's evolution towards true virtual prototyping; the relativistic magnetron is being simulated before it is built at the lab. The details of the device that will eventually be built, including the geometric structure and the externally generated magnetic field distribution, will be based on these simulations. Scientific visualizations are used for three focuses. First, it is used for communication of complex physics. Second, it is useful for debugging ICEPIC software as well as the input files. Lastly, it can be used to uncover new and unexpected emergent physics.

Figure 2. This shows the Titian/PSI A6 magnetron simulated in ICEPIC. This snap shot shows the electric field and particles 50 ns after the start of the applied voltage. The camera is pointing upstream toward the pulse power. The iso-surfaces in this figure are the electric field pointing around the cathode (theta direction). Red is in the clockwise direction when facing upstream, green is in the counter clockwise direction. The power extracted from the magnetron into the wave-guides shows a pi phase advance between the two cavities. The desired mode has a 2pi phase advance for the extractors, this magnetron is operating in the wrong mode. The phase advance from cavity to cavity is not constant in this design. The phase advance for the extracting cavities and the cavity between is pi/2. The rest of the cavities have a 3pi/4 advance, which makes the average phase advance 2pi/3.



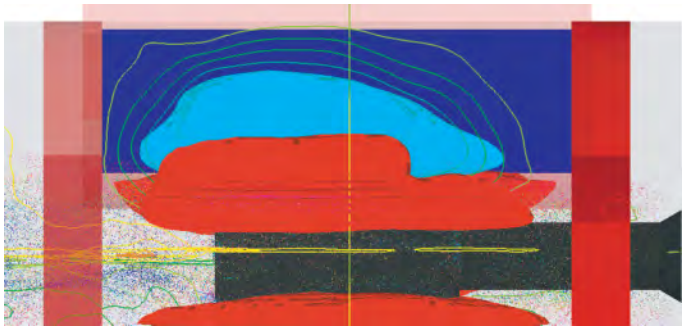


Figure 3. This shows the Titian/PSI A6 magnetron simulated in ICEPIC. This snap shot shows the electric field and particles 50 ns after the start of the applied voltage. The peak electric field for these modes is not in the center of the anode block as expected, but downstream (left) of the center (vertical) yellow line.

The Titan/PSI A6 magnetron design is improved through extensive ICEPIC simulations. The simulations allow studies of the consequences of changing the vane depth and extraction slots to force the tube into the pi-mode. Using simulation results, the parasitic mode is reduced in amplitude to ten percent of the desired pi-mode, and cathode end caps are designed to reduce the upstream and downstream loss current. The reduced loss current increases the efficiency of the magnetron. Plans are to build the improved design in late 2002 and to compare to experimental results to simulation results from ICEPIC.

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CTA: Computational Electromagnetics and Acoustics

Computer Resources: IBM SMP [ARL, ERDC, MHPCC], IBM Netfinity [MHPCC], and Compaq SC40 [ERDC]

Multiphase CFD Simulations of Solid Propellant Combustion in Modular Charges and Electrothermal-Chemical (ETC) Guns

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The Army is exploring a variety of gun propulsion options for indirect and direct-fire weapons for the legacy force and the Future Combat System. As it transforms, the Army has identified requirements for hypervelocity projectile launch for strategic Army missions. Among these gun systems are those that use solid propellant — granular form loaded in modules (indirect-fire) or disk/strip form for high-loading-density cartridges (direct-fire) — along with electrothermal-chemical (ETC) augmentation. Advanced indirect-fire gun systems with complex grain and container geometries are being investigated for the Modular Artillery Charge System (MACS) that has been developed for all fielded 155 mm cannons. The gun propulsion-modeling environment has been one in which separate codes (some 1-D, some 2-D) are used, with no single multi-dimensional code able to address the truly 3-D details of all of these systems. This situation renders comparison of ballistic performance cumbersome and inconclusive. In contrast, the multiphase continuum equations that represent the physics of gun propulsion comprise a set of general equations applicable to all of these systems. Thermodynamic state equations and constitutive laws, as well as boundary conditions, represent the relevant differences in system details.

NGEN – The Army's Next Generation Interior Ballistics Model

The Army's next generation interior ballistics model, NGEN, is a multi-dimensional, multi-phase CFD code that has been under development at ARL for a number of years. The NGEN code incorporates 3-D continuum equations along with auxiliary relations into a single code structure that is both modular and readily transportable between scaleable, high performance computer architectures. Since interior ballistics involves flowfield components of both a continuous and a discrete nature, an Eulerian/Lagrangian approach is used. The components of the flow are represented by the balance equations for a multi-component reacting mixture. This describes the conservation of mass, momentum, and energy on a sufficiently small scale of resolution in both space and time. A macroscopic representation of the flow is adopted using these equations derived by a formal averaging technique applied to the microscopic flow. These equations require a number of constitutive laws for closure including molecular transport terms, state equations, chemical reaction rates, intergranular stresses, and interphase transfer. The numerical representation of these equations as well as the numerical solution is based on a finite-volume discretization and high-order accurate, conservative numerical solution schemes.

"The success of this modeling effort has yielded a code that stands as a singular computational simulation tool providing the Army with the unique capability to simulate current and emerging gun propulsion systems. These simulations serve to both streamline testing and aid in the optimization of interior ballistics performance."

The success of this modeling effort has yielded a code that stands as a singular computational simulation tool providing the Army with the unique capability to simulate current and emerging gun propulsion systems. These simulations serve to both streamline testing and aid in the optimization of interior ballistics performance. High performance computing resources and scientific visualization tools are essential to efficiently use these numerical simulations, because the NGEN code solves the governing equations in a high-resolution 2-D and 3-D mode. In one particularly significant application, the NGEN code was used to

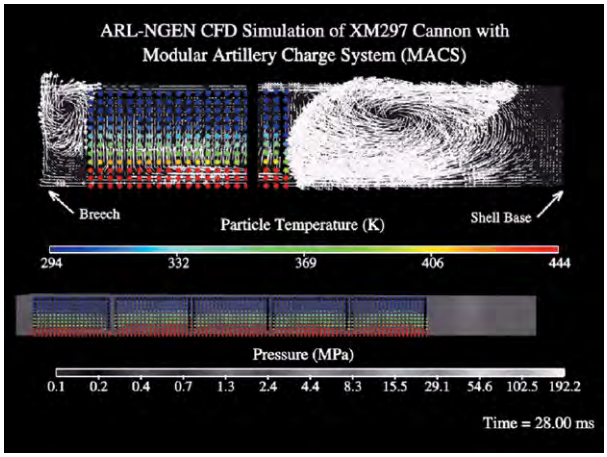

Figure 1. Scientific visualization of the MACS charge (five modules) showing the location of propellant particles (colored by temperature) and formation of gas dynamic vortices in the gun chamber

simulate the MACS propelling charge, that is being developed at the Armament Research Development and Engineering Center for all fielded 155mm cannon, and for the XM297 Crusader cannon (developed by PM-Crusader). Figure 1 displays a scientific visualization of the MACS using NGEN. The NGEN code simulations for the M231, low-zone MACS charge, aided in the successful type classification of the charge. For the high-zone charge, NGEN code simulations were used to uncover previously unknown physical phenomena for the M232 charge that only occurs during charge fallback in an elevated gun tube. This is a particularly acute concern at top zone since bag charges positioned adjacent to the breech lead to large-amplitude pressure waves that can destroy the weapon. NGEN simulations of these modular charges proved that the prevailing gas dynamic process (when the charges are positioned adjacent to the breech face) causes the modules to be displaced forward. This mitigates pressure wave formation — a fact confirmed by actual gun tests performed a year later.

Encouraged by these successes, the scientists at ARL used the NGEN code to investigate the loading of M232 charges that are at the ambient temperature along with modules that have been initially temperature conditioned. This combination emulates taking modules from different loading pallets and assembling a single propelling charge. The important questions were whether such a charge would lead to high-amplitude pressure waves in the gun chamber and what level of performance gain or loss could be expected. Figure 2 shows a scientific visualization of the case of three hot modules loaded in the forward position along with two ambient modules comprising the final charge. In this situation (considered a worst-case scenario) hot propellant impacts the projectile base, as predicted by the NGEN code. This leads to a noticeable amplification of pressure waves in the chamber but still non-threatening to the weapon's structural integrity. The predicted projectile velocity was shown to be slightly enhanced by this type of charge.

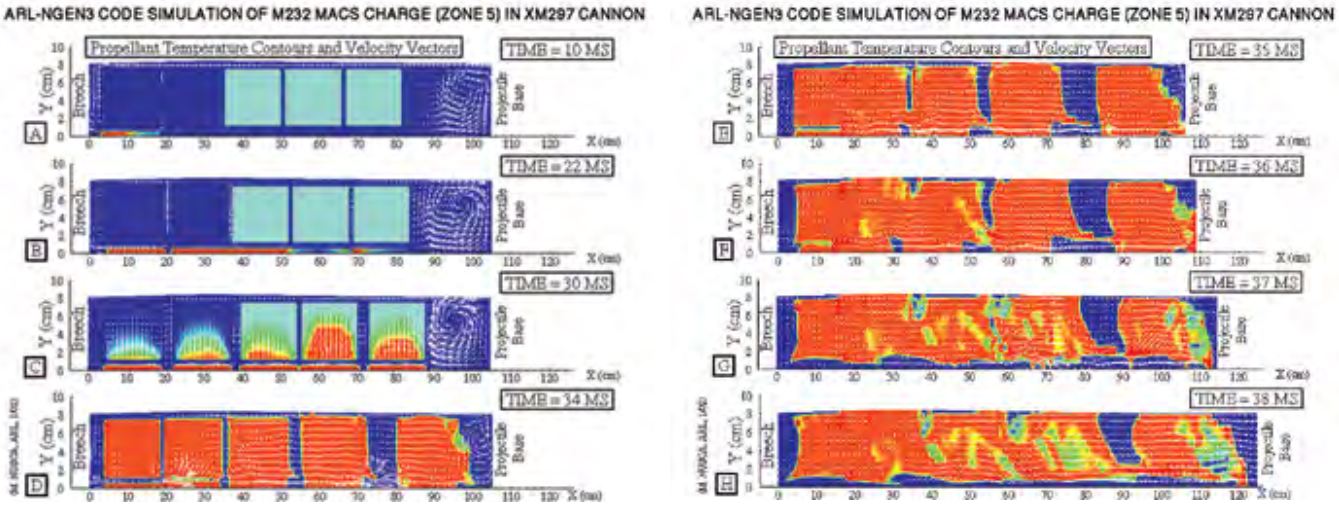

Figure 2. Scientific Visualization of the MACS charge (five modules with three forward modules at initially elevated temperature) showing the location of propellant modules (colored by temperature) at eight times in the flamespreading process. Note the impact of hot propellant on the projectile base (E,F).

Direct-Fire Gun Simulation

In another application, this time to direct-fire gun systems, the ARL researchers used the NGEN code to simulate solid propellant charges ignited using an ETC igniter. A simulation of a high-loading-density (HLD) M829A1 120mm tank charge composed of disk and granular solid propellant media demonstrated the ability of the NGEN code to accommodate ignition and flamespreading through a novel charge. This simulation included the effects of projectile afterbody intrusion and movement as well as compression and the resulting ignition delay in the propellant. Figure 3 is a scientific visualization of this gun charge. These simulations revealed, for the first time, that the igniter, positioned at the gun breech, could forcefully compress the disk charge. This compression closed critical flow paths in the charge, preventing effective flamespreading and even ignition. The simulations showed that the low molecular weight plasma, generated by an ETC igniter, could circumvent this problem. The plasma establishes a convectively driven flame that propagates faster than the material compression wave in the disk propellant, permitting an even ignition of the charge. A basic design tenet for using high-loading-density charges was established; that pressure waves in the gun chamber generated by the conventional igniter, when paired with the disk propellant charge, were avoided by using an ETC igniter.

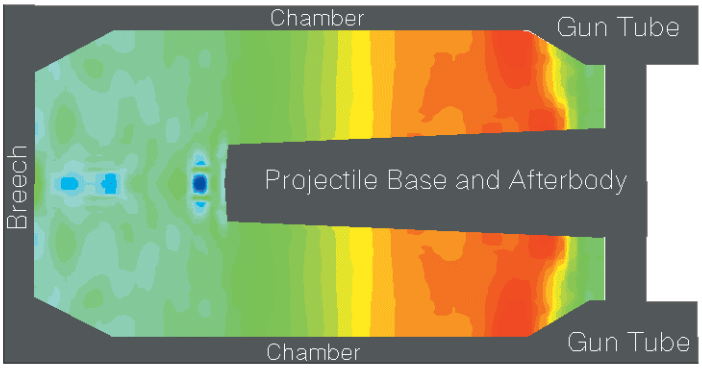

Figure 3. Scientific Visualization of a HLD charge (disk propellant) showing gas pressure (colored by pressure up to red at about 100 MPa). Note the higher pressure forward on the projectile afterbody.

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CTA: Computational Fluid Dynamics

Computer Resources: SGI Origin 2000 [SMDC] and Cray SV1 [NAVO]

The Effects of Propellant Deformation During a Gun Firing

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The US Army is studying the use of increased amounts of propellant in tank and artillery gun rounds to increase the range and lethality of the guns. One of the technical challenges posed by larger amounts of propellant is ensuring that all of the propellant burns rapidly enough while keeping the pressure in the gun below certain levels. Usually, higher pressure is an effect of faster propellant burning. If the projectile leaves the gun before the propellant has finished burning, the energy released by combustion after the projectile exits is wasted. On the other hand, if the pressure in the gun is too high, the gun can be damaged.

Army researchers want better control of the tradeoff between the speed at which the propellant burns and the pressure in the gun. In order to achieve that control, they first need a better understanding of some of the detailed phenomena that occur while the gun is being fired. For instance, propellant disks can be placed in the gun (Figure 1), and they start to burn because hot gas from the igniter reaches them and raises their surface temperature. The hot gas will also cause the propellant disks to move, deform, and possibly break. This interaction between the gas and the propellant is not yet well understood, but knowing how it works will help researchers control the burning of the propellant.

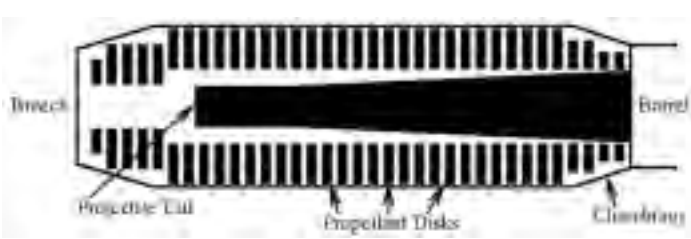

Figure 1. Sketch of disks of solid propellant in a gun round

Numerical Study of Gas and Propellant Interaction Underway

Studying the interaction between the gas and propellant is difficult to do experimentally. An effort to study this numerically is underway using HPC resources available at AHPCRC. In order to study this problem in detail, the motion, pressure, and temperature of the gas have to be computed in each time step using conservation of mass, momentum, and energy equations. The motion, stresses, and strains of the propellant are computed by using the equations of motion complemented by an appropriate strength model and an equation of state. This all has to be done on a very fine grid, with the distance between grid points on the order of 0.008 inches. The HPC systems have the memory and computing speed needed to study this problem.

"Army researchers want better control of the tradeoff between the speed at which the propellant burns and the pressure in the gun. This interaction between the gas and the propellant is not yet well understood, but knowing how it works will help researchers control the burning of the propellant."

Scientific visualization, specifically the FV2 and PRESTO visualizers developed at the AHPCRC, has played an important role in understanding the data generated by the numerical model. In the study of gas interacting with the propellant, the formation and motion of pressure waves in the gas is a very important phenomenon. Creating animations of the pressure in the gas allows researchers to see how it happens, which aids in understanding it.

Numerical Study Gives New Insight

The numerical study of the interaction between the gas and the propellant on the HPC systems has given new insights into some of the effects of the interaction. For instance, many researchers agree that the propellant disks will break if they are involved in a high-speed collision. But the HPC study shows that the gas can bend the disks around the neighboring propellant and break them even though the disks are moving at very low speeds (Figure 2). The inclusion of combustion and fracture models in the simulation of the propellant will allow the code to generate new details about the interactions. Such insights will give researchers more information as they develop a fuller understanding of the gun firing, which in turn will develop the control needed to safely increase the amount of propellant in the tank and artillery gun rounds.

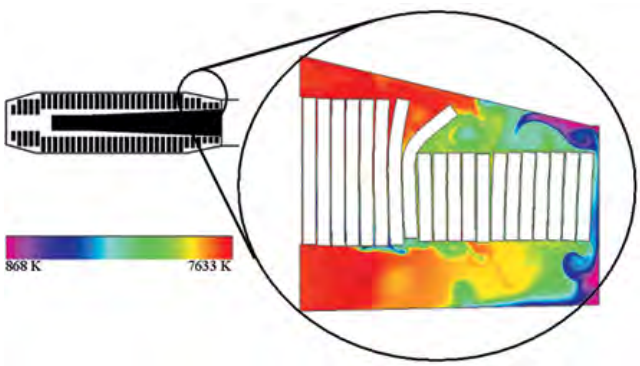

Figure 2. Gas temperature in barrel end of the gun. Notice how one disk is bending over its neighbor; this disk is fracturing.

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CTA: Computational Fluid Dynamics
Computer Resources: Cray T3E [AHPCRC]

Modeling and Simulation of Nanoparticle Formation and Growth in Turbulent Reacting Flows

Sean Garrick
Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN

Simulations can be used in the production and characterization of nanoscale energetic particles and composites. There are several technologies that can be employed in the manufacture of nanoscale materials. Vapor-phase methodologies are by far the most favored because of the chemical purity and cost considerations. When driven from gas phase precursors, there are several phenomena, which need to be addressed: vapor-phase chemistry, particle formation, and growth (coagulation, coalescence, condensation, etc.) among others.

Researchers at AHPCRC are developing tools to simulate the production of nanoenergetic particles — propellants or explosives. Energetic nanoparticles have been targeted as one of the propellants for the Army's FCS because they exhibit very high reaction rates. However, the Army currently has no source of these materials. The manufacture of nanoparticles is difficult because all of the relevant mechanisms/dynamics are not completely understood. To mitigate this, tools are being developed to determine the effects of chemistry, flow/temperature dynamics, and particle-particle interactions on nanoparticle formation and growth in realistic flow systems, such as those employed in cost-effective processes like vapor-phase synthesis. In this way, the Army can have particles in a specified size range, chemical composition, and physical structure.

Simulating Nanoscale Particle Production

The numerical simulation of nanoscale particle production through gas phase synthesis involves the solution of a large number of coupled, non-linear integro and partial differential equations. These models represent turbulent reacting flows with length scales spanning seven orders of magnitude. With the addition of nucleation, coagulation, and other particle-particle interactions, a rather diverse range of phenomena is under investigation. The primary objective is to improve our physical understanding of particle formation and growth in a turbulent reacting environment.

To illustrate the underlying phenomena, simulations of several turbulent flows were performed. A turbulent planar jet was simulated with a domain comprised of 24,500,000 grid points. In this calculation, the time steps are on the order of 10^{-9} seconds and the dynamics of particles between 1 and 10 nanometers were captured. The concentration of 4 nanometer diameter particles is shown in Figure 1(a). From this image, one can see that the particles are engulfed in the vortical structures and are effectively segregated from the rest of the flow. The characteristic flow time of the particles, the length of time the particles remain in specific regions of the flow, and the temperature of these regions are key areas of investigation. These are just a few of the issues which can be answered with the capability facilitated by advanced simulation.

"Energetic nanoparticles have been targeted as one of the propellants for the Army's FCS because they exhibit very high reaction rates. Tools are being developed to determine the effects of chemistry, flow/temperature dynamics, and particle-particle interactions on nanoparticle formation and growth in realistic flow systems, such as those employed in cost-effective processes like vapor-phase synthesis."

High performance computing resources were required to run the direct numerical simulation of the turbulent jet. The exact solution required 96,265 CPU hours. Other solution methodologies had to be explored for the more complex flow geometries. Large-eddy simulations can provide reasonably accurate simulations in a fraction of the time required by direct numerical simulation. However, the effect of turbulence on both the flow and particle fields must be modeled.

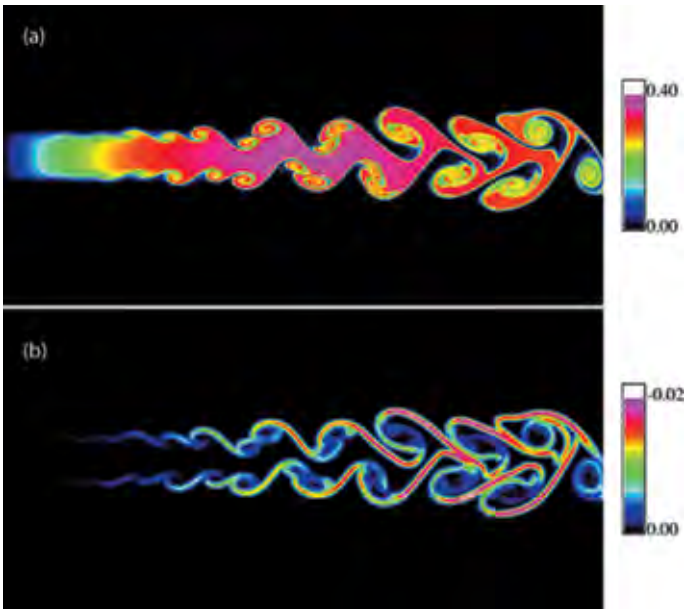


Figure 1. Nanoparticle coagulation in a turbulent jet: (a) Concentration of 4 nm diameter particles; (b) Turbulent growth rate

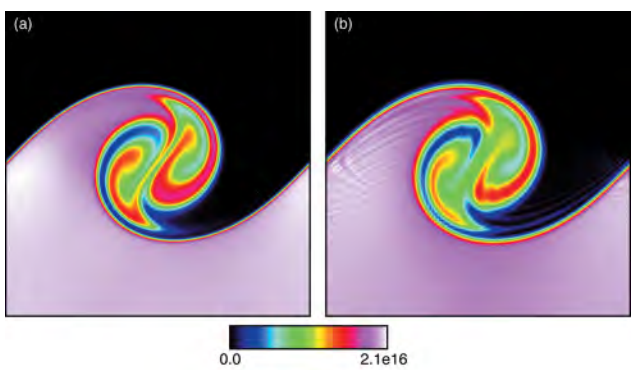


Figure 2. Nanoparticle growth in temporal mixing layer: (a) Direct numerical simulation (450 CPU hours); (b) Large-eddy simulation (1 CPU hour)

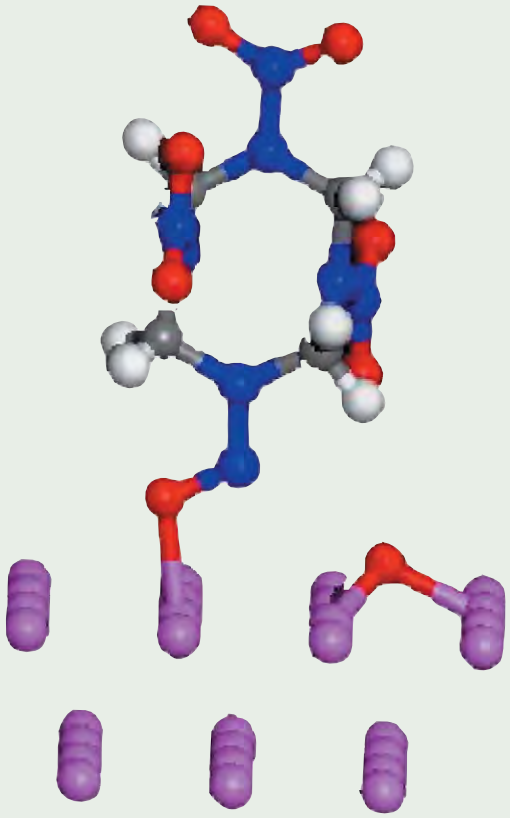
The effect of turbulence on the particle growth rate is shown in Figure 1(b). The figure reveals that the effect is more pronounced as the flow develops and is as high as 20%. This resulted in the development of the first large-eddy simulation of nanoparticle growth in turbulent flows, which represents the particle field in a manner which allows for the capture of the underlying physics and chemistry of particle coagulation.

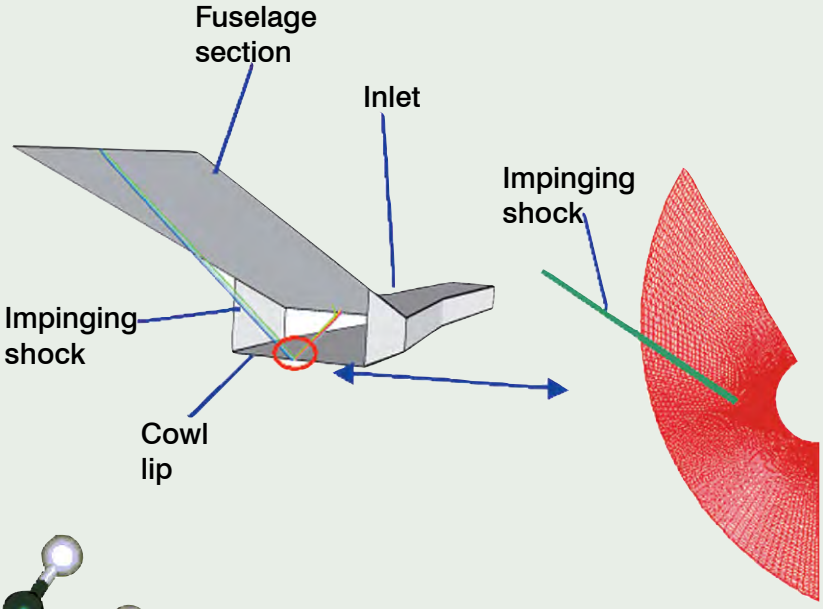
Large-Eddy Simulation versus Direct Numerical Simulation

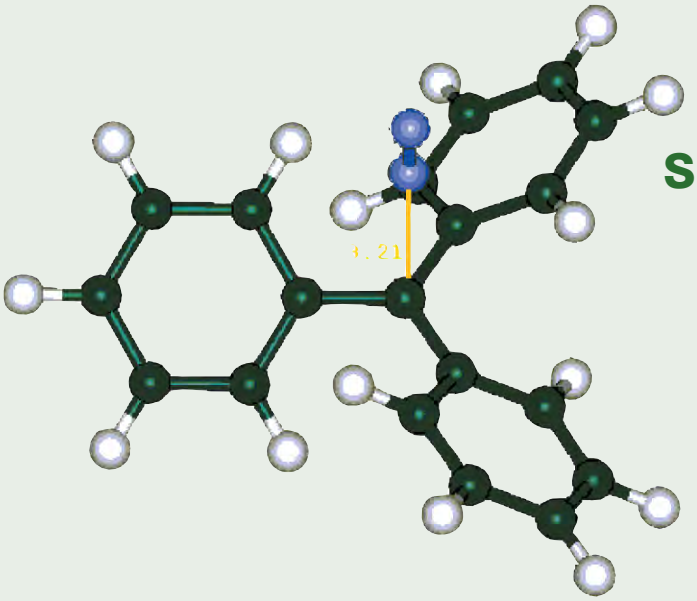
To test the methodology, both large-eddy simulations and direct numerical simulations of nanoparticle coagulation in temporal mixing layers, which are subsections of the turbulent planar jet were performed. The results are shown in Figure 2. The concentration of 4 nanometer diameter particles obtained through direct numerical simulation is shown in Figure 2(a) and the concentration obtained through large-eddy simulation is shown in Figure 2(b). The large-eddy simulation yields very good results while reducing the CPU time by a factor of more than 400. The use of large-eddy simulation will greatly affect the development of advanced nanostructured materials such as composites, which are being considered as the next generation of propellants because of the large surface-to-volume ratio, and thus are highly reactive.

CTA: Computational Fluid Dynamics
Computer Resources: Cray T3E [AHPCRC]

Enhance the Capability and Survivability of Space Systems







Space Surveillance

Space Access

Sub-Orbital Space Vehicle

References (from top to bottom):

Simulations of Energetic Materials for Rocket Propulsion: Getting More Bang for the Buck by Jerry Boatz

Final configurations of an HMX molecule on an aluminum (111) surface. In the final configuration, one of the oxygen atoms is bonded to two surface aluminum atoms and is completely dissociated from the initial NO2 group. The other oxygen atom also forms a bond with aluminum but remains bonded to the nitrogen atom in the original NO2 group.

Scramjet Shock-on-Cowl-Lip Load Mitigation with Magnetogasdynamics by Datta Gaitonde

Schematic of shock-on-cowl-lip problem

New Polynitrogen Molecules – Energetic "Air" as a Next-Generation Propellant? by Jerry Boatz

MP2/6-31G(d) optimized structure of triphenylmethyldiazonium cation, $[C_{19}N_2H_{15}]+$. The predicted C-N internuclear distance of 3.21 angstroms indicates that this cation is unstable with respect to dissociation to triphenylmethyl cation and N2.

Enhance the Capability and Survivability of Space Systems

The overarching strategic goal for the DoD is to maintain US global superiority in space while making space access and operations easily affordable. From space, a whole range of critical information collection and distribution functions becomes possible with both robust global reach and little forward-based infrastructure. Information provided to US military personnel by space-based systems includes weather, forces location/movement, environmental monitoring, transportation routes, advanced warning on weapons deployment, and weapons targeting. Future space systems could allow application of space-based force against ballistic missiles and other threats. The number of space-faring nations and their capabilities is increasing and, with that, the possibility of threat to US forces. Space systems based on current technology are highly expensive to acquire and operate. This high cost threatens US dominance of space.

One of the ways to reduce the costs of future space systems is to reduce the weight of the vehicle. A common area for advancement to reduce the weight of launch vehicles is in the propellants. Propellants comprise 70–90% of a launch vehicle's weight and accounts for 40–60% of the cost of the vehicle. Added to this, the manpower required to load the propellants into the space vehicle and the costly safety procedures and apparel that are intrinsic in this, research in more efficient and safer propellants is ongoing.

Another focus is the development of rocket propulsion engines and motors with improved performance for transition into existing or new systems. Boost and orbit transfer propulsion systems will demonstrate improvements in specific impulse, mass fraction, thrust to weight, reliability, reusability, and cost. Spacecraft propulsion systems will demonstrate improvements in specific impulse, thruster efficiency, and mass fraction.

Both of the above areas have one commonality — designing the item prior to developing the item. High performance computing is the key to these design efforts. The articles by Boatz, Sorescu, and Thompson; by McQuaid; and another article by Boatz describe quantum mechanical calculations to determine which proposed propellants will provide sufficient energy as a propellant, if there is a feasible path to produce it, and if it is less toxic. All three of these characteristics must be considered prior to the development of new propellants. In the article by Gaitonde, the design of facets of supersonic engines is studied to alleviate problems with sustained hypersonic flight.

We believe that using HPC in the early stages of developing new space technologies helps ensure continued US superiority in space.

Dr. Leslie Perkins

High Performance Computing Modernization Program Office, Arlington, VA

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Simulations of Energetic Materials for Rocket Propulsion: Getting More Bang for the Buck

Jerry Boatz
Air Force Research Laboratory (AFRL), Edwards Air Force Base, CA
Dan C. Sorescu
University of Pittsburgh, Pittsburgh, PA
Donald L. Thompson
Oklahoma State University, Stillwater, OK

Powdered aluminum has long been used as an energetic ingredient in rocket propellant formulations, comprising approximately 15–20% of some conventional ammonium perchlorate solid propellants. However, the performance of aluminum is reduced because of the rapid formation of an aluminum oxide overcoat on aluminum particles before combustion, which inhibits efficient burning. Furthermore, formation of the oxide overcoat severely reduces the potential advantages of using high surface-to-volume-ratio ultrafine aluminum particles, which have highly desirable properties such as enhanced burn rates.

Inhibiting Formation of Oxide Overcoat

In order to inhibit the rapid formation of an oxide overcoat on the ultrafine aluminum particles without simultaneously degrading performance, coating the aluminum particles with an energetic material such as 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) has been proposed. One of the objectives of this challenge project is to characterize the interactions between energetic compounds such as HMX and aluminum surfaces in order to understand, at an atomic level, the chemistry at the metal-molecule interface. Specifically, *ab initio* quantum chemical calculations are used to determine if HMX and/or other classes of energetic materials will effectively inhibit the formation of an oxide overcoat on the surface of aluminum.

Using Quantum Chemical Calculations

Conventional techniques for determining the feasibility of new ideas such as this have relied heavily on costly and time-consuming experimental synthesis and testing. However, the availability of HPC resources has significantly lessened the need for these empirical approaches by enabling the application of reliable high-level quantum chemical calculations to address complex issues such as the nature of the interactions between energetic materials and metallic surfaces. A key advantage of using HPC is the ability to efficiently screen a variety of energetic materials as potential metallic coatings and focus subsequent experimental efforts on only the most promising candidates.

"A key advantage of using HPC is the ability to efficiently screen a variety of energetic materials as potential metallic coatings and focus subsequent experimental efforts on only the most promising candidates."

Spin-polarized generalized gradient approximation (GGA) density functional theory, using ultrasoft Vanderbilt-type pseudopotentials and the PW91 exchange-correlation functional in a plane-wave basis, has been used to characterize the interactions between the energetic molecules nitromethane (NM), HMX, and 1,1-diamino-2,2-dinitroethylene (FOX-7) and the aluminum (111) surface (Figure 1). Two different models have been used to approximate the (111) surface of aluminum: a $(\sqrt{7}\mathrm{x}\sqrt{7})\mathrm{R}19.1^{\circ}$ slab

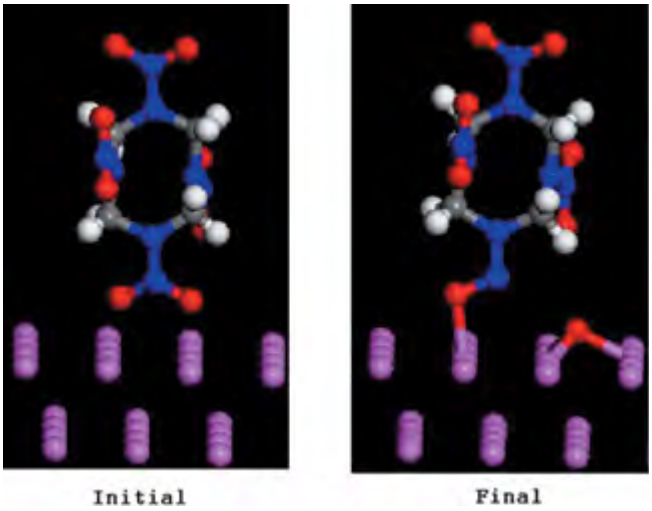

Figure 1. Initial (left) and final (right) configurations of an HMX molecule on an aluminum (111) surface. In the final configuration, one of the oxygen atoms is bonded to two surface aluminum atoms and is completely dissociated from the initial NO_2 group. The other oxygen atom also forms a bond with aluminum but remains bonded to the nitrogen atom in the original NO_2 group.

model with four layers (28 aluminum atoms) used for NM and a four-layer (3x3) slab (36 atoms) for the larger molecules (HMX and FOX-7). All calculations were performed using the Vienna as Initio Simulation Package (VASP) code.

Preliminary predictions of the interactions between the energetic molecules NM, HMX, and FOX-7 have indicated a common propensity for oxidation of the aluminum surface by the oxygen-rich nitro groups (NO_2) present in these molecules. Dissociation of the nitro groups and formation of strong Al-O bonds appears to be a common mechanism for these molecules. These results suggest that nitro-containing energetic compounds are not likely to be effective coating materials for preventing rapid oxidation of aluminum.

Scientific visualization is used for the construction of the initial atomic configurations for crystals, surfaces and gas-solid systems, using the Crystal and Surface Builders modules available in Cerius2 package.

Interactions of Several Ionic Systems

Future work will extend this set of investigations to first principles density functional theory calculations of the interactions of several ionic systems such as ammonium nitrate or ammonium dinitramide with an Al surface. In these investigations, key reaction pathways of these energetic salts on an aluminum surface will be computed. Researchers will attempt to understand the type of chemical processes that can take place at the interface of aluminum hydrides with different classes of energetic materials. In this case, they will focus on the case of ammonium nitrate and RDX crystals where the detonation properties are significantly affected by the interaction with aluminum hydrides.

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CTA: Computational Chemistry and Materials Science

Computer Resources: SGI Origin 2000 [ARL], Cray T3E [NAVO], and IBM SP P3 [ASC]

A New Design Approach to Hydrazine-Alternative Hypergols for Missile Propulsion

Michael McQuaid
Army Research Laboratory (ARL), Aberdeen Proving Ground, MD

Providing an extremely reliable basis on which to design intermittent and/or variable thrust propulsion systems, hypergolic liquid (or gel) fuel-oxidizer combinations—i.e., those that react spontaneously upon mixing—are candidates for propelling beyond line-of-sight weapons for the Army's FCS, an example being the Loitering Attack Missile being developed under the NetFires technology demonstration program.

Finding Viable Alternatives to Toxic and Carcenogenic Fuels

One of the drawbacks to "standard" hypergolic fuel-oxidizer combinations is that the fuels are derived from hydrazine, monomethylhydrazine (MMH), and/or unsymmetrical dimethylhydrazine (UDMH)—all of which are acutely toxic and suspected carcinogens. Fielding weapons systems with them necessitates the implementation of burdensome and costly handling procedures. Moreover, the only US producer of hydrazines is in danger of closing. Searching for alternatives to hydrazine-based fuels, the Army, in collaboration with the Air Force and the Navy, is investigating the use of secondary and tertiary amine azides in various propulsion applications. One of the formulations within this class of compounds receiving considerable attention is 2-azido-N,N-dimethylethanamine [$(CH_3)_2NCH_2CH_2N_3$]. Also referred to as DMAZ, this fuel has shown great promise as a hypergolic fuel, performing competitively with Aerozine 50 (a 50/50 mixture of hydrazine and UDMH) in inhibited red fuming nitric acid (IRFNA) oxidized systems. DMAZ-IRFNA systems do not, however, meet "ignition delay" standards set by MMH-IRFNA systems. This shortcoming negatively impacts engine design and may preclude the fielding of DMAZ.

Gaining Insights Through Computational Chemistry in a High Performance Computing Environment

Based on traditional chemical insights, proton transfer to the amine nitrogen has been hypothesized as an important initial step in the ignition of DMAZ-IRFNA systems. Therefore, attempts to address the ignition delay issue have been based on synthesizing 2-azidoethanamines with amine substituents other than the methyl groups found in DMAZ, with the hope being to increase the nucleophilic nature of the amine lone pair electrons. However, a computational quantum chemistry study of DMAZ identified that in its lowest energy configuration (Figure 1), the amine nitrogen is shielded from proton attack by the azide group, and therefore may be a barrier to the ignition process. Moreover, it is not possible to prevent azide group shielding of the amine lone pair in alternately substituted 2-azidoethanamines. The finding stimulated a search for molecular designs that prevented shielding, but did not otherwise significantly compromise DMAZ's features and thermophysical properties. Proposing to achieve this goal by introducing a cyclic structure between the amine and azide groups, ballistic performance-relevant properties of the *cis* and *trans* isomers of a notional compound—2-azido-N,N-dimethylcyclopropanamine (ADMCPA)—were computationally evaluated. (The *trans* form of ADMCPA prevents direct amine-azide interaction).

> "The ability to computationally screen the properties and predict the performance of notional hypergols through this environment has provided firm justification for further investment in this high-risk development effort."

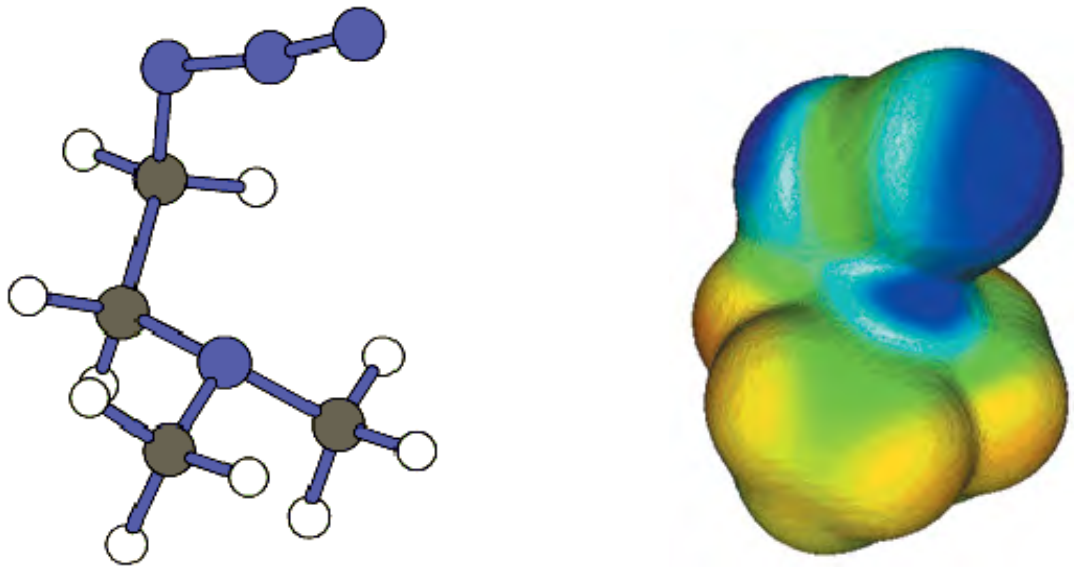

Figure 1. Molecular structure of the lowest energy DMAZ structure (left) and its electrostatic potential on an electron isodensity surface (right). Dark blue regions of surface indicate sites to which nitric acid will transfer a proton, the amine site being screened by the azide group.

Molecular stability and gas-phase heats of formation were established through computational quantum chemistry, and liquid densities and heats of vaporization were estimated via molecular dynamics simulations. The results were then used as input to thermochemical calculations of ballistic potential. Finding that the ADMCPA isomers merit further investigation as hypergols, their synthesis is now being pursued by the Army Aviation and Missile Research, Development, and Engineering Center as an option for its Impinging Stream Vortex Engine—a top launch package candidate for the Loitering Attack Missile.

Without the insight provided by computational quantum chemistry in a high performance computing environment, the new design approach could not have been identified. Moreover, the ability to computationally screen the properties and predict the performance of notional hypergols through this environment has provided firm justification for further investment in this high-risk development effort.

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CTA: Computational Chemistry and Material Science

Computer Resources: SGI Origin 2000 and SGI Origin 3000 [ARL]

New Polynitrogen Molecules – Energetic "Air" as a Next-Generation Propellant?

Jerry Boatz
Air Force Research Laboratory (AFRL), Edwards Air Force Base, CA

The identification, development, and formulation of new energetic materials for advanced rocket propulsion applications are areas of long standing interest to the Air Force. The performance limits of currently used propellants have been reached, so new energetic compounds are required to significantly improve the ability of the warfighter to access and control space.

Polynitrogen species such as the recently discovered N5+ cation (a positively charged ion) are of interest as potential energetic ingredients in new propellant formulations. The recent successful synthesis of N5+ in macroscopic quantities has prompted the search for additional polynitrogen compounds. Computational chemistry plays a central role in determining the stabilities, potential synthetic pathways, and key spectroscopic "fingerprints" of new polynitrogen species.

> "The performance limits of currently used propellants have been reached, so new energetic compounds are required to significantly improve the ability of the warfighter to access and control space."

Characterizing New Materials

Conventional techniques for characterizing new materials such as polynitrogens have relied heavily on costly and time-consuming experimental synthesis and characterization. However, the availability of HPC resources has significantly lessened the need for these more empirical approaches by enabling the application of high-level quantum chemical calculations to reliably predict important properties such as heats of formation, stabilities, mechanisms of formation and decomposition, and spectroscopic constants. A key advantage of using HPC in this regard is the ability to efficiently "screen" a large number of potential polynitrogen molecules and focus subsequent experimental efforts on the subset of only the promising candidates.

Computing Chemical Characteristics Using *Ab Initio* Methods

The structures, stabilities, vibrational frequencies, and infrared intensities of several potential synthetic precursors to new polynitrogen species have been computed using *ab initio* electronic structure theory, at the second order perturbation theory level (MP2, also known as MBPT(2)), using the 6-31G(d) valence double-zeta polarized basis set. Shown in Figure 1 is the predicted structure of triphenylmethyldiazonium cation, also known as trityldiazonium, which is a possible precursor to new polynitrogen compounds such as pentazole, a 5-membered ring system. The calculated structure shows that this cation is unstable

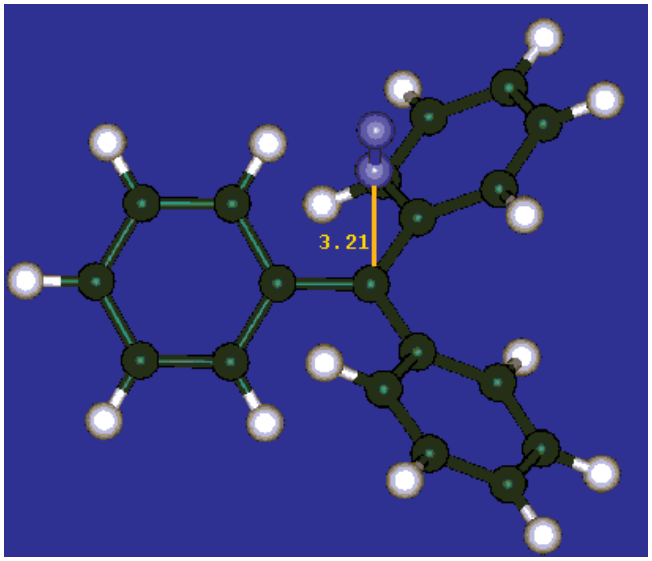

Figure 1. MP2/6-31G(d) optimized structure of triphenylmethyldiazonium cation, $[C_{19}N_2H_{15}]+$. The predicted C-N internuclear distance of 3.21 angstroms indicates that this cation is unstable with respect to dissociation to triphenylmethyl cation and N2.

with respect to dissociation of N2. Therefore, these calculations predict that this cation is not a viable polynitrogen precursor.

Although this is a negative result in the sense that it indicates that trityldiazonium is not a stable precursor, it is nonetheless a highly useful result in multiple ways. First, it saves significant time and effort by eliminating from consideration subsequent attempts at synthesis of a compound that is not likely to be stable. Furthermore, it suggests ways in which the trityldiazonium cation may be chemically modified in order to overcome its instability (e.g., by judicious placement of electron-withdrawing groups on the trityl moeity.)

Derivatives of Polynitrogen Precursors

Future work in this area will examine such derivatives of the trityldiazonium cation, as well as other classes of promising polynitrogen precursors.

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CTA: Computational Chemistry and Material Science
Computer Resources: IBM SP P3 [ASC], SGI Origin 3800 [AFFTC]

Scramjet Shock-on-Cowl-Lip Load Mitigation with Magnetogasdynamics

Datta Gaitonde
Air Force Research Laboratory (AFRL), Wright-Patterson AFB, OH

Advances in sustained hypersonic flight (exceeding five times the speed of sound) will impact future strike capability, ease access-to-space, and influence military strategy. Developing vehicles to survive the harsh high-speed aerodynamic environment for lengthy periods poses major challenges. Key limitations are imposed by poor efficiency of current air-breathing propulsion technologies and by excessive heat transfer and drag loads, which can affect design viability and cause mission failure. Supersonic combustion ramjets or scramjets will play a critical role by overcoming many of these constraints. Effective design will require informed compromise, coupled to revolutionary flow control techniques. The problem considered here stems from a mass-capture standpoint; scramjets function best when external compression shock waves are focused on cowl lips (Figure 1). Figure 2 shows Mach contours of the flow pattern resulting near the cowl lip without control. The crucial feature of this so-called Edney Type IV interaction is the nearly wall-normal supersonic jet, which impacts the surface. The stagnation process yields extremely high, unsteady heat loads, which can exceed forty times nominal values and lead to catastrophic failure.

> "These problems require months to solve on stand-alone workstations but can be solved in days on the high-speed HPC systems."

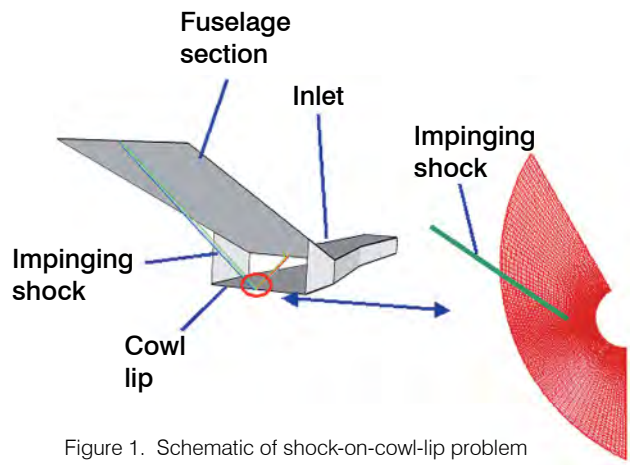

Figure 1. Schematic of shock-on-cowl-lip problem

Exploring Revolutionary Flow Control Techniques

Traditional approaches to flow control and heat transfer mitigation have not proven successful at high speeds. This has motivated exploration of more revolutionary techniques. Since hypersonic flow is, or can be artificially made to be electrically conducting, an innovative method calls for a properly established electromagnetic field to provide surface shielding. The advantages of magnetogasdynamics (MGD) include the absence of moving parts, short control response times, and the possibility of leveraging the massive scales and advanced technological state of electrical engineering. Ground testing difficulties dictate that the development of these techniques will be led by modeling, with simulations providing insight into the flow physics as well as guidance on experimental test-bed configuration.

The problem is fundamentally multidisciplinary since it requires integration of the Navier-Stokes and Maxwell equations, together with models of thermo-chemical, non-equilibrium phenomena. This yields a large non-linear equation set and requires intelligent simplifications for computer modeling. The current effort employs elements of first principles and phenomenological approaches for the MGD formulation. Thus, the Lorentz forces and energetic interactions are treated as source terms; the electric field is obtained by solving the Poisson equation arising from the current continuity constraint and the current is obtained from the generalized Ohm's law.

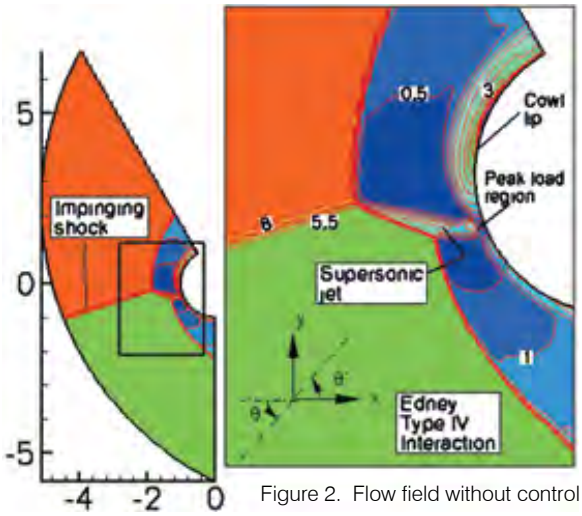

Figure 2. Flow field without control

Alleviating High Heat Transfer Rates

Massive computational resources are mandated by the mathematical complexity of the governing equations coupled with the need for fine spatio-temporal discretizations to assure solutions of high fidelity. Despite the use of a unique algorithm, which blends high-resolution upwind, high-order compact-difference/filtering and implicit time-integration schemes, these problems require months to solve on stand-alone workstations but can be solved in days on the high-speed HPC systems. This greatly facilitates numerical exploration of the parameter space to characterize effectiveness and identify promising candidates for further study in ground-test facilities.

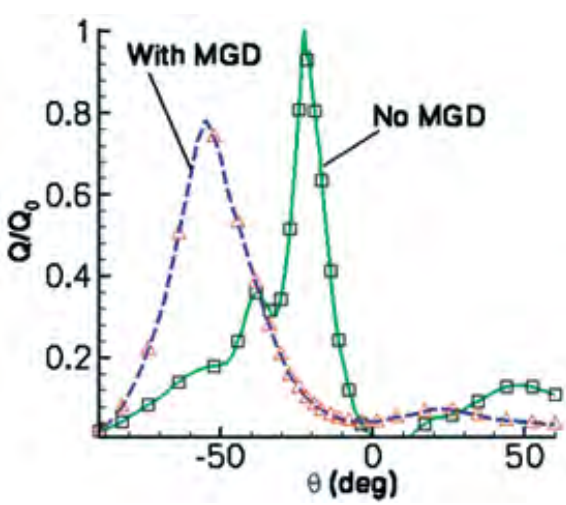

Figure 3. Effect of MGD-control on heat transfer rates

To alleviate the high heat transfer rates, a circumferential, radially decaying magnetic field is imposed on the flow, consistent with an axially directed current. Various electrical conductivity distributions are enforced in an electrodeless setup to reduce the strength of the jet and to modify the fluid dynamic bifurcation. Figure 3 shows the effect of one of the more promising control configurations in which the primary triple point is modified with an ionized hot-spot, reducing peak heat transfer rate by over 20%. Surface pressures also diminish to a similar extent. Furthermore, parametric studies demonstrate that these benefits increase as the second power of magnetic field strength and first power of electrical conductivity. Post processing yields invaluable insight into the mechanics of flow control. Figure 4 shows that the magnetic field has modified the pattern from Type IV to that classified as Type III, and the supersonic jet does not form at all. Energy balance analyses indicate a highly efficient and reversible flow field energy extraction process, which raises the possibility of even more effective control through realization of successive flow bifurcations.

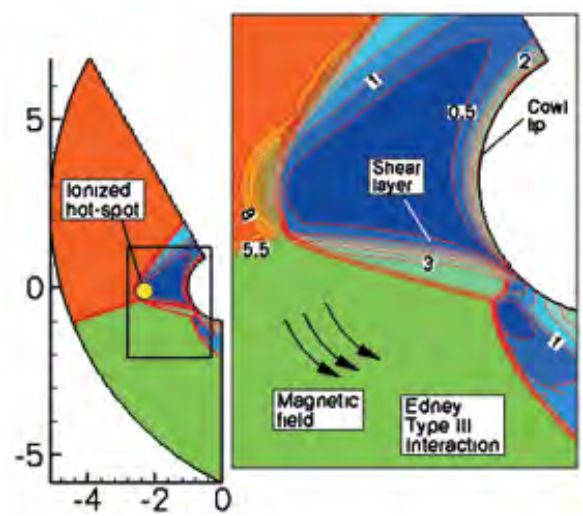

Figure 4. Effect of MGD-control on flow field

The analysis of advanced flow control techniques is greatly facilitated by visualizing the results. Although the primary goal is often to influence quantities on the surface itself, many promising possibilities leverage the large gains obtained by modifying the overall flow structure. Scientific visualization aids in understanding the fluid dynamics and control response and fosters out-of-the-box thinking.

Future of Scramjets

This work clearly shows the ability of advanced electromagnetic force-based methods to alleviate or eliminate problems encountered in sustained hypersonic flight.

Significant challenges remain both in enhancing the theoretical model and in comprehensively evaluating and exploiting the potential of these revolutionary proposals. Phenomenological aspects of the formulation are presently being replaced with first principles approaches, particularly in the modeling of high-temperature effects. The use of wall electrodes and non-equilibrium ionization techniques opens exciting new possibilities in managing global energy budgets of scramjet operation. MGD-assisted diffusers, nozzles and combustors promise efficiency enhancements unthinkable with conventional methods, and may provide the key breakthrough to make sustained hypersonic flight feasible.

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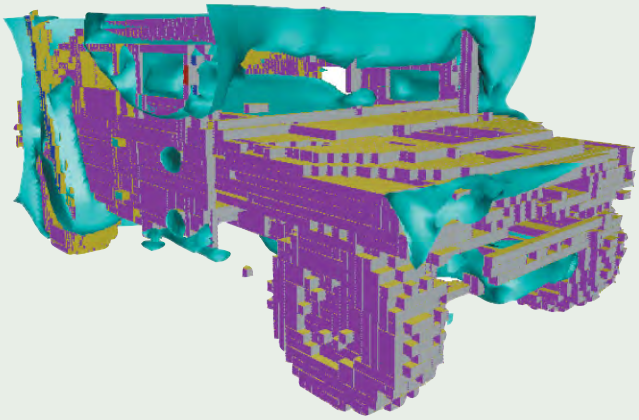
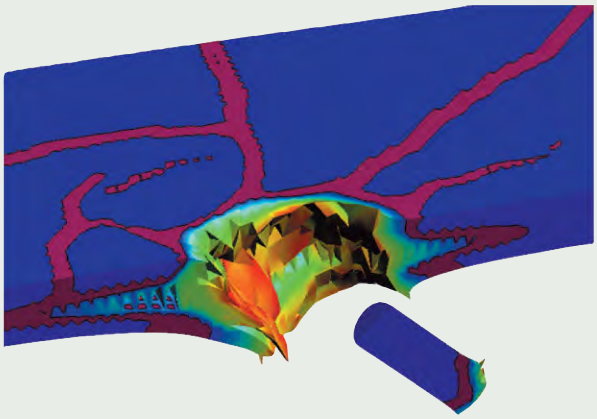
CTA: Computational Electromagnetics and Acoustics

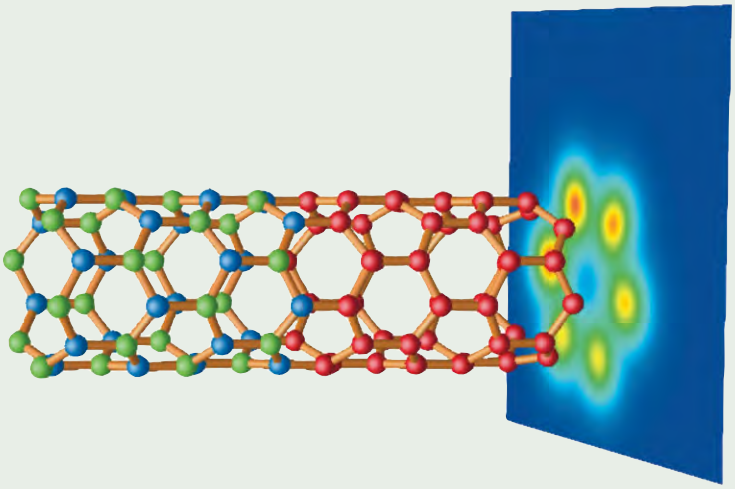
Computer Resources: Cray SV1 [NAVO] and IBM SP3 [ASC]

Leveraging Information Technology



End-to-End Interoperable Communications
Survivable Strategic Communications





References (from left to right):

Mixed Electromagnetic — Circuit Modeling and Parallelization for Rigorous Characterization of Cosite Interference in Wireless Communication Channels by Costas Sarris
Electric field magnitude iso-surfaces on a military vehicle staircase model at 50 MHz

"Presto": Parallel Scientific Visualization of Remote Data Sets by Andrew Johnson
View of the Presto interface showing the results of a CSM simulation. Damage and material stress is shown for a projectile-armor penetration

Novel Electron Emitters and Nanoscale Devices by Jerry Bernholc
Electron distribution near a tip of a BN/C nanotube in a field emitter configuration

Leveraging Information Technology

A Native American Indian chief once remarked that the words written on the medallions worn on necklaces of his tribesmen are but a visual reminder of the words written on their minds and souls. The words on the Air Force Research Laboratory coin from General Hap Arnold read, "The First Essential of Airpower is Pre-Eminence in Research." The mind and soul of America's transformational department of defense exist in a body fundamentally dependent on pre-eminence in research; a body fed by HPC technology. The following seven articles exemplify the importance of HPC in the transformational defense power the US DoD is becoming.

To support soldiers in the field and scientists in the laboratory, an effort from the Army High Performance Computing Research Center provides a persistent data repository for data producers and consumers. The *Virtual Data Grid* described in the article by Weissman provides just-in-time data production and delivery for data intensive HPC applications. This data management system assimilates and fuses data for real time and as-fast-as-possible computational systems, pumping valuable information into the 21st century battlespace. The Virtual Data Grid may enable modeling the evolution of toxic agents in public places, providing support to homeland defense organizations. Leveraging Virtual Data Grid information technology enables US and allied forces to project power into remote environments with integrated multi-source data access.

The technical capability discussed by Flemming, Perlman, Sarris, Thiel, Czarnul, and Tomko in *Mixed EM-Circuit Modeling and Parallelization* characterizes cosite interference problems relevant to military communication ad-hoc network architectures. This modeling tool mixes electromagnetic wave propagation and circuit modeling equations to simulate the effects of collocating electronic equipment on the same vehicle, station, or base. Specific communications impact to US forces projected anywhere in the world can be realized by leveraging this advanced communication focused information technology.

While the Virtual Data Grid technology provides US and allied forces access to data on a wide area network structure and the cosite electromagnetic interference technology models the communication channels connecting the troops to that data and its derivatives, the third effort, *Parallel Scientific Visualization of Remote Data* by A. Johnson, dramatically reduces the necessary network traffic and client machine requirements to get the data to the user by providing remote parallelized visualization of large data sets. This client-server approach to visualization of massive data puts visual data not only in the scientists' hands, but projects information into the deployed soldiers' battlefield. These first three articles describe rapid advances in information technology that connect the battlespace to large amounts of real-time and near-real-time data. Since this third technology reduces network traffic, an alternative application might enhance space operations by enabling data visualization across limited communication channels.

The article by Samios and Welday, *Connecting the Navy Research Lab to the Department of the Navy's Chief Information Officer* describes a successful effort that physically connects the two locations with asynchronous, real time variable bit rate transfer capability. This advanced information technology employment provides permanent virtual circuits upgrade throughout the core fabric of the defense research and engineering network wide area network (DREN WAN). In addition to VTC link, this connection enables real time experiments with secondary benefactors including modeling and simulation, test and evaluation, and research and development users on the DREN WAN. This article details a terrific example of leveraging rapid advances in commercially available network technology to improve US communication connectivity.

Included in this section is *Novel Electron Emitters and Nanoscale Devices* by Bernholc, that describes an exciting application of the nation's HPC resources. The authors were able to accomplish computationally intensive nanoscale device analysis to investigate and predict the properties of new

materials and technologies. Impacts of this particular analysis includes flat panel displays and electron emitters. This study from the Office of Naval Research provides an excellent example for how HPC plays a vital role investigating revolutionary concepts in a field cited in the quadrennial defense review as having a potentially large impact on US military capability.

The final two articles describe evolutionary enhancements to two battlefield simulation systems. *An Integrated Missile Defense Approach* by Johnson and Robertson improves the Missile Defense Agency's (MDA) wargaming capability by using the DoD HPC resources in conjunction with Missile Defense Wargame and Analysis Resource. Under this effort, the Joint National Integration Center (JNIC) improved MDA's homeland defense simulation realism by increasing the simulation size, including fog of war error simulation, adding a target assignment decision aid, and enabling data collection in parallel without performance degradation. The final article entitled *Successfully Operating WG2000 Simulation* by Fuller describes a JNIC developed simulation tool, Wargame 2000 (WG2000), that leverages HPC capability and high-speed high-volume communication network technology. WG2000 provides simulated battles for military planners around the world to exercise command and control human-in-control analysis. When coupled with the Virtual Data Grid technology, these evolutions in parallelization of wargame simulation tools provide the next generation of homeland defense simulation modeling.

These seven examples comprise a subset of HPC projects with current and future impact to the joint warfighting team. Secretary of Defense Rumsfeld has stated that: "It is not only about changing the capabilities at our disposal, but changing how we think about war. Imagine for a moment that you could go back in time and give a knight in King Arthur's court an M-16. If he takes that weapon, gets back on his horse, and uses the stock to knock his opponent's head, it's not transformational. Transformation occurs when he gets behind a tree and starts shooting." Our nation's High Performance Computing resources are an essential tool in a battlespace demanding information superiority and advanced technology. When used in the transformational sense Mr. Rumsfeld describes, this computational and algorithmic power enables US forces to employ an arsenal of leading edge technologies in transformational manners.

1st Lt John Gulick, USAF

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The Virtual Data Grid: Just-in-time Data Delivery … and Data Production for HPC Applications

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Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN

A persistent data repository for data producers and consumers is needed to support soldiers in the field and scientists in the laboratory. Increasingly, data from a large variety of sources must be available quickly and reliably. Earlier solutions did not attempt to provide a single coherent infrastructure for data management. HPC is needed to produce data on the fly such as in battlefield simulation scenarios. HPC applications will also critically rely on data products (e.g., battlefield visualization).

Virtual Data Grid

This project supports and extends HPC technology to a wide-area Grid. The digitally enhanced battlefield of the future requires a distributed data and computation infrastructure. As shown in Figure 1, this infrastructure must provide for the storage and delivery of distributed, heterogeneous, data sources including geographic information systems data, weather, sensor grids (e.g., the Information Grid, NSOFT) and a variety of national assets. Often times, the data of interest is large, and distributed across different remote storage locations and data delivery networks. In addition, connection to remote data networks may be intermittent (e.g., sensor networks). A reliable, efficient, persistent data network called the Virtual Data Grid (VDG) is being developed for this purpose. The VDG allows data producers and consumers to see a consistent infrastructure for data exchange. The VDG also allows data produced from high performance simulations to be stored and made

> "The digitally enhanced battlefield of the future requires a distributed data and computation infrastructure."

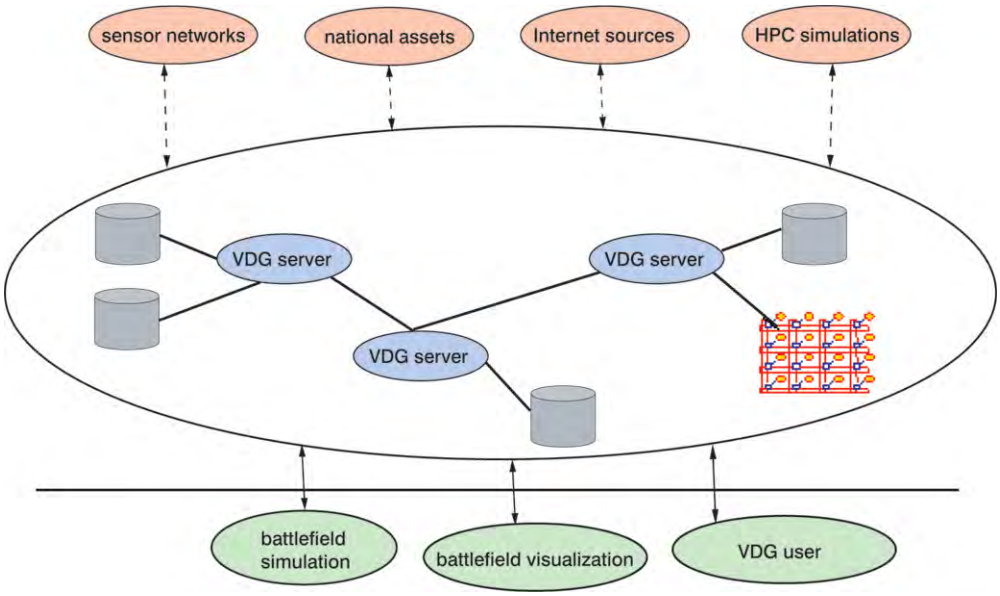

Figure 1. Virtual Data Grid

available by launching such simulations on-the-fly to produce needed data on demand. A publish-subscribe applications programming interface (API) for data producers and consumers is provided.

The VDG leverages existing metacomputing Grid technologies and solutions to meet its requirements. For example, it uses the Globus toolkit support to connect a grid of VDG servers that manages a set of persistent storage depots. Internally, the VDG implements data scheduling algorithms for performance, including intelligent caching, staging, and prefetching of data based on application patterns of access (an API for expressing access patterns has been developed). Data scheduling considers the demand for a particular data object by concurrent users. Novel data scheduling algorithms have also been developed. Data is moved close to the consumer before the data is actually required. Popular data objects are moved to a location near the consumer base. In some cases, popular data objects are replicated. Large data objects are also striped across several VDG server depots for increased performance. Fault tolerant delivery of data objects is achieved by intelligent replication schemes.

Currently, the VDG represents core infrastructure in support of the AHPCRC's efforts in Virtual Computing Environments. One application is predicting and simulating the evolution of toxic agents in large public places (e.g., stadiums). Data from many sources must be integrated and simulations must be launched quickly to solve this problem.

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CTA: Forces Modeling and Simulation/C4I

Computer Resources: Cray T3E and IBM SP2 [AHPCRC]

Mixed Electromagnetic — Circuit Modeling and Parallelization for Rigorous Characterization of Cosite Interference in Wireless Communication Channels

T. Flemming and B. Perlman

Communication-Electronics Command (CECOM), Fort Monmouth, NJ

C. Sarris, W. Thiel, and P. Czarnul

University of Michigan, Ann Arbor, MI

K. Tomko

University of Cincinnati, Cincinnatti, OH

The objective of this research is to characterize cosite (collocation of electronic equipment on the same vehicle, station, or base) interference problems relevant to military communication ad-hoc network architectures, in complex, arbitrary environments, through scaleable computational techniques for the numerical modeling of electromagnetic wave propagation (Maxwell's equations) and transmitter-receiver geometries (circuit equations).

The numerical tools developed in this research provide, for the first time, the opportunity of performing end-to-end characterization of military radio network performance under cosite interference conditions including realistic vehicle models and advanced receiver architectures in environments as complex as a forest. Two applications evolved from this work. The first application was a physics-based optimization of the system design (such as choice of coding scheme and power levels). The second application was an educated, simulation-based planning of exercises in tactical communication scenarios.

Relying on Measurement-Based Models

Despite the high interest that cosite interference problems present from both a research and an application point of view, few efforts have been made towards their rigorous theoretical characterization. Straightforward calculation of interfering power levels is not possible because of the close proximity of interferers and the presence of complex scatters and antenna platforms. Therefore, some previous studies have relied on measurement-based models that omit the influence of system-specific parameters on communication link performance. On the other hand, time-domain methods for the solution of Maxwell's equations hold the promise of fully accounting, not only for the effect of platforms on radiation properties of vehicular antennas, but also for the operation of front-end electronics, through a state-equation description of the latter.

> "These techniques allow for the accurate, physics-based evaluation of system performance via mixed electromagnetic-circuit simulations and provide the tactical communication analyst with a reliable simulation tool that takes into account critical electromagnetic interactions within complex, real-life environments."

The computational cost of time-domain techniques grows large, however, when more complex operation environments are considered for cosite interference scenarios. An example of particular interest is the case where communication between a receiver and a transmitter, under cosite interference conditions, is attempted within a forest environment at very high frequency (VHF) band military radio frequencies.

Using a Method of Moments Approach

A hybrid solution has been implemented for modeling a multi-antenna, mobile communication system with a time-domain technique and its interaction with its forest environment by means of the MoM approach. In addition, advanced circuit models are included through a recently developed circuit simulator (TRANSIM), that allows for fast time-domain analysis of linear and nonlinear components.

Time domain electromagnetic modeling is based on the Haar wavelet based Multiresolution - Time Domain technique (MRTD), which allows for dynamically adaptive gridding throughout the computational domain. Using a novel, efficient thresholding algorithm, wavelet operations are not carried out at regions of the domain where slow field variations are observed. That effectively amounts to establishing a multigrid with a cell aspect ratio of 1:8 (since one wavelet level is used in all three dimensions). In addition, wavelet operations dictate an adaptive, global repartitioning algorithm for periodic load balancing, which improves the performance of the parallel code.

Using Communication Scenario Simulations

Communication scenarios have been simulated involving the interaction of neighboring transmit-receive modules, communicating with a remote peer, within a forest environment. The simulation showed the effects of platform, multi-path and forest-induced attenuation of electromagnetic waves on network performance (Figure 1). Realistic models of vehicular platforms have been incorporated and several radiation properties of those have been brought to light (Figure 2).

The US Army Communication-Electronics Command scientists have predicted interfering power levels at multi-antenna vehicular systems and compared architectures showing the effect of the vehicle positioning on the performance of the radio network. The results have highlighted such issues as the dependence of parasitic interference between neighboring platforms on the shape of the vehicle and geometry-specific scattering effects and resonance.

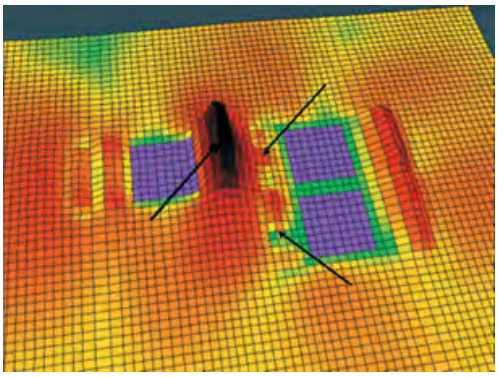

Figure 1. Interference pattern for three vehicular platforms (shown in lily) at 50 MHz, at the plane of the gap of the monopole antennas, mounted on them. Thick arrow indicates the position of a transmitting antenna and the thin arrows the position of receiving antennas.

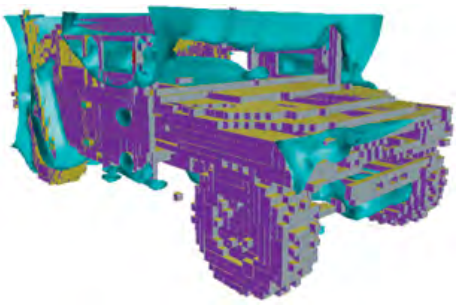

Figure 2. Electric field magnitude iso-surfaces on a military vehicle staircase model at 50 MHz

Scientific visualization was used to gain insight into the physical phenomena of interest for this research effort and has led to several important conclusions related to the effect of vehicle positioning on radio network performance based on inspection of visualization tool output.

Implementing Efficient, Scaleable Computational Techniques

Efficient, scaleable computational techniques for end-to-end characterization of cosite interference in military radio networks have been proposed and implemented in this project. These techniques allow for the accurate, physics-based evaluation of system performance through mixed electromagnetic-circuit simulations and provide the tactical communication analyst with a reliable simulation tool that takes into account critical electromagnetic interactions within complex, real-life environments.

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CTA: Computational Electronics and Nanoelectronics

Computer Resources: SGI Origin 2000 and IBM SP3 [ASC]

"Presto": Parallel Scientific Visualization of Remote Data Sets

Andrew Johnson
Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN

Presto is an interactive data visualization tool developed at AHPCRC which provides researchers, using their desktop workstations, the capabilities of a large and expensive visualization laboratory for visualizing large numerical simulation data sets. These data sets are computed on, and reside at, remote HPC systems. This is accomplished by implementing a closely coupled client-server paradigm that leverages the parallel computing technology of remote HPC systems. The client (i.e., the user's desktop system) and the server (i.e., the remote HPC resource) only need to be linked through a typical Internet or other dedicated network connection.

Limitations of Current Computing Models

A new visualization tool such as Presto is required due to various limitations with current computing and/or data processing models. Traditionally, a researcher would compute a large numerical simulation on a HPC resource that is physically located at a remote, central computing center such as a MSRC or DC. They would download the entire completed data set to their local workstation for post-processing and visualization. Today, researchers are computing data sets of between 1 and 200 gigabytes in file size or larger. Transfer of this amount of data across a network is impractical. Also, researchers do not typically have local computing resources powerful enough to load, process and visualize the entire data set effectively. These bottlenecks have limited the size and scope of the numerical simulations that researchers can create and process effectively.

Presto Solves Limitations

Presto solves both of these problems through its client-server implementation and parallel computing capabilities. The client-server implementation means that Presto actually consists of two separate components. The "Presto Client" runs on the user's desktop workstation, either Windows or UNIX-based, and handles all user interaction and displays all visualization geometry sent to it by the server. Visualization is accomplished through traditional boundary shadings, cross-sections, iso-surfaces, streamlines and volume rendering. The "Presto Server" runs on the remote HPC resource, and is written using the distributed-memory parallel programming model based on MPI, which is portable to almost all HPC systems such as the Cray T3E, Cray X1, IBM SP, SGI Origin servers, and PC clusters. The server is responsible for loading and processing the large 3-D data set, and generating and/or extracting any visualization geometry requested by the client component. The parallel implementation is fully scalable, so the size of the data set that can be visualized from the desktop is only limited by the size of the remote HPC resource.

"Presto has been built to visualize 3-D unstructured mesh data sets composed of either scalor or vector variables, and is typically being used to visualize CFD and CSM data sets."

Presto has been built to visualize 3-D unstructured mesh data sets composed of either scalor or vector variables, and is typically being used to visualize CFD (Figure 1) and CSM (Figure 2) data sets. Typically, unstructured mesh data sets containing between 1 and 40 million tetrahedral elements are visualized using up to 32 processors of a Cray T3E. Data sets containing over 1 billion tetrahedral elements have been visualized with Presto using 1024 processors. Currently, Presto is being used in a production environment, and several future updates

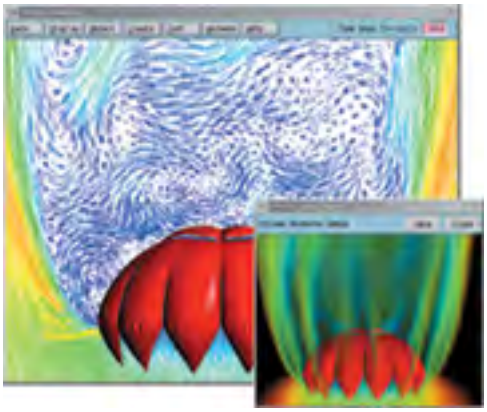

Figure 1. View of the Presto interface showing the results of a CFD simulation. Velocity vectors are shown as well as a volume-rendered image showing velocity magnitude.

are being planned which include implementing a tighter client-server security model as well as geometry compression techniques to reduce Presto's network bandwidth requirements.

Advantages of Presto

Presto provides three advantages to the researcher: 1) Visualizes remote data sets: Basically, the researcher just leaves the data set on the large work disks of the HPC system that computed the results. The "Server" part of Presto runs on that HPC system and is responsible for loading and processing the numerical simulation results. The user never needs to transfer their data set off of the HPC system that generated it. Data sets located on any HPC system can be visualized from any remote location as long as an Internet connection (TCP/IP) can be created between the user's local workstation and the remote HPC system. 2) Scalability: The Presto Visualization "server" is fully parallel based on the MPI library. This means that the server runs on any parallel architecture and is fully scalable in terms of memory. When visualizing a small data set, the user can use only a few processors to load the data set. When visualizing a large data set, the user may have to use more processors. Typically, around 8 to 16 processors are used, but Presto has been tested with as many as 1024 processesors on a Cray T3E. This many processors were required to visualize one of the largest data sets ever, which involved an unstructured mesh containing 1 billion tetrahedral elements. 3) Easy-to-use: The "client" part of Presto handles all of the GUI user interface and displays all of the graphics components sent to it by the server over the Internet. The client runs on Windows or any UNIX flavor (Linux, SGI, etc.). Once the connection between the client and remote server is made, the application behaves as any traditional desktop application.

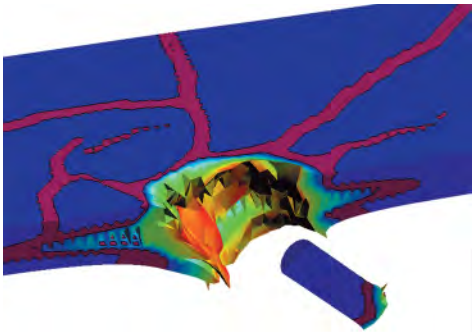

Figure 2. View of the Presto interface showing the results of a CSM simulation. Damage and material stress is shown for a projectile-armor penetration.

Presto saves time and money (i.e., users can use their traditional workstations and not an expensive visualization system) and effectively uses HPC parallel resources for post-processing and visualization. A user from almost any type of desktop system can visualize data sets of almost any size quickly and efficiently. This makes the use of numerical simulation by researchers more effective, efficient, and easier, especially for large data sets.

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CTA: Computational Fluid Dynamics and Computational Structural Mechanics

Computer Resources: Cray T3E ,IBM SP, and Cray X1 [AHPCRC] and SGI Origin 2000 [ARL]

Connecting the Naval Research Laboratory to the Department of the Navy's Chief Information Officer

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Just prior to September 11, 2001, the Department of Navy (DON) Chief Information Officer (CIO) approached the Network Infrastructure Services Agency (NISA) to support a high-speed permanent virtual path (PVP) between their offices and the Defense Research and Engineering Network (DREN) node in the Pentagon (NISA supports both locations and the cross-connection). After September 11, 2001, available bandwidth on some of the links was reduced and the original request could no longer be easily accommodated. As a result, the request for a 40-Mbps PVP was reduced to 6 Mbps. The Naval Research Laboratory (NRL) looked to DREN to provide the link.

The technical problem centered around how to connect multiple DoD sites using real-time variable bit rate virtual circuits, which have very low latency and jitter. Resolution of the problem will have a wider impact to DoD Science and Technology, Modeling and Simulation, and Test and Evaluation communities within the Navy.

Early Issues

There were several early issues that were identified: physical connectivity from the closest NISA Asynchronous Transfer Mode (ATM) switch to the DREN ATM switch at the Pentagon, availability, cost, and characteristics of the PVP had to be determined. Security also had to be considered; the existing security on the DON CIO workstations could not be compromised. Any traffic between these workstations and the NISA-supported systems would leave PT-1, tunnel through to the DREN wide area network (WAN), enter the NISA enclave and existing NISA security mechanisms through the same path that Unclassified but Sensitive Internet Protocol Router Network and Internet traffic follows, without interacting with the NISA infrastructure.

In the past, procuring many independent unclassified and classified connections between each site would have solved this problem. But separate circuit solutions are very difficult to manage, very expensive, and usually result in severe limits on bandwidth availability.

"In September of 2002, a solution was completed, that connects several TeraMedia VTC sessions between NRL and DON CIO spaces. This was done by using real-time variable bit rate (rt-VBR) setups over DREN."

Connection Established

In September of 2002, a solution was completed that connects several TeraMedia VTC sessions between NRL and DON CIO spaces. This was done by using real-time variable bit rate (rt-VBR) setups over DREN. Figure 1 shows the connection using ATM-connected Macinstosh workstations and a Sun server at DON CIO (PT-1).

This project brought to the fore other ATM requirements in the HPMCP community for rt-VBR permanent virtual circuits (PVCs). As a result, DREN WAN switches throughout the core fabric were upgraded to support rt-VBR PVCs as well as switched virtual circuits.

The Future of ATM and the Use of PVCs With DREN

Even as long haul WAN providers move away from ATM based networks to increasingly sophisticated IP based networks, there will be ATM-oriented Quality of Service requirements that will be difficult to meet with

the new architectures for some time to come. At the start of this project, DREN could not handle the low jitter requirements that drove a rt-PVCs solution; today it can. The beneficiaries of this innovation are not only the original testers but, a much wider group of communities that includes modeling and simulation, test and evaluation, and research and development. Today, "hardware-in-the-middle" or "man-in-the-loop" simulations and tests can be done in real-time. Without this capability, the experiments cannot be done remotely, and assumptions had to be made by researchers to simulate the "real-time" effect put on their test or experiment.

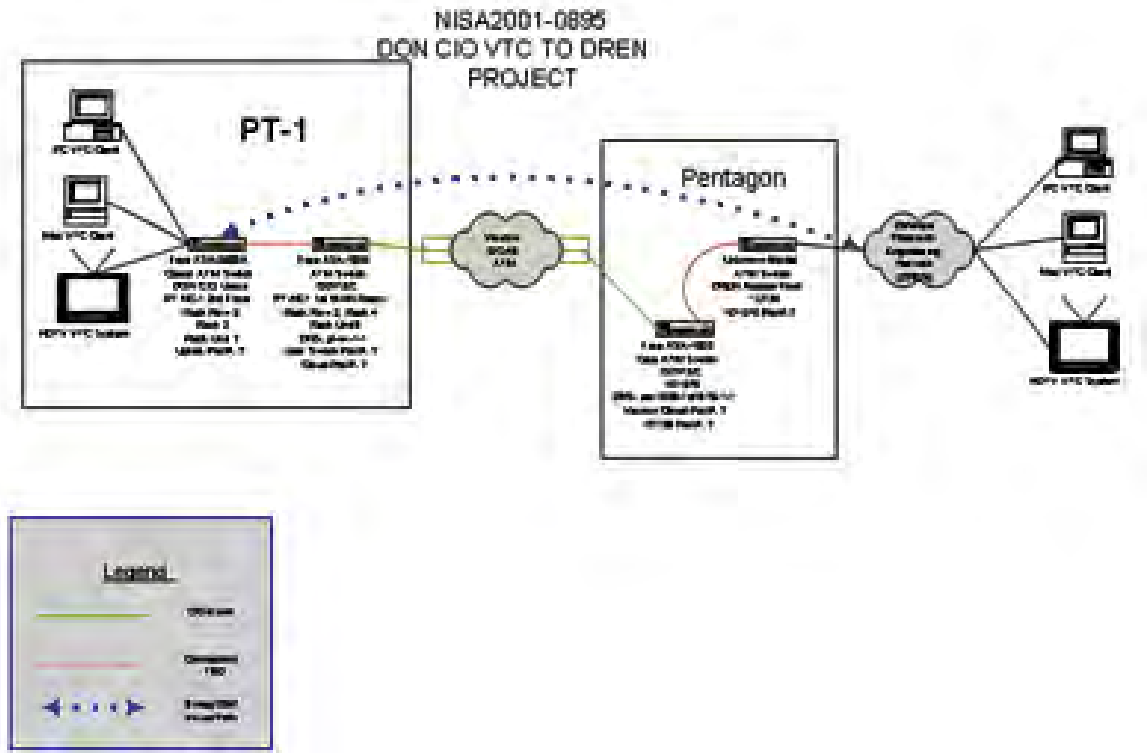

Figure 1. The box on the left shows an ATM switch in the PT-1 wiring closet under NISN control. From the PT-1 ATM switch, there is a 6-Mbps rt-VBR PVP through the NISN cloud to the DREN switch in the Pentagon. The PT-1 switch signals with the DREN switch (and is using a subset of its ATM NSAP address space). The DREN/PT-1 switches fully signals with DREN so direct end-to-end ATM connection are possible. The LECS, LES, and BUS are running on the DREN switch and an ELAN was created for this project.

Novel Electron Emitters and Nanoscale Devices

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Sponsor: Office of Naval Research (ONR), Arlington, VA

Nanotubes are one of the most interesting new materials to emerge in the past decade. Several layered materials form tubular structures, but the most prevalent are carbon (C) and boron nitride (BN) nanotubes. The discovery of carbon nanotubes as a material with outstanding mechanical and electrical properties has led to a quest for other novel graphene-based structures with technologically desirable properties. The closely-related boron nitride (BN) nanotubes and mixed BN/C systems, which are now being produced in gram quantities, have electronic properties that are complementary to pure carbon nanotubes and could thus be useful in a variety of electronic devices.

The focus of this work was to use Challenge-level HPC resources to investigate and predict properties of advanced new materials and technologies critical to the DoD's needs. This research has shown that BN/C nanotube structures can be used for effective band-offset engineering in nanoscale devices, and for robust field emitters with efficiencies of up to two orders in magnitude higher than those built from carbon nanotubes.

Using Sophisticated *ab initio* Techniques

Until very recently, the design and prediction of advanced materials has been an empirical undertaking. The advent of HPC enabled the use of sophisticated *ab initio* techniques, which can predict the properties of complex materials. The simulations were carried out using a novel, real-space multigrid method developed especially for very large-scale quantum calculations. Plane-wave-based methods have also been used for independent crosschecking of the key results. The use of multigrid techniques permits efficient calculations on ill-conditioned systems with multiple length scales and/or high-energy cutoffs. The multigrid codes have been very well optimized for massively parallel computers and their execution speed scales linearly with the number of processors. The calculations required up to 128 processors of the Cray T3E supercomputer. The calculations were carried out in a supercell geometry, using up to 6 layers of boron nitride and carbon. In a periodic super lattice of polar and non-polar materials (such as BN and C), any spontaneous polarization field manifests itself as a periodic oscillation in the electrostatic potential of the system, due to periodic boundary conditions. The full potential then displays a saw tooth behavior that is the signature of a spontaneous polarization field superimposed onto a periodic crystalline potential. In order to obtain the value of this field, the planar average of the electrostatic potential along the nanotube axis has been evaluated. This average, which is over the plane perpendicular to the tube, displays strong oscillations due to the varying strength of the ionic potentials. To subtract out this effect, the corresponding "bulk" averages have been subtracted out, and thereby the one-dimensional macroscopic average of the electrostatic potential of the system was calculated. Since nanotube calculations include a sizable vacuum region surrounding the nanotube, the band offsets could be computed directly by referring the highest occupied levels to the vacuum level.

"This research has shown that BN/C nanotube structures can be used for effective band-offset engineering in nanoscale devices, and for robust field emitters with efficiencies of up to two orders in magnitude higher than those built from carbon nanotubes."

Symmetry of Nanotube Important

It is clear that symmetry of the nanotube plays an important role in determining the magnitude of the spontaneous polarization field. The strongest effects will be observed in the (k, 0) zigzag nanotubes, since this geometry maximizes the dipole moment of the BN bond. This study has primarily concentrated on

zigzag nanotubes with diameters of up to 12 E. The value of the polarization field obtained from the slope of the macroscopic average potential for zigzag tubes is shown in Figure 1. In contrast, the (k, k) armchair nanotubes are not expected to display any spontaneous polarization field. This is because any individual nanotube ring must be charge neutral, so that no fields are possible. This has been directly verified for the case of a (5,5) BN/C super lattice.

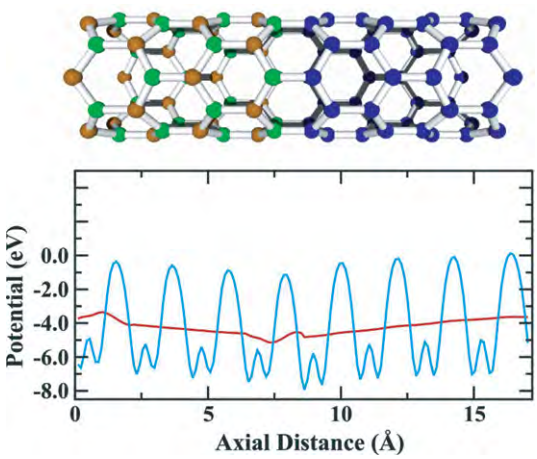

Figure 1. The structure of a BN/C nanotube superlattice (top), the average electrostatic potential (blue) and its macroscopic average (red). The slope in the macroscopic potential leads to an electric field inside the nanotube.

Chiral nanotubes will have fields that are between the zigzag and armchair values.

From the calculated band-offsets, it is clear that the valence state of the BN/C super lattices is always spatially localized in the carbon region. This state plays an important role in determining the response to the macroscopic electric field induced by the BN section. In particular, the oscillatory behavior observed as a function of the helicity index can be understood from the symmetry property of the valence state, displayed in Figure 2 for two zigzag nanotubes. Figure 2 directly shows that the valence state is localized within the carbon section. For small diameter nanotubes, it displays either a longitudinal or a transverse symmetry as exemplified by the (7,0) and (8,0) tubes, respectively. Specifically, for (k = 3p+1, 0) nanotubes such as the (7,0) tube, the valence state always assumes a longitudinal character. The axial distribution of valence electrons will therefore induce a depolarization field that is opposite to the one intrinsic to the BN section. This field is quite effective in small diameter nanotubes in reducing the polarization, so that for the (7,0) nanotube the screening is almost total and the observed macroscopic field is close to zero. For larger diameter nanotubes, the symmetry of the valence state gradually loses its peculiar axial or longitudinal character and the macroscopic field asymptotically approaches the value obtained for a flat BN sheet in the "zigzag" direction.

Assessing the Effectiveness of BN/C Systems

Despite the screening by the valence electrons distributed over the carbon portion of the BN/C superlattices, a net polarization field is built up along any zigzag structure. The existence of an intrinsic macroscopic field will clearly influence the extraction of electrons from BN/C systems, when these are used as field emitting devices. Qualitatively, a good electron emitter is characterized by a large geometrical field enhancement factor, due to the needle-like shape of nanotubes, and a small work function that is an intrinsic property of the emitter material (Figure 3). Quantitatively, the current at the emitter tip is calculated from the so-called Fowler-Nordheim relationship. To assess the effectiveness of BN/C systems as emitters, the field enhancement factor for tubes of length 15.62 E and an applied field of 0.11 V/E have been computed. As expected, the applied field is very well screened inside the system and the local field enhancement factors were similar for different BN/C systems. Since the field enhancement factor increases linearly with the size of

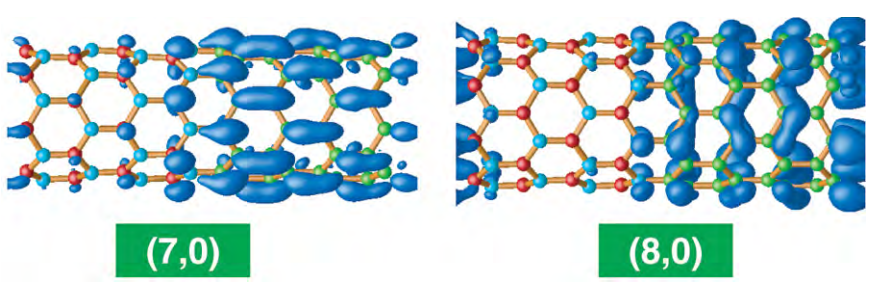

Figure 2. Electron distribution in the top valence state for (7,0) and (8,0) BN/C nanotubes. Note that the symmetries of the two states are quite different.

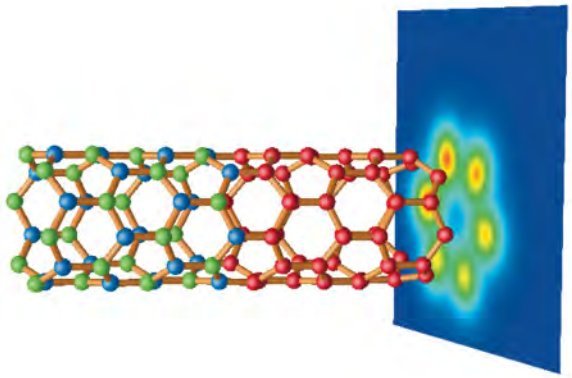

Figure 3. Electron distribution near a tip of a BN/C nanotube in a field emitter configuration

the nanotubes, large enhancement factors are possible for long nanotubes. However, the polarization field can clearly be used to further enhance the field emitting properties. In order to examine this effect quantitatively, researchers have built-up a set of finite sized (6,0) zigzag structures using B, N, and C in various combinations. The work functions were then computed as the difference between the vacuum level and the Fermi energy of the system. The former was obtained by the previously discussed potential average procedure, while the latter was simply given by the highest occupied eigen state-of-the-system. With this method, we calculated a work function of 5.01 eV for a (10,10) carbon nanotube, in close agreement with previously published values. For the smaller diameter (6,0) carbon nanotube, we found a considerably larger work function of 6.44 eV. This is primarily due to curvature effects.

Turning to the heterostructures, the researchers considered a finite NB/C (6,0) system consisting of four alternating N and B layers followed by 8 C layers, giving a total of 96 atoms. Due to the net polarization field experienced by the electron, the work function is reduced to 5.04 eV at the C tip and increased to 7.52 eV on the N tip. The same trend is observed for the BN/C system, for which the work function on the B tip is equal to 5.00 eV while it takes a value of 6.45 eV on the C tip. Therefore, the work function decreases by a significant 1.40 eV, as compared to the pure carbon system. This is large enough to lead to significant macroscopic effects. According to the Fowler-Nordheim relationship, the current density depends exponentially on the work function. It follows that the insertion of BN segments in C nanotubes will increase the current density by up to two orders in magnitude as compared to pure carbon nanotube systems.

Future Uses for Nanotubes

Nanotubes are prime candidates for novel electron emitters, to be used in ultrahigh resolution flat panel displays and cold-cathode-based microwave amplifiers. The hundred-fold increase in the emission current density would obviously have a major effect on the use and efficiency of electron emitters at the battlefield and in support systems. The variability of the band offsets in BN/C systems as a function of their radius offers substantial flexibility when designing novel nanoscale electronic devices.

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CTA: Computational Electronics and Nanoelectronics
Computer Resources: Cray T3E [NAVO]

An Integrated Missile Defense Approach

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The Missile Defense Agency (MDA) uses a series of operator-in-the-loop wargames to examine Ballistic Missile Defense System (BMDS) issues for the near-term (2004–2006) and far-term (2012). The primary means of examining these issues is to use DoD HPC resources in conjunction with Missile Defense Wargame and Analysis Resource (MDWAR) and other federated simulations. To achieve optimal realism within its war games, MDWAR explicitly models threats, interceptors, sensors, and communication systems (including passing tactical message contents in near-native formats). This approach permits MDWAR to enhance field exercises and other HWILT by providing high-level integration between simulated future missile defense system elements and today's real battle management, command, control, communications, computers and intelligence equipment. Planners can evaluate the practical effectiveness of adding an additional family of systems interoperability features by extending the tactical messages set within MDWAR's joint data network communications model.

MDWAR Innovations

MDWAR's design includes extensive data collection and information retrieval capabilities that provide insight into the tactical messages and engagement event outcomes. The data collected during a wargame are available worldwide using the Secret Internet Protocol Routed Network (SIPRNET) and any commercially available Internet browser. Multiple innovations are a direct result of the HPC contributions. One innovation is that MDWAR is the first successful Optimistic, Parallel, Discrete Event Simulation (O-PDES) framework. In achieving MDWAR's vision, the designers committed to the use of an O-PDES framework as the basic simulation engine. The decision to use O-PDES as the foundation for a real-time, interactive, simulator destined to participate or even lead Distributed Interactive Simulations and High Level Architecture federations is not without controversy. Synchronous Parallel Environment for Emulation and Discrete-Event Simulation (SPEEDES) is the most significant advancement in state-of-the-art discrete event simulation in the last five years and was the only mature framework. Its primary use is in as-fast-as-possible (AFAP) academic applications but it is available as a government off-the-shelf product.

MDWAR expands the scalability envelope. The primary reason for replacing the previous wargaming tool is to achieve the performance needed to simulate more objects at higher fidelity. In the past, problem size and fidelity were reduced to achieve real-time execution. MDWAR's goal is to maintain the desired problem size and fidelity and "dial-up" the computer power to achieve real-time performance

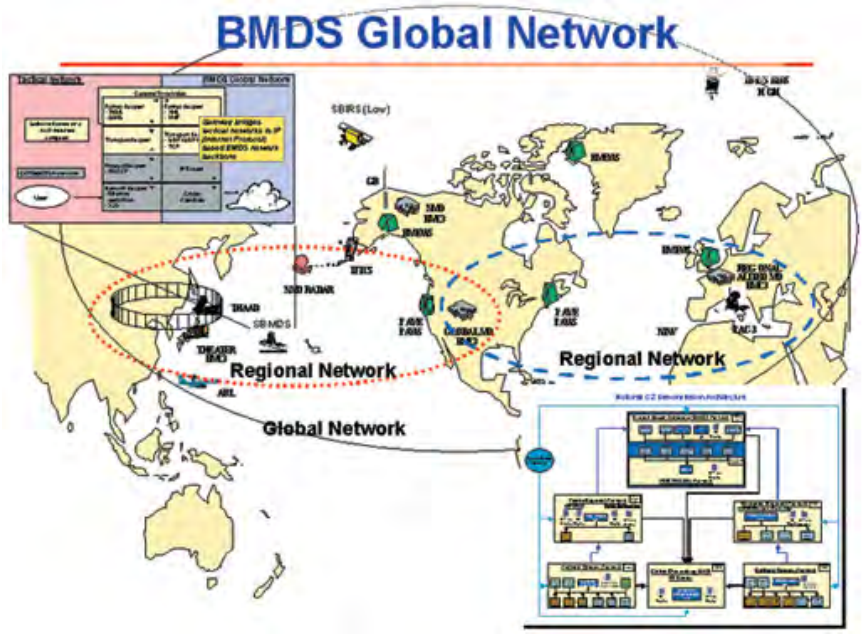

Figure 1. BMDS System

through the use of distributed processing technologies. The first National Missile Defense wargame in 1999 was run on twelve CPUs and involved six radars, a simple point-to-point communications model, tens of threat objects, tens of interceptors and 25 non-interactive player positions. Seven months after its implementation, MDWAR was simulating 56 radars, 3,000 interceptors, 50 threat objects, 59 fully independent battle managers, and a theater-wide Joint Tactical Information Distribution System (JTIDS) communication system operating in an imperfect space track environment. It supports 32 fully interactive player positions at three command and control levels and runs on 25 CPUs. Two months later, MDWAR was handling an approximately 50 percent increase in the threat load through the modeling of duplicate tracks in an imperfect Single Integrated Air Picture. Test problems are being run on 88 CPUs in preparation for even larger problems. The practical demonstration of this kind of scalability is another important advancement in the state-of-the-art.

O-PDES Techniques Eliminates Simulation Constraints

MDWAR changes the fundamental nature of the capability versus performance tradeoff in force-on-force level, real-time simulators. With previous missile defense simulators, it was often necessary to simplify the simulation to achieve real-time execution by reducing modeling detail and resolution or scenario complexity. MDWAR pioneers the application of O-PDES techniques to harness the processing capability of today's high-performance, multi-processor computers. MDWAR's advanced technology all but eliminates the need to constrain the simulated scenario definition for real-time execution. MDWAR maintains real time performance, simulates more defense elements at higher fidelity, and operates in more complex and realistic environments than previously possible with other wargaming tools. Its high-end capabilities are impressive; yet it retains its predecessor's variable fidelity and portability.

MDWAR overcomes the customary constraint to model the perfect information situation. In a Joint Theater and Missile Defense Organization wargame, the JNIC did test the introduction of fog-of-war contributors to evaluate joint command and control modes and firing doctrine in the presence of imperfect information. Real-world location and alignment biases (errors) were intentionally introduced into MDWAR sensor models; the perceived tracks were passed to a simulated JTIDS communications network where explicit correlation algorithms produced realistic track "drops," "swaps," and "duals" as well as "Reporting Responsibility dueling" behaviors.[1] The sensor biases and correlation control parameters were tuned to achieve the target space track picture quality necessary to satisfy the game objectives. This represents an advance in the state-of-the-art because it is the only real-time, interactive simulator with both the fidelity and capacity to look at the theater-wide ballistic missile defense operational behaviors in the presence of uncertain information.

"With previous missile defense simulators, it was often necessary to simplify the simulation to achieve real-time execution by reducing modeling detail and resolution or scenario complexity. MDWAR pioneers the application of O-PDES techniques to harness the processing capability of today's high-performance, multi-processor computers. MDWAR's advanced technology all but eliminates the need to constrain the simulated scenario definition for real-time execution."

Target Assignment Decision Aid Developed

MDWAR also provides a test environment within which a variety of test articles, concepts of operations (CONOPS), tactics, techniques and procedures, algorithms, decision aids, real world systems, and prototypes are embedded and their human in control aspects analyzed. In an early application, MDWAR developers were asked to automate the specified joint firing doctrine in a way that allows the operators to control the theater ballistic missile engagements using a management by exception approach. By designing the Automated Weapon Target Assignment to be fully compatible with MDWAR's mission (e.g., operate in a fog-of-war environment), the developers have produced a prototype of what is believed to be the first theater-wide automated weapon target assignment decision aid. This first generation prototype was successfully exercised in an imperfect information environment in its very first exposure.

MDWAR has a heavy data collection concept that eliminates performance impacts. The primary purpose of any simulator is to generate data and MDWAR is no exception. It is common practice on

[1] R2 Dueling refers to reporting rules for radar data. Conflicts arise in radar data coming in and they must be deconflicted.

many (even non-real-time) simulators to turn off data collection in an effort to get acceptable runtime performance. MDWAR has the goal of collecting data with little or no impact on runtime performance. MDWAR's architecture, which consists of a combination of shared memory buffering and a separate dedicated data collection application, satisfies this goal. The contents of every tactical message and data on every simulated event (typically one to two million) produce one to two gigabytes of data that are collected in real-time with no measurable negative impact on runtime performance.

Technical Enhancements Spark Improvements

Through the use of HPC and state-of-the-art advances in simulation, MDA and the HPCMP have taken wargaming to a new level. MDWAR's design goal is to examine and to develop CONOPS, doctrine, tactics, techniques and procedures through the use of operator-in-the-loop experiments that include real-world fog-of-war challenges. The combination of advanced simulation technologies, performance oriented architecture, state-of-the-art HPC computers, and unique gaming facilities put this goal well within the reach of the air and missile defense communities. These technical enhancements translate into a number of improvements in the support provided to the MDA wargaming customers: a dramatic increase in the numbers of runs during game times; significant improvement in quantitative data collection leading to better analysis and understanding of emergent behaviors; and a rapid prototyping laboratory for analyzing operational concepts, battle management, mission function automation, and operator displays. The end result is a flexible tool that can be readily configured to represent desired modes of command and control, system architecture, and threat.

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CTA: Forces Modeling and Simulation (FMS)/C4I
Computer Resources: SGI Origin 2000 [JNIC]

Successfully Operating the Wargame 2000 Simulation

David Fuller
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The JNIC provides the nation a center of excellence for joint missile defense interoperability testing, wargaming, exercises simulation, modeling, and analysis. JNIC uses a locally developed simulation, Wargame 2000 (WG2000). WG2000 is intended to provide a simulated combat environment that will allow warfighting commanders, their staffs, and the acquisition community to examine missile and air defense CONOPS.[1] In the AFAP mode (non-real-time), WG2000 has a significant economic advantage in executing test simulations in parallel on the Origin 2000 servers instead of the serial execution seen on most real-time programs. The Air and Missile Defense Simulation, or AMDSim, is the core software computational component of WG2000. AMDSim contains the code for all functional simulation elements including battle management, sensors, communications nodes, missile threat and defense elements, and graphics displays. Using WG2000, military planners from around the world exercise command authority in simulated battles for command and control (C^2) human-in-control analysis.

SPEEDES Provides Wargame 2000 Framework

Jet Propulsion Laboratory's state-of-the-art SPEEDES framework forms the underlying basis for WG2000's high-performance, object-oriented, discrete-event, real-time simulation support. With its forte in time and multi-CPU management, SPEEDES supports both conservative and optimistic synchronization strategies. WG2000 improves upon the previous generation MDA/JNIC Advanced Real-time Gaming Universal Simulation. This is a pursuit for higher fidelity, greater realism, and configuration flexibility with significant parallel CPU execution supported by meaningful graphics. JNIC human-in-control C^2 wargame pioneering efforts remain a challenging effort.

> "In 2001, WG2000 achieved success at the eleven CPU scaling level. Today, scaling from 22 to 25 CPUs represents more than a 100 percent scaling improvement."

A WG2000 simulation execution results in a 35 to 60 minute consumption of from 3 to 25 CPUs in either dedicated or shared modes. Most executions use 22–25 CPUs in shared mode. In the shared mode, up to six complete copies of the simulation may execute simultaneously per server. WG2000 simulation executions most frequently occur in the AFAP mode on the shared servers. WG2000 does not require the use of special hardware such as aircraft cockpits or communication devices often seen in other simulator types.

WG2000 server utilization nearly doubled in 2001[2]. Such a huge execution success on HPC servers cannot occur with a traditional real-time simulation product due to serial operation dependencies. Consequently, with this economic model, the MDA program realizes extraordinary execution productivity that enhances the quality of the delivered software.

Parallelization Offers Time Savings

Large-scale servers seen today with anywhere from 256 to 512 CPUs at the MSRCs and up to 128 CPUs at the JNIC DC offer their respective sites the capacity to scale their products with the use of more

[1] http://WWW.JNTF.OSD.MIL/pROGRAMS/mODELING/WG2K.ASP

[2] Approximately 10,000 simulation executions occurred in 2000 and 19,144 occurred in 2001, a performance level enhanced by improved communication and a server upgrade. Up to 30,000 may be achieved in 2003.

CPUs applied in parallel to the problem space. In effect, a problem that started as a serial sequence of events, becomes divided into parallel tasks that execute on either dynamically or statically assigned CPUs. The parallel architecture model should produce more work in the same period of time, when compared with the serial model. However, the launch, detection, and defense against a threat missile obviously present a serial time sequence of events. Consequently, the composition of parallel tasks demands much from the software designers. In 2001, WG2000 achieved success at the eleven CPU scaling level. Today, scaling from 22 to 25 CPUs represents more than a 100 percent scaling improvement.

The combination of the WG2000 execution model and large-scale servers provide the MDA with a successful, low-cost per execution model through the unique application of large server technology. WG2000 expects to expand to even faster large-scale servers to produce even more product during its life cycle.

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CTA: Forces Modeling and Simulation/C4I
Computer Resources: SGI Origin 2000 [JNIC]

Section 3

High Performance Computing Modernization Program

Introduction

The DoD HPCMP is a strategic national defense initiative that exists to enable over 4,000 scientists and engineers to address the engineering challenges of the S&T and T&E communities. The program provides an unparalleled collaborative environment, linking users at over 100 DoD laboratories, test centers, universities, and industrial sites. Because the HPCMP is managed as a DoD-wide corporate asset, expert teams are guaranteed access to a world-class, commercial, HPC capability based on mission priority rather than on the size or budget of their organizations.

A User-Centered Management Focus

Traditional HPC programs are built around a single central facility that acts as the "center of gravity" for all activities. The HPCMP, in contrast, provides a world-class HPC capability accessible over a single network service, the DREN. All the program's MSRCs and DCs are available to HPCMP users, with the allocation of resources determined independently by the Services and Defense Agencies. Additionally, users have a direct role in overall policy and implementation through the HPC User Advocacy Group (UAG) and through their CTA leaders, who unify the HPCMP community.

Integrated Program Strategy

The program has evolved beyond an initial phase of procurement and program development to field, in FY 1996, a world-class HPC infrastructure for the DoD S&T and the T&E communities. Figure 1 depicts the HPCMP integrated program strategy. The infrastructure is comprised of three components: HPC Centers, Networking, and Software Applications Support. Each of these components will be discussed in detail in this section.

The HPCMP continually acquires the best commercially available, high-end, high performance computers. The program also acquires and develops common-use software tools and programming environments, expands and trains the DoD HPC user base, and exploits the best ideas, algorithms, and software tools emerging from the national HPC infrastructure.

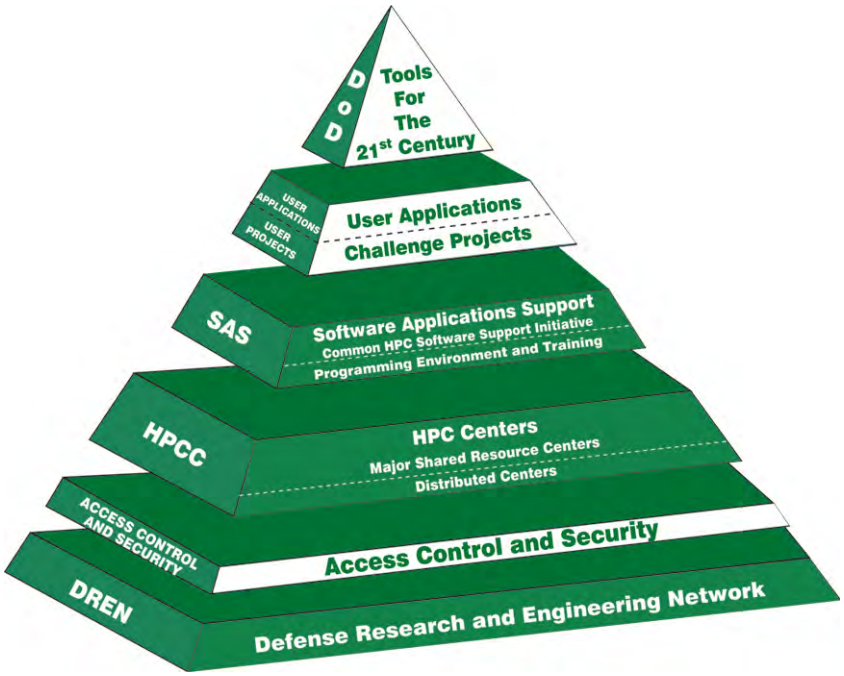


Figure 1. Integrated Program Strategy of the Department of Defense High Performance Computing Modernization Program

User Requirements

The requirements process, developed and employed by the program, includes an annual survey of the DoD S&T and T&E communities, coupled with site visits to discuss requirements and provide information to user groups. The program obtains additional feedback through user satisfaction surveys, annual user group conferences, and advisory panels who establish policies and procedures at the HPC centers.

HPC systems performance metrics are tracked throughout the year at the computational project level to ensure projects receiving allocations are able to use the resources effectively and efficiently. This process provides feedback to the Services and Agencies before allocating resources the following fiscal year. The overall integrated process furnishes accurate and timely data on which to base program decisions.

World-Class Shared HPC Capability

The HPCMP provides almost 27 teraflops of peak computing capability, an integrated computing environment, and a full complement of specialized and general user support. The program provides a variety of architectures and classes of systems, ranging from the most powerful commercial configurations available from major US HPC vendors to more specialized systems configured for specific types of mission applications. HPC capability is upgraded regularly to ensure that DoD users are among the first to use the new generations of HPC capabilities. During FY 2002, the HPCMP completed its third technology upgrade at the MSRCs and continued to fund special capabilities at selected DCs. The program will continue to make major upgrades to capabilities at the MSRCs in FY 2003.

DoD HPC Challenge Projects

HPCMP allocates approximately 25 percent of its HPC resources each fiscal year to competitively selected DoD Challenge Projects. These high-priority, computationally intensive projects develop and use pathfinding applications that meet mission-critical warfighting and science and technology requirements. Forty-one projects were selected for implementation in fiscal year 2002. Many of the projects use multiple hardware platforms and in some cases, multiple shared resource centers. Table 2 lists the fiscal year 2002 DoD HPC Challenge Projects.

HPCMP Computational Technology Areas

The DoD HPCMP user community is organized around ten broad CTAs. Each CTA has a designated leader, a prominent DoD scientist or engineer, working in the discipline. Users of HPCMP resources address challenges in the following computational areas:

- Computational Structural Mechanics, Mr. Michael Giltrud, Defense Threat Reduction Agency, Alexandria, VA
- Computational Fluid Dynamics, Dr. Robert Meakin, Army Aviation and Missile Command, Moffett Field, CA
- Computational Chemistry and Materials Science, Dr. Ruth Pachter, Air Force Research Laboratory, Materials/Manufacturing Directorate, Wright-Patterson AFB, OH

Table 2. DoD High Performance Computing Challenge Projects (Fiscal Year 2002)

Project	Project Leader(s)	Organization
Computational Structural Mechanics		
Evaluation and Retrofit for Blast Protection in Urban Terrain	James Baylot, Tommy Bevins, James O'Daniel, Young Shon, David Littlefield, and Chrisopher Eamon	Engineer Research and Development Center, Vicksburg, MS
Modeling Complex Projectile Target Interactions	Kent Kimsey and David Kleponis	Army Research Laboratory, Aberdeen Proving Ground, MD
Three-Dimensional Modeling and Simulation of Bomb Effects for Obstacle Clearance	Alexandra Landsberg	Naval Surface Warfare Center, Indian Head Division, Indian Head, MD
Computational Fluid Dynamics		
3-D Computational Fluid Dynamics Modeling of the Chemical Oxygen-Iodine Laser (COIL)	Timothy Madden	Air Force Research Laboratory, Kirtland AFB, NM
Active Control of Fuel Injectors in Full Gas Turbine Engines	Suresh Menon	Army Research Office, Research Triangle Park, NC
Airdrop System Modeling for the 21st Century Airborne Warrior	Keith Stein, Richard Benney, Tayfun Tezduyar, James Barbour, Hamid Johari, and Sonya Smith	Army Soldier & Biological Chemical Command, Natick, MA
Analysis of Full Aircraft with Massive Separation Using Detached-Eddy Simulation	Kenneth Wurtzler, Robert Tomaro, William Strang, Matthew Grismer, Capt James Forsythe, Kyle Squires, and Phillipe Spalart	Air Force Research Laboratory, Wright-Patterson AFB, OH
Applied CFD in Support of Aircraft-Store Compatibility and Weapons Integration	John Martel	Air Force Seek Eagle Office, Eglin AFB, FL
High-Fidelity Analysis of UAVs Using Nonlinear Fluid/Structure Simulations	Reid Melville and Miguel Visbal	Air Force Research Laboratory, Wright-Patterson AFB, OH
High-Resolution Adaptive Mesh Refinement (AMR) Simulation of Confined Explosions	John Bell, Marcus Day, Charles Rendleman, Mike Lijewski, Vincent Beckner, and Allen Kuhl	Defense Threat Reduction Agency, Alexandria, VA
Hybrid Particle Simulations of High Altitude Nuclear Explosions in 3-D	Stephen Brecht	Defense Threat Reduction Agency, Alexandria, VA
Large-Eddy Simulation of Steep Breaking Waves and Thin Spray Sheets Around a Ship: The Last Frontier in Computational Ship Hydrodynamics	Ki-Han Kim, Dick Yue, and Douglas Dommermuth	Naval Surface Warfare Center, Carderock Division, Bethesda, MD
Large-Eddy Simulation of Tip-Clearance Flow in Stator-Rotor Combinations	Parviz Moin, Meng Wang, Donghyun You, and Rajat Mittal	Office of Naval Research, Arlington, VA
Modeling of Microbubble Drag Reduction Physics	Parney Albright and James Uhlman	Defense Advanced Research Project Agency, Arlington, VA
Multiphase CFD Simulations of Solid Propellant Combustion in Modular Charges and Electrothermal-Chemical (ETC) Guns	Michael Nusca and Paul Conroy	Army Research Laboratory, Aberdeen Proving Ground, MD

Table 2—*Continued*. DoD High Performance Computing Challenge Projects

Project	Project Leader(s)	Organization
Computational Fluid Dynamics (continued)		
Numerical Modeling of Wake Turbulence for Naval Applications: Vortex Dynamics and Late-Wake Turbulence in Stratification and Shear	Michael Gourlay, Donald Delisi, David Fritts, Maria-Pascale LeLong, James Riley, Robert Robins, and Joe Werne	Office of Naval Research, Arlington, VA
Parallel Simulations of Weapons/Target Interactions Using a Coupled CFD/Computational Structural Dynamics (CSD) Methodology	Joseph Baum	Defense Threat Reduction Agency, Alexandria, VA
Three-Dimensional, Unsteady, Multi-Phase CFD Analysis of Maneuvering High Speed Supercavitating Vehicles	Robert Kunz, Jules Lindau, and Howard Gibeling	Office of Naval Research, Arlington, VA
Time-Accurate Aerodynamics Modeling of Synthetic Jets for Projectile Control	Jubaraj Sahu, Sukumar Chakravarthy, and Sally Viken	Army Research Laboratory, Aberdeen Proving Ground, MD
Time Accurate Computational Simulations of Ship Airwake for DI, Simulation and Design Applications	Susan Polsky	Naval Air Warface Center Aircraft Division, Patuxent River, MD
Unsteady RANS Simulation for Surface Ship Maneuvering and Seakeeping	Ki-Han Kim, Joseph Gorski, Fred Stern, Lafayette Taylor, and Mark Hyman	Naval Surface Warfare Center, Carderock Division, Bethesda, MD
Computational Chemistry and Materials Science		
Characterization of DoD Relevant Materials and Interfaces	Emily Carter	Air Force Office of Scientific Research, Bolling AFB, DC
Computational Chemistry Models Leading to Mediation of Gun Tube Erosion	Cary Chabalowski, Margaret Hurley, Dan Sorescu, Roger Ellis, Donald Thompson, Betsy Rice, and Gerald Lushington	Army Research Laboratory, Aberdeen Proving Ground, MD
First Principles Studies of Technologically Important Smart Materials	Andrew M. Rappe	Office of Naval Research, Arlington, VA
Interactions of Chemical Warfare Agents with Acetlycholinesterase	Jeffery Wright, Gerald Lushington, and William White	Edgewood Chemical and Biological Center, Aberdeen Proving Ground, MD
Multiscale Simulations of High Temperature Ceramic Materials	Rajiv Kalia, Aiichiro Nakano, and Priya Vashista	Air Force Office of Scientific Research, Bolling AFB, DC
Multiscale Simulation of Nanotubes and Quantum Structures	Jerry Bernholc	Office of Naval Research, Arlington, VA
Multi-Scale Simulations of High Energy Density Materials	Jerry Boatz	Air Force Research Laboratory, Edwards AFB, CA
New Materials Design	Jerry Boatz, Ruth Pachter, Mark Gordon, Gregory Voth, and Sharon Hammes-Schiffer	Air Force Office of Scientific Research, Bolling AFB, DC

Table 2—*Continued*. DoD High Performance Computing Challenge Projects

Project	Project Leader(s)	Organization
Computational Electromagnetics and Acoustics		
Airborne Laser Challenge Project II	Wilbur Brown, Jeremy Winick, and Robert Beland	Air Force Research Laboratory, Kirtland AFB, NM
Directed High Power RF Energy: Foundation of Next Generation Air Force Weapons	Keith Cartwright	Air Force Research Laboratory, Kirtland AFB, NM
Radar Signature Database for Low Observable Engine Duct Design	Kueichien Hill	Air Force Research Laboratory, Wright-Patterson AFB, OH
Seismic Signature Simulations for Tactical Ground Sensor Systems and Underground Facilities	Mark Moran, Stephen Ketcham, George McMechan, Stig Hestholm, Roy Greenfield, Thomas Anderson, James Lacombe, Michael Shatz, Robert Haupt, Richard Lacoss, and Robert Greaves	Cold Regions Research and Engineering Laboratory, Hanover NH
Signature Modeling for Future Combat Systems	Raju Namburu, Theresa Gonda, Peter Chung, Margaret Hurley, Steve Bunte, William Coburn, Christopher Kenyon, Calvin Lee, John Escarsega, and William Spurgeon	Army Research Laboratory, Aberdeen Proving Ground, MD
Climate, Weather, and Ocean Modeling and Simulation		
1/32 Degree Global Ocean Modeling and Prediction	Alan Wallcraft, Harley Hurlburt, Robert Rhodes, and Jay Shriver	Naval Research Laboratory, John C. Stennis Space Center, MS
Basin-scale Prediction with the HYbrid Coordinate Ocean Model	Eric Chassignet	Office of Naval Research, Arlington, VA
Coupled Environmental Model Prediction (CEMP)	Wieslaw Maslowski, Julie McClean, Albert Semtner, Robin Tokmakian, Yuxia Zhang, Ruth Preller, and Steve Piacsek	Naval Postgraduate School and Naval Research Laboratory, Monterey, CA
Coupled Mesoscale Modeling of the Atmosphere and Ocean	Richard Hodur	Naval Research Laboratory, Monterey, CA
High Fidelity Simulation of Littoral Environments	Richard Allard and Jeffery Holland	Naval Research Laboratory, John C. Stennis Space Center, MS and Engineer Research and Development Center, Vicksburg, MS
Submerged Wakes in Littoral Regions	Patrick Purtell, Roger Briley, Joseph Gorski, and Douglas Dommermuth	Office of Naval Research, Arlington, VA
Signal/Image Processing		
Automatic Target Recognition Performance Evaluation	Timothy Ross	Air Force Research Laboratory, Wright-Patterson AFB, OH

- Computational Electromagnetics and Acoustics, Dr. Kueichien Hill, Air Force Research Laboratory, Sensors Directorate, Wright-Patterson AFB, OH
- Climate/Weather/Ocean Modeling and Simulation, Dr. William Burnett, Naval Oceanographic Office, John C. Stennis Space Center, MS
- Signal/Image Processing, Dr. Anders Sullivan, Army Research Laboratory, Aberdeen Proving Ground, MD
- Forces Modeling and Simulation/C4I, Dr. Larry Peterson, Space and Naval Warfare Systems Center, San Diego, CA
- Environmental Quality Modeling and Simulation, Dr. Jeffrey Holland, US Army Corps of Engineers, Engineer Research and Development Center, Vicksburg, MS
- Computational Electronics and Nanoelectronics, Dr. Barry Perlman, Army Communications-Electronics Command Research Development and Engineering Center, Ft. Monmouth, NJ
- Integrated Modeling and Test Environments, Mr. Jere Matty, Arnold Engineering Development Center, Arnold AFB, TN

Program Components

The program is organized into three components to achieve its goals. The components are HPCMP HPC centers, networking, and software applications support. The components allow the program to focus on the most efficient means of supporting the S&T and T&E communities' requirements. The components align to the program goals as follows:

High Performance Computing Centers

The High Performance Computing Modernization Program currently supports four MSRCs and eleven DCs. The large MSRCs provide a wide range of high performance computing (HPC) capabilities designed to support the ongoing needs of the DoD HPC community.

Each MSRC supports complete centralized systems and services. The MSRCs also provide vector machines, scalable parallel systems, clustered workstations, scientific visualization resources, and access to training. Storage capabilities include distributed file and robotic archival systems. The four MSRCs are:

- Air Force Aeronautical Systems Center (ASC), Wright-Patterson AFB, OH
- Army Research Laboratory (ARL), Aberdeen Proving Ground, MD
- Engineer Research and Development Center (ERDC), Vicksburg, MS
- Naval Oceanographic Office (NAVO), John C. Stennis Space Center, MS

The DCs provide specialized HPC capability to users. HPC systems have been established at DCs where there is a significant advantage to having local HPC systems and where there is a potential for advancing DoD applications using investments in HPC capabilities and resources (e.g., a test activity with real-time processing requirements).

The DCs are divided into two categories: “Allocated” and “Dedicated”. Allocated Distributed Centers associates the annual service/agency project allocation and/or challenge project allocation process with these centers. Dedicated Distributed Centers associates the dedicated project or projects for which each independent DDC was awarded with their respective center. The DCs have the following goals:

- Apply commercial HPC hardware and software as rapidly as it becomes available.
- Complement, balance, and supplement the major shared resource centers by enabling local expertise to be developed and leveraged by the larger DoD community.
- Support small and medium-size HPC applications, leveraging the larger MSRCs that support large applications.
- Foster reuse of software tools and application software components as well as appropriate use of communication standards, interface standards, and graphics visualization standards across DoD.
- Support local HPC requirements at selected sites where there is potential for advancing DoD applications.
- Promote the development of new software tools and application area specific software.
- Leverage HPC expertise and assets located in industry, academia and other federal laboratories in addition to DoD facilities.

The DCs are :

Dedicated Distributed Centers

- Air Force Research Laboratory, Information Directorate (AFRL/IF), Rome, NY
- Arnold Engineering Development Center (AEDC), Arnold AFB, TN
- Fleet Numerical Meteorology and Oceanography Center (FNMOC), Monterey, CA
- Naval Air Warfare Center Aircraft Division (NAWCAD), Patuxent River, MD
- Naval Research Laboratory (NRL-DC), Washington, DC
- Simulation and Analysis Facility (SIMAF), Wright-Patterson AFB, OH
- White Sands Missile Range (WSMR), White Sands Missile Range, NM

Allocated Distributed Centers

- Arctic Region Supercomputing Center (ARSC), Fairbanks, AK
- Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN
- Maui High Performance Computing Center (MHPCC), Kihei, HI
- Space and Missile Defense Command (SMDC), Huntsville, AL

The MSRCs and DCs provide state-of-the-art HPC capabilities operating in several classification environments and ensuring the DoD science and technology and test and evaluation user communities have the computational tools needed to retain the US warfighter’s technological advantage.

Figure 2. DREN Connections, High Performance Computing Centers, and Other Network Access Points

Networking

Defense Research and Engineering Network

The DREN is DoD's recognized research and engineering network. The DREN is a robust, high bandwidth, low latency network that provides connectivity between the High Performance Computing Program's geographically dispersed user sites and high performance computing centers. (See Figure 2)

DREN networking services are provided as a Virtual Private Network over the public infrastructure. DREN currently supports both cell-based and packet-based traffic over core infrastructures such as Multi Protocol Layer Service and ATM. DREN Service Delivery Points are specified in terms of WAN bandwidth access, network protocols, and local interfaces for connectivity. Minimal access to a site is DS-3 (45 Mbps) with potential high end access of OC-768 (40 Gbps) over the next 10 years. Current site connectivity to the DREN ranges from DS-3 at some user sites to OC-12 (622 Mbps) at MSRCs and selected DCs and Internet Network Access Points (NAP).

Since its inception, DREN has been very active in transferring leading edge network and security technologies across DoD and other Federal agencies. Our leading edge, defense-in-depth security model is now viewed by experts as the best way to protect resources both internally and externally. Layered defense extends from access control lists at the NAPs through sophisticated, high bandwidth intrusion detection monitored by our HPC Computer Emergency Response Team.

Hardware pre-authentication, strong configuration management, and periodic physical security assessments all contribute to hardened resources that are still accessible to the DoD research scientists from wherever they need to work. Well designed WAN security coupled with strong server and user security, allows DREN to truly deploy leading-edge, defense-in-depth protection of DoD resources.

DREN services are currently provided to sites throughout the continental United States, Alaska, Hawaii, and can be extended overseas where necessary. Incorporating the best operational capabilities of both the DoD and the commercial telecommunications infrastructure, DREN provides DoD a secure, world-class, long-haul research network in support of DoD's S&T and T&E communities. DREN also extends services to DoD's Modeling & Simulation community and the MDA.

Security

The HPCMP has also designed and deployed a Secret DREN (SDREN) using a common Secret systems high key with National Security Agency certified Type-1 encryptors. SDREN can transport classified traffic at OC-3 (155 Mbps).

The Defense Information Systems Agency Information Security Program Management Office has certified the DREN for sensitive but unclassified information and encrypted classified traffic. Access to high performance computing systems is controlled by enhanced security technology and user procedures.

Software Applications Support

"Software Applications Support" is new terminology that captures the evolutionary nature of the Program's efforts to acquire and develop joint need HPC applications, software tools, and programming environments and educate and train DoD's scientists and engineers to effectively use advanced computational environments. This component contains two areas: the CHSSI, which has been producing efficient applications software codes for the last several years and PET, which is realigned from the HPC MSRCs. As the program has evolved, the potential synergy of re-focusing PET activities caused the HPCMP to realign PET from a shared resource center-centric orientation to a broader program-wide focus. This realignment offers significant opportunities for leveraging and collaborating with CHSSI.

Common High Performance Computing Software Support Initiative

CHSSI consists of a set of focused software development activities. These activities are designed to provide recognized communities of DoD computational scientists and engineers with common HPC technical codes that exploit scalable computer architectures. Each CHSSI application is selected based on DoD needs and technical quality. The products have application across a significant portion of the DoD S&T and T&E HPC user community.

CHSSI provides efficient, scalable, portable software codes, algorithms, tools, models, and simulations that run on a variety of HPC platforms for use by a large number of S&T and T&E scientists and engineers. CHSSI, which is organized around ten CTAs and eight portfolios, involves many scientists and engineers working in close collaboration across government,

industry, and academia. CHSSI teams include algorithm developers, applications specialists, computational scientists, computer scientists, and engineers.

Currently, the CHSSI program invests $20 million per fiscal year in 55 software projects. These support a mix of single and multi-disciplinary projects. These projects are providing "state-of-the-art" or advanced computer modeling capabilities. Prominent scientists and engineers from the DoD lead the projects. These development efforts leverage the considerable expertise and assets of industry, academia, and other federal agencies. CHSSI software products are rigorously tested, documented, and reviewed as part of their structured development process.

Programming Environment and Training

PET activity focuses on improving DoD HPC productivity by creating an information conduit between DoD HPC users and top academic and industry experts. PET is responsible for gathering and deploying the best ideas, algorithms, and software tools emerging from the national high performance computing infrastructure into the DoD user community. PET acquires world-class technical support, develops strategic partnerships, and focuses on HPC tool development and deployment.

PET is divided into four components and each component executes a program that supports the designated functional area, as shown in Table 3.

The functional areas are grouped to encourage synergy among related CTAs, collaboration and interaction between CTA and cross-community functions, and to balance the workload across the four components.

PET activities consist of short- and long-term strategic efforts. Short-term efforts lasting less than three years include short collaborative projects with users. Two of the long-term efforts focus on distance learning and metacomputing. PET teams anticipate and respond to the needs of DoD users for training and assistance. The teams have a strong on-site presence at HPCMP major shared resource centers.

Table 3. CTA Component Functional Areas

Component Number	CTAs and Functional Areas
1	Climate/Weather/Ocean Modeling and Simulation Environmental Quality Modeling and Simulation ***Computational Environment***
2	Forces Modeling and Simulation/C4I Integrated Modeling and Test Environments Signal/Image Processing ***Enabling Technologies***
3	Computational Fluid Dynamics Computational Structural Mechanics ***PET Online Knowledge Center*** ***Education, Outreach, and Training Coordination***
4	Computational Chemistry and Materials Science Computational Electromagnetics and Acoustics Computational Electronics and Nanoelectronics ***Collaborative and Distance Learning Technologies***

Section 4

Acronyms

Acronyms

1-D	one-dimension (dimensional)
2-D	two-dimensions (dimensional)
3-D	three-dimensions (dimensional)
3DVAR	three-dimensional variational data assimilation
AAA	Anti-Aircraft Artillery
AATD	Aviation Applied Technology Directorate
AChE	acetylcholinesterase
ADCIRC	ADvanced CIRCulation Model
ADCP	Acoustic Doppler Current Profiler
ADH	ADvanced Hydraulics
ADMCPA	2-azido-N,N-dimethylcyclopropanamine
ADVISR	Advanced Visualization for Intelligence, Surveillance, and Reconnaissance
AFAP	as-fast-as-possible
AFB	Air Force Base
AFOSR	Air Force Office of Scientific Research
AFRL	Air Force Research Laboratory
AFWA	Air Force Weather Agency
AHPCRC	Army High Performance Computing Research Center
AIRMS	Airborne Infrared Measurement System
AL	aluminum
ALE	Arbitrary Lagrangian Eulerian
AMDSim	Air and Missile Defense Simulation
AMR	Adaptive Mesh Refinement or Automatic Mesh Refinement
AoA	Analysis of Alternatives or angle of attack
API	applications programming interface
ARL	Army Research Laboratory
ARO	Army Research Office
ASC	Aeronautical Systems Center
ATD	Advanced Technology Demonstrator
ATM	Asynchronous Transfer Mode
ATR	Automatic Target Recognition
AWS	Abrupt Wing Stall
BAD	Behind-armor debris
BLOS	beyond-line-of-sight
BMDS	Ballistic Missile Defense System
BN	boron nitride
C	carbon
CAD	computer aided design

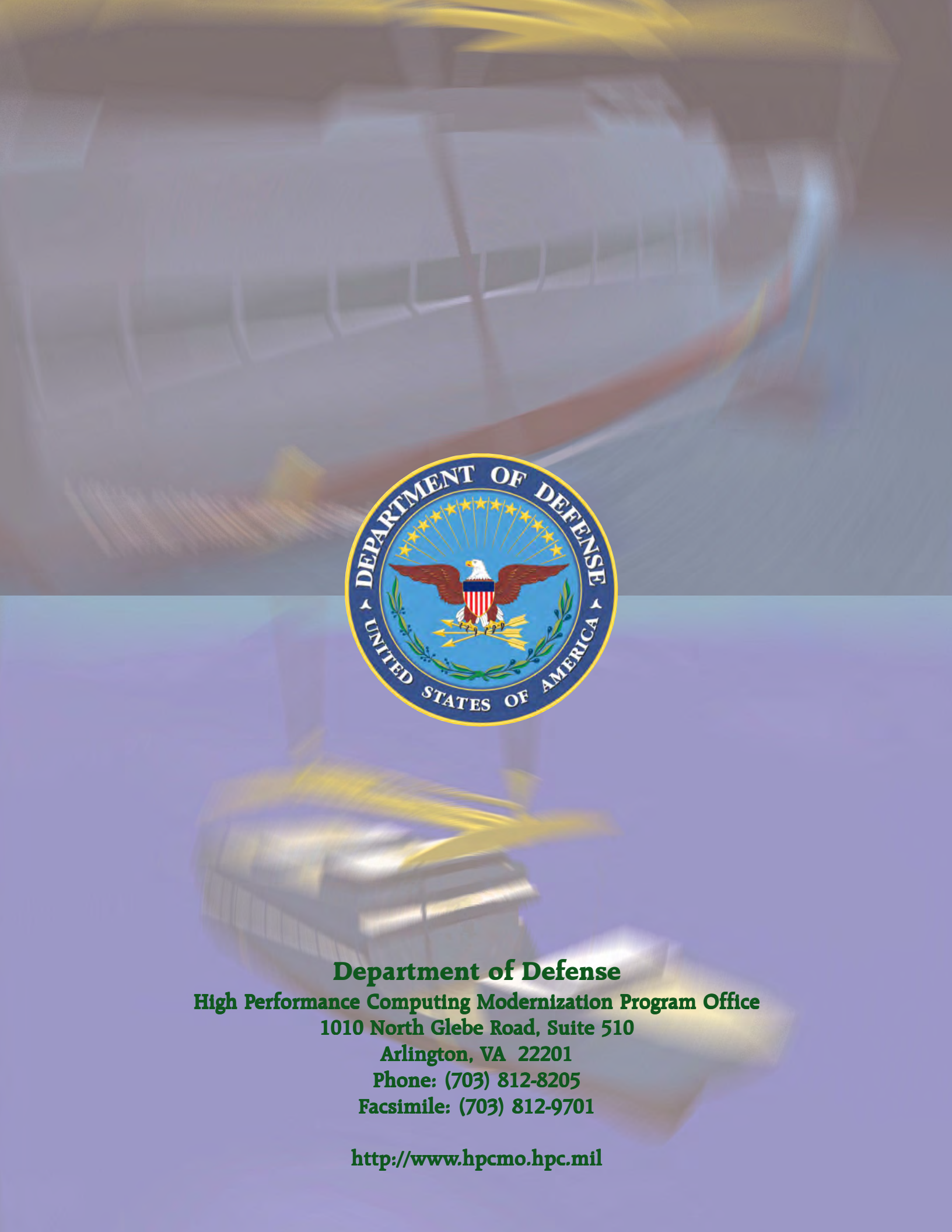
C/B	chemical/biological
CCM	Computational Chemistry and Materials Science
CEA	Computational Electromagnetics and Acoustics
CEM	Computational Electromagnetics
CEN	Computational Electromagnetics and Nanoelectronics
CFD	Computational Fluid Dynamics
CHSSI	Common High Performance Computing Software Support Initiative
CIO	Chief Information Officer
COAMPS	Coupled Ocean Atmosphere Mesoscale Prediction System
CODESSA	COmprehensive DEscriptors for Structural and Statistical Analysis
COMPOSE	COmposite Manufacturing PrOcess Simulation Environment
CONOPS	concept of operations
CSD	Computational Structural Dynamics
CSM	Computational Structural Mechanics
CTA	Computational Technology Area
CWO	Climate/Weather/Ocean Modeling and Simulation
DARPA	Defense Advanced Research Projects Agency
DC	Distributed Center
DES	Detached-Eddy Simulation
DFT	density functional theory
DMAZ	2-azido-N,N-dimethylethanamine
DNS	direct numerical simulation
DoD	Department of Defense
DOF	Degrees of Freedom
DON	Department of Navy
DREN	Defense Research and Engineering Network
DSD	Deforming-Spatial-Domain
DTRA	Defense Threat Reduction Agency
EQM	Environmental Quality Modeling
ERDC	US Army Corps of Engineers, Engineer Research and Development Center
ETC	electrothermal-chemical
FCS	Future Combat Systems
FDTD	Finite Difference Time Domain
FE	ferroelectric
FEM	Finite Element Method
FeO	iron oxide
FMM	fast multipole method
FMS	Forces Modeling and Simulation
FNC	Future Naval Capabilities
FNMOC	Fleet Numerical Meteorology and Oceanography Center
FOX-7	1,1-diamino-2,2-dinitroethylene

FSI	fluid-structure interaction
FY	fiscal year
GB	gigabyte
GW	giga-watt
HE	high explosives
HFM	Hyperbolic Frequency Modulated
HFSOLE	High Fidelity Simulations of Littoral Environments
HLD	high-loading-density
HMX	1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane
HPC	high performance computing or high performance computer
HPCMP	High Performance Computing Modernization Program
HPCMPO	High Performance Computing Modernization Program Office
HPM	high power microwave
HVRB	history variable reactive burn
HWILT	hardware-in-the-loop test
HYCOM	HYbrid Coordinate Ocean Model
IBCTs	Interim Brigade Combat Teams
ICE	Interdisciplinary Computing Environment
ICEPIC	Improved Concurrent Electromagnetic Particle-in-Cell
IMT	Integrated Modeling and Test Environment
I/O	input/output
IP	Information Processor or Internet protocol
IRFNA	inhibited red fuming nitric acid
JNIC	Joint National Integration Center
JSF	Joint Strike Fighter
JTIDS	Joint Tactical Information Distribution System
KE	Kinetic Energy
LANL	Los Alamos National Laboratory
LB/TS	Large Blast and Thermal Simulator
LBE	Lattice-Boltzman Equation
LES	Large-Eddy Simulations
LO	Low observables/observability
LOB	line-of-bearing
M&S	Modeling and Simulation
MACS	Modular Artillery Charge System
MBPT(2)	Many-body perturbation theory (second order)
MCEL	Model Coupling Environmental Library
MCM	mine countermeasures
MDA	Missile Defense Agency
MDWAR	Missile Defense Wargame and Analysis Resource
MEMS	micro-electro-mechanical systems

METOC	Meteorology and Oceanography Community
MGD	magnetogasdynamics
MILO	magnetically insulated line oscillator
MLFMA	multi-level fast multipole algorithm
MMH	monomethylhydrazine
MoM	method of moments
MP2	Moller-Plesset perturbation theory (second order)
MPI	Message Passing Interface
MPRS	Multi-Point Refueling System
MRTD	Multiresolution-Time Domain
MSRC	Major Shared Resource Center
MW	mega-watt
NAP	Network Access Point
NAVAIR	Naval Air Systems Command
NAVMETOCCOM	Naval Meteorology and Oceanography Command
NAVO	Naval Oceanographic Office
NAWCAD	Naval Air Warfare Center Aircraft Division
NE	nuclear explosive
NGEN	The Army's Next Generation Interior Ballistics Model
NIAB	Non-Ideal Air Blast
NISA	Network Infrastructure Services Agency
NLOS	non-line-of-sight
NM	nitromethane
NMR	Nuclear Magnetic Resonance
NOGAPS	Navy Operational Global Atmospheric Prediction System
NRL	Naval Research Laboratory
ns	nanosecond
NWP	Numerical Weather Prediction
ONR	Office of Naval Research
O-PDES	Optimistic, Parallel, Discrete Event Simulation
PDF	pair distribution function
PenRen	Pentagon Renovation Office
PET	Programming Environment and Training
P-I	pressure-impluse
POPS	Primary Oceanographic Prediction System
PVC	permanent virtual circuit
PVP	permanent virtual path
PZT	lead zirconate titanate
QC	quantum-chemical
QM/MM	quantum mechanics/molecular mechanics
QSPR	Quantitative Structure-Property Relationships

R&D	research and development
RANS	Reynolds Averaged Navier-Stokes
RCS	radar cross section
RDT&E	Research, Development, Test, and Evaluation
RF	radio frequency
RHA	rolled homogenous armor
RMS	Root Mean Square
RPM	rate per minute
ROC	Receiver Operating Characteristic
rt-PVC	real-time permanent virtual circuit
rt-PVP	real-time permanent virtual path
rt-VBR(s)	real-time variable bit rate(s)
SAFEDI	Ship Aircraft Airwake Analysis for Enhanced Dynamic Interface
SALVOPS	Salvage Operation(s)
SBCCOM	Soldier Biological and Chemical Command
SDOF	single-degree-of-freedom
SDREN	Secret Defense Research and Engineering Network
SGI	Silicon Graphics Inc.
SHAMRC	Second-order Hydrodynamic Automatic Mesh Refinement Code
SHARC	Second-order Hydrodynamic Advanced Research Code
SHMEM	SHared MEMory
SIP	Signal/Image Processing
SIPRNET	Secret Internet Protocol Routed Network
SONAR	SOund Navigation and Ranging
SPAWAR	Space and Naval Warfare Systems Command
SPE	Scalable Processing Environment
SPEEDES	Synchronous Parallel Environment for Emulation and Discrete-Event Simulation
SSC	SPAWAR Systems Center
SSCSD	SPAWAR Systems Center, San Diego
SSHB	Short Strong Hydrogen Bond
SST	Stabilized Space-Time
S&T	science and technology
STWAVE	STeady-state WAVE
SVC	Scientific Visualization Center
SWAFS	Shallow Water Analysis and Forecast System
SWAN	Simulating WAves Nearshore
TARDEC	Tank Automotive Research, Development and Engineering Center
TBC	Thermal Barrier Coating
T&E	test and evaluation
Ti	titanium
UAG	User Advocacy Group

UAV	Unmanned Air Vehicles
UDMH	unsymmetrical dimethylhydrazine
UGS	Unattended Ground Sensor
UHF	Ultra High Frequency
UNCLE	Unsteady Computations of Field Equations
U.S.	United States
UWB	ultra-wideband
UXO	Unexploded Ordnance
VASP	Vienna as Initio Simulation Package
VCMD	variable-charge molecular dynamics
VDG	Virtual Data Grid
VHF	very high frequencies
VV	Vertical Transmit-Vertical Receive
WAN	wide area network
WG2000	Wargame 2000
WLS	weighted, least-squares
WRF	Weather Research and Forecast
WSMR	White Sands Missile Range
YSZ	yttria-stabilized zirconia
Zr	zirconate



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