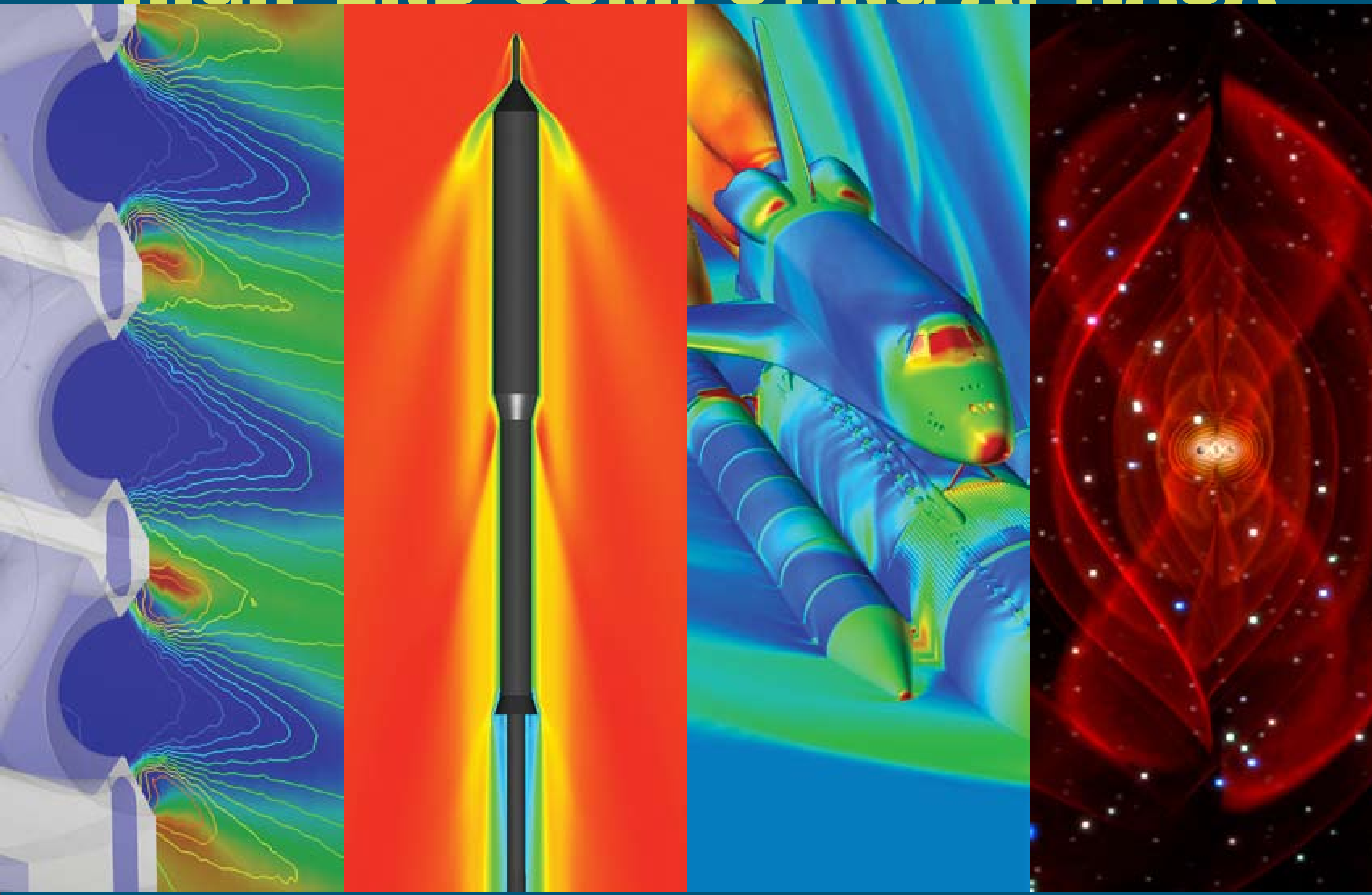
National Aeronautics and Space Administration

HIGH-END COMPUTING AT NASA



Highlights of science and engineering achievements on NASA's supercomputers during the past 18 months

2006

VISION STATEMENT

NASA's HEC resources are relied on as an essential and pervasive partner by the breadth of Agency science, engineering, and technology activities, enabling rapid advances in insight and dramatically enhancing mission achievements.

Images shown on cover (from left to right):

- Cross-section of the computational fluid dynamics analysis of an engine combustor geometry, confirming experimental results—that the NASA Hydrogen Lean Direct Injection concept produces low amounts of nitrogen oxide.
- Flowfield surrounding a Crew Launch Vehicle concept computed using OVERFLOW-2, showing Mach contours in a plane of symmetry for supersonic flow.
- Pressure coefficient on the Space Shuttle Launch Vehicle and in the near-body flowfield.
- Gravitational waves radiating from two inspiraling black holes.

November 1, 2006

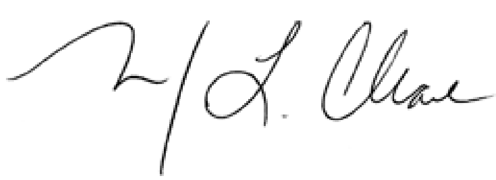
Members of the Scientific Research and Engineering Community:

We are extremely pleased to present the inaugural report from NASA's newly established High-End Computing (HEC) Program. This publication captures remarkable science and engineering accomplishments enabled by the HEC Program's shared high-end computing systems and services.

For several decades, high-end computing has played an important role in supporting NASA's missions, with advancements as broad as preparing the Space Shuttle for Return to Flight, assimilating vast quantities of Earth observational data into climate models, and developing astrophysical calculations that help us better understand the origins of our universe. Today, our Program is committed to maintaining a stable, service-oriented computing environment for all four of the Agency's mission directorates—Aeronautics Research, Exploration Systems, Science, and Space Operations—as well as NASA's Engineering and Safety Center, external collaborators, and the nation.

In this report, you will read about the technologies that help make NASA's HEC Program successful. As described in the *Program Overview*, our user community encompasses more than 1,000 researchers from NASA field centers, government laboratories, academia, and industry across the United States. In partnership with them to achieve mission impact, we provide premier computing systems, high-speed networks, a huge data storage capacity, extensive programming and visualization expertise, and responsive user and training services. This increasingly integrated computing environment has fostered significant achievements within each mission directorate. In *Science and Engineering Highlights*, our principal investigators relate their successes.

As NASA embarks on a new era of space exploration, scientific discovery, and aeronautics research, our HEC Program is committed to providing computing resources and services to help achieve NASA's mission. With renewed emphasis on delivering a stable, service-driven computing environment that maximizes scientific discovery and engineering optimization, we will continue enabling NASA to turn today's far-reaching dreams into tomorrow's reality.



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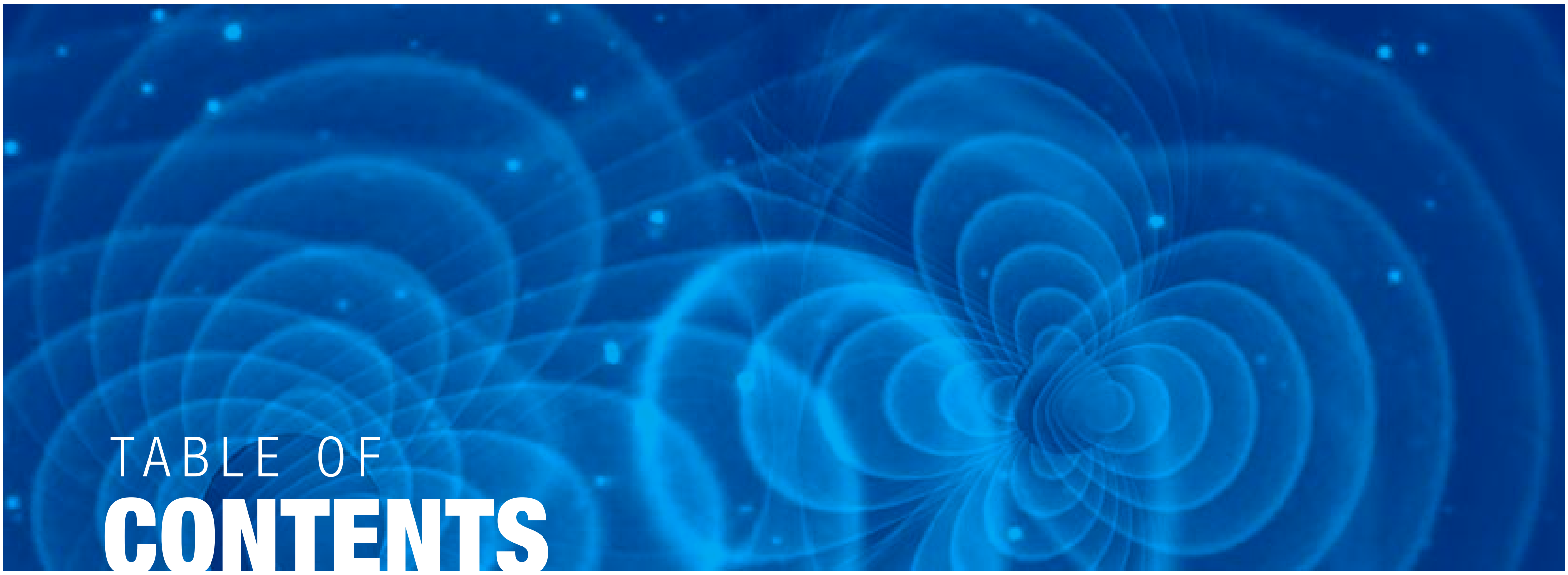

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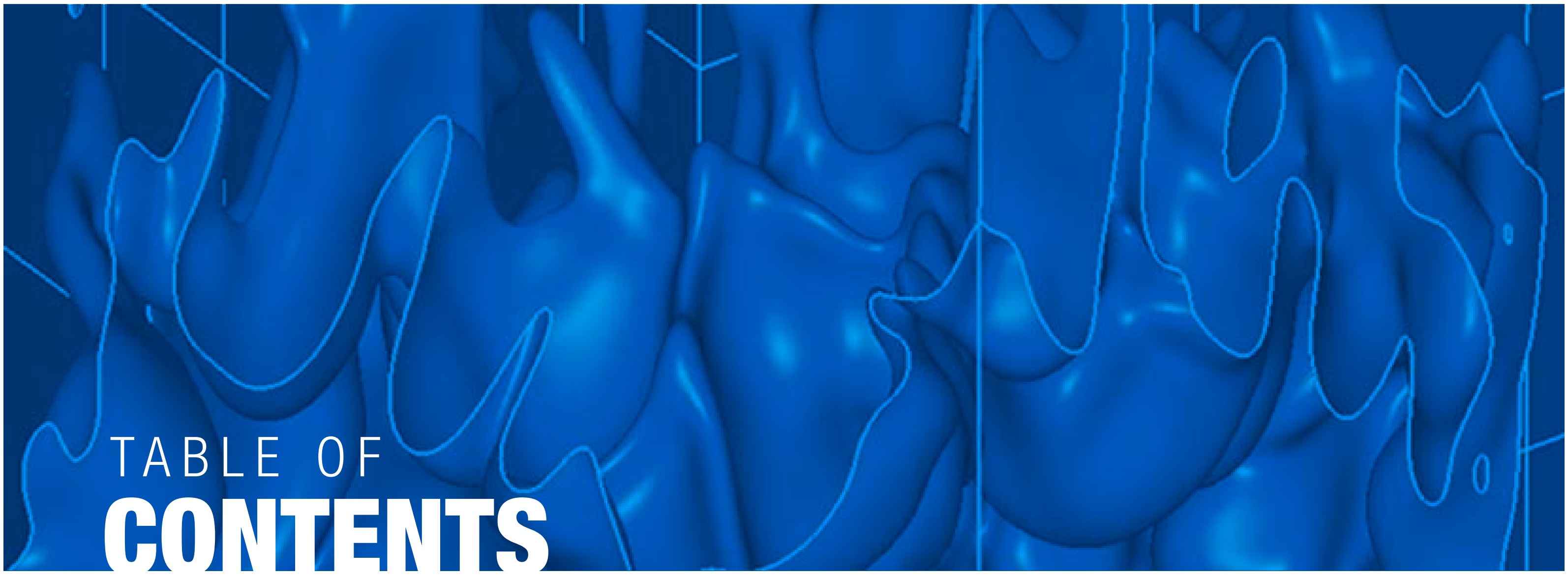

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EXECUTIVE SUMMARY

NASA's challenging mission to explore space and to understand the universe and the Earth within it increasingly requires supercomputing, also known as high-end computing or HEC, as a powerful leading-edge tool. Computing capability has advanced exponentially for decades, to the point that computational modeling and simulation has become an equal partner to experiment and theory for scientific and engineering progress. As a result, HEC is now broadly used in support of NASA's mission achievements.

For over 30 years, NASA has invested in a comprehensive, mission-focused set of HEC resources and integrated services that enables the Agency to rapidly address the specific challenges of its computation- and data-intensive science and engineering endeavors. Recently, NASA created the HEC Program to demonstrate a long-term commitment to funding and supporting HEC as an Agency-wide asset. Program funding flows through the Shared Capability Assets Program and the Science Mission Directorate.

The HEC Program provides high-level oversight and coordination of NASA's two HEC projects, ensuring efficient, effective, and reliable service to its users, NASA management, and other stakeholders. These projects are the High-End Computing Columbia (HECC) Project operated by the NASA Advanced Supercomputing (NAS) Division at Ames Research Center in Moffett Field, California, and the NASA Center for Computational Sciences (NCCS) Project operated by NCCS at Goddard Space Flight Center in Greenbelt, Maryland.

The NASA HEC Program's computing resources and integrated services environment enable and enhance progress in hundreds of projects supporting all four NASA mission directorates. NASA's HEC users number well over 1,000 and come from virtually every NASA center, as well as universities, industry, and other agencies. This document presents 40 user projects, chosen because of their importance to the Agency, their impact during the reporting period (past 18 months), and their technical maturity. Notable highlights reported by each mission directorate are captured here.

Aeronautics Research

- Scientists and engineers are using computational tools, enabling NASA to investigate more fuel-efficient, lower-noise, and reduced-emissions aircraft.

Exploration Systems

- Engineers are using HEC resources to develop complete aerothermodynamics databases across the entire flight envelope of the Orion Crew Exploration Vehicle, dramatically reducing the number of wind tunnel tests needed, thus decreasing effort, time, and cost.

Science

- Astrophysicists are testing new theories for how large-scale structures in the universe formed—against rapidly improving observational evidence.
- Earth scientists are developing comprehensive models for weather and climate applications, incorporating NASA's satellite observations to advance our understanding of processes related to climate variability and change, and to improve our modeling and prediction of the Earth system.

Space Operations

- Engineers were able to rapidly validate the redesign of the Space Shuttle's external fuel tank to aid its return to flight, increasing overall safety of human spaceflight.

This report contains three primary messages for NASA management, NASA's HEC community, and the public:

- NASA's supercomputing-enabled projects are addressing the most daunting science questions and engineering challenges in pursuit of NASA mission success;
- NASA's HEC Program has strong Agency support and a commitment from its own program and project managers to serve the needs of its users and stakeholders; and
- The HEC Program will continue to enhance the performance, usability, and productivity of its resources and services, in support of these projects.

EXECUTIVE SUMMARY

The HEC Program is vigorously pressing forward on many fronts to improve the performance, usability, and productivity of its resources and services, and to improve communication with stakeholders. An example is the publication of this inaugural Program overview and accomplishments report. Another key effort is the “Unified HEC Environment” initiative, which is pursuing 10 activities to move NASA towards a seamless, multi-facility environment for HEC users and system administrators. The HEC Program is also forming a Board of Advisors to represent the strategic interests of each mission directorate. Also planned are a customer board with representation from major NASA programs and a user board to represent the interests of HEC users. A HEC requirements workshop is being planned for 2007 to better understand and predict NASA’s HEC needs and potential mission impacts.

Many colleagues at the HEC centers contributed long hours and dedicated effort to producing this initial report of the NASA HEC Program. We are especially grateful to the technical publications teams at NAS and NCCS, without whose much appreciated hard work and critical expertise this report would not have been remotely possible to produce.

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PROGRAM OVERVIEW

INTRODUCTION

Since its inception in 1958, the National Aeronautics and Space Administration (NASA) has pushed to expand the boundaries of science and technology to enable and enhance NASA missions. Today in Aeronautics Research, the Agency is working to pioneer new flight technologies. In Exploration Systems, the Agency is creating new capabilities for affordable, sustainable human and robotic exploration beyond the Earth environment. In Science, NASA is exploring the Earth, moon, Mars, and the universe. In Space Operations, NASA is providing critical enabling technologies through the Space Shuttle, the International Space Station, and human spaceflight support. Increasingly, these scientific and engineering pursuits require the development and utilization of leading-edge capabilities and technologies—including reliable, high-end computing resources. Recognizing these needs, NASA has created the Agency-wide High-End Computing (HEC) Program. Its mission is to:

> *"Deliver high-performance computational capability to NASA's science, exploration, aeronautics, and space operations communities, facilitating the rapid development and application of advanced knowledge and technology for mission success."*

Managed by the Science Mission Directorate (SMD) and funded through the Agency's Shared Capability Assets Program (SCAP) and SMD (Figure 1), the HEC Program is partnering with each mission directorate to ensure specific resource requirements and user needs are identified and addressed. Across all levels, the HEC Program will be responsive, accountable, and dedicated to the high-end computing requirements of its user communities.

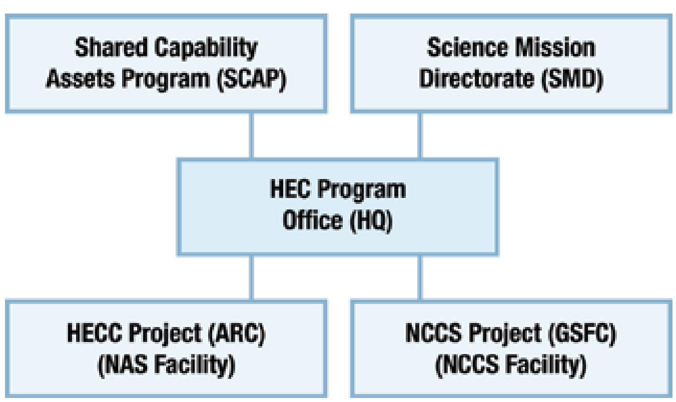


Figure 1: *NASA HEC Program management structure.*

The HEC Program has established an integrated management approach for NASA's high-end computing systems and services currently located at the NASA Advanced Supercomputing (NAS) facility at Ames Research Center, Moffett Field, California, and the NASA Center for Computational Sciences (NCCS) at Goddard Space Flight Center in Greenbelt, Maryland. Both facilities have a long history of providing users with advanced computational technologies, mass storage systems, and network solutions for cutting-edge science and engineering problems. For several decades, Ames has been a leader in computational fluid dynamics and thermal protection systems, and Goddard has been a leader in climate and weather modeling research. NASA is committed to continuing this tradition of scientific and technical excellence with the broader HEC Program.

The configuration management, supporting documentation, and strategic upgrades that have been hallmarks of NAS and NCCS will continue, but in a unified HEC environment. Although physically separate and located on opposite coasts, the systems and resources will be managed logically as one integrated computing environment. Whether located at NASA centers or external partner organizations, users will have remote access to a common user environment and a standard set of services. Systems will be right-sized to meet the computing and storage demands of NASA's growing user community; and new technologies will be introduced gradually to ensure minimal disruption to the users. All of these efforts underscore the HEC Program's dedication to understanding its user community's needs and to providing the best services to users across the Agency's four mission directorates.

HIGH-END COMPUTING FACILITIES

NAS and NCCS are home to the Program's most valuable resources—the supercomputers and the people who keep them operational on a daily basis, support their users with a variety of services, and implement new technologies to ensure the Agency's future science and engineering problems can be solved in a timely manner.

NASA Advanced Supercomputing Facility

The NAS Division was formally established in the early 1980s by Congress with the initial charter of providing high-end computing capabilities for carrying out numerical simulations of proposed commercial and military aircraft designs. Since its initial charter, NAS has adapted to meet the changing needs of the Agency. In mid-2004, the NAS Division acquired a 10,240-processor supercomputer named Columbia (Figure 2). This computational resource and its facility became part of the HEC Program, designated the High-End Computing Columbia (HECC) Project. Since Columbia's installation in 2004, and especially in the last 18 months, the HEC Program has made many modifications to the system to enhance performance. These include the development of a shared-memory architecture across four of Columbia's twenty 512-processor nodes, which has enabled ground-breaking science and engineering for all four mission directorates. In parallel with Columbia's growth, new visualization techniques have been developed on the hyperwall (a 100-processor visualization system) that enhance Columbia's impact.

Figure 2: *Bird's-eye view of the Columbia supercomputer, a 10,240-processor SGI Altix system comprised of 20 nodes, each containing 512 processors.*

NASA Center for Computational Sciences

The NCCS was formed in 1990 with the arrival of the first Cray supercomputers at Goddard, carrying on a role dating from the 1960s to provide computing and data services to NASA's science community. Today, NCCS is housed within the Sciences and Exploration Directorate at Goddard and supports modeling and analysis activities for SMD users in the Earth Sciences, Heliophysics Science, Solar System Exploration, and Astrophysics Science Divisions. SMD researchers are developing and using atmospheric, ocean, land surface, space, and solar models as well as coupled modeling systems. The NCCS operates a diverse collection of hardware, including the 1,152-processor Explore (Figure 3), 1,392-processor Halem, and 128-processor Courant computing systems. In addition, the NCCS maintains and preserves a petabyte-scale archive of data from SMD science missions and projects.

Figure 3: *SGI Altix 3700 BX2 supercomputer Explore (top), and SGI Origin 3800 system, Courant (bottom) are housed at the NASA Center for Computational Sciences.*

HIGH-END COMPUTING SERVICES

Combined, NASA's HEC Program resources (Columbia, Explore, Discover, Halem, and Courant) provide NASA researchers and scientists with over 13,000 processors and more than 75 teraflops (peak) of computing power. The Program offers NASA and its research partners with far more than computing cycles, however. Users are provided with a wide variety of value-added services to help them quickly and efficiently accomplish their mission computing needs. High-End Computing Systems Development, System Performance, Mass Storage, High-Speed Networking, User Services Support, Application Optimization, and Advanced Visualization are all a part of NASA's integrated HEC environment (Figure 4) aligned to support each of NASA's four mission directorates and the NASA Engineering and Safety Center (an organization chartered to perform value-added independent testing, analysis, and assessments of NASA's high-risk projects to ensure safety and mission success).

High-End Computing Systems Development

NASA's HEC Program strives to provide users with computing architectures well-suited for their applications. The Program also aims to deliver a full-service HEC offering, ensuring applications are running well and producing the desired science and engineering results; resources are operating efficiently and securely; users are being provided with effective ways to move and exploit their data; system utilization needs are balanced; and resources are being managed prudently. Striking a balance between upgrading HEC technologies and minimizing impact on users is of utmost importance, along with maintaining a high level of system availability and providing uninterrupted access to computational resources and user data.

System Performance

The Program is also dedicated to ensuring proper management and allocation of its resources—for example, determining appropriate shares of the resources for each NASA mission directorate and closely tracking usage to ensure maximum productivity.

The Program has seen a dramatic increase in usage of its HEC resources over the past 3 years: a nearly four-fold increase in processor-hours consumed in Fiscal Year (FY) 2004 as compared to FY 2006 (Figure 5). This increase, due to the creation of higher-fidelity models generating larger amounts of data,

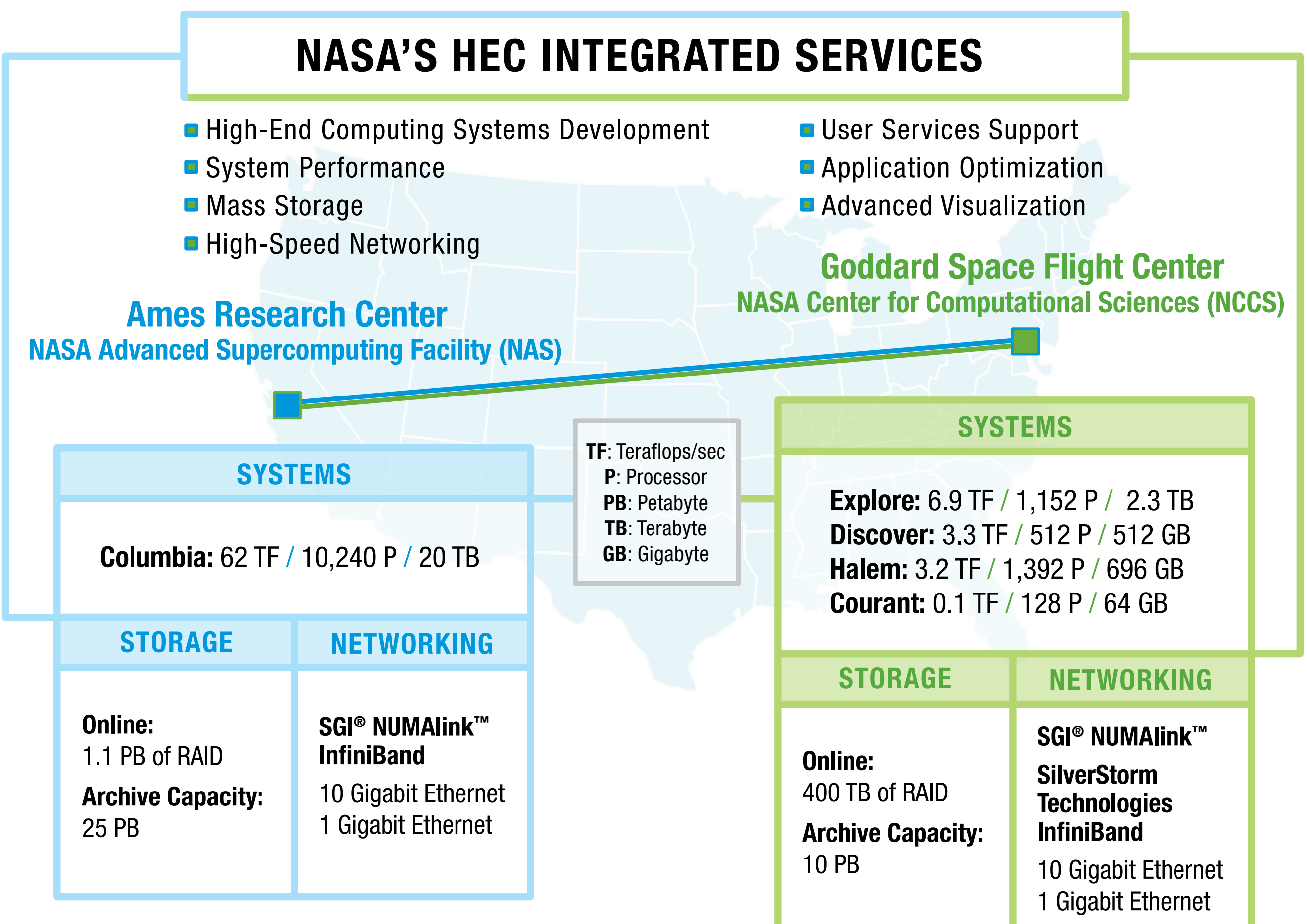


Figure 4: NASA's integrated HEC services environment.

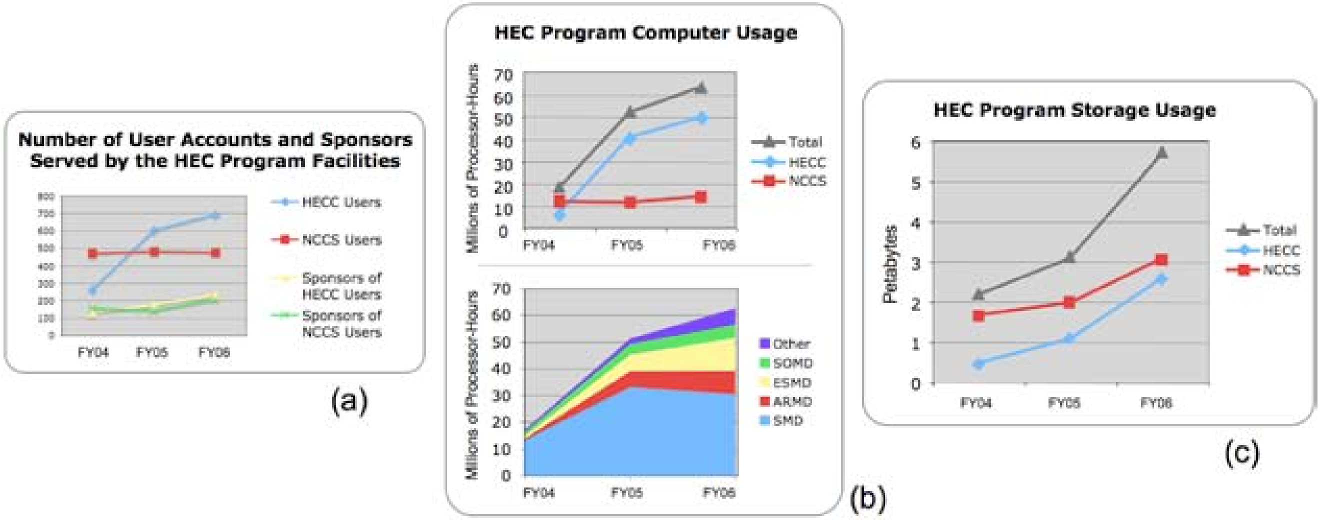


Figure 5: *Growth trends for the NASA HEC Program over the past 3 Fiscal Years, shown by project and mission directorate. (a) shows user accounts and sponsors, (b) shows processor-hours used, and (c) shows mass storage utilization.*

has prompted Program staff to look at alternative methods for making data available to users for post-processing—to help researchers better understand their results.

Mass Storage

With the massive amounts of data generated every day in support of NASA's missions, users must have a place to store it all—and be able to access it quickly, reliably, and securely for post-processing and future reference. The Program strives to provide users with ample archival capacity to help off-load on-line data—so that there is always room for computational runs on the Program's computing resources. The NAS facility provides 25 petabytes of tertiary storage capacity and over a petabyte of disk capacity while the NCCS furnishes users with 10 petabytes of tertiary storage capacity. With an average of 10 terabytes (TB) of data being generated in a single day at the NAS and NCCS facilities combined, this is no small task for Program storage specialists.

In a 2-year period—from the beginning of FY 2005 through the end of FY 2006, storage needs at the NAS facility increased over 700%, and in the last 12 months, archive data volume at NCCS grew by more than 60%, and the number of files grew by nearly 17 million (approximately 43%). To stay on top of increasing demands for data storage, several upgrades are planned for the near future including increasing archive capacity bandwidth on Columbia, after which the average data transfer is expected to be 12 TB/day with a peak of 44 TB/day, and installing new robotic libraries at NCCS, which will add more than 6 petabytes of capacity.

High-Speed Networking

High-speed network connectivity is a necessity for users to take full advantage of NASA's HEC resources. The Program provides end-to-end operational networking support for both local area networks (LAN) and wide area networks (WAN), in addition to engineering support to accommodate users' new requirements for local and distributed applications—all while adhering to NASA's increasingly stringent security requirements. Program network engineers are also constantly monitoring connections to and from all HEC systems using custom-designed network analysis tools. These tools are used to both pinpoint problems before users encounter them, and identify areas for improving network performance—from both an aggregate and individual user perspective.

One of the Program's greatest efforts over the past 18 months in the area of high-speed networking—an effort that is expected to grow as computational model sizes increase and users gravitate toward time-based modeling—is the exploration and development of methodologies for increasing network bandwidth for NASA applications. This work encompasses working directly with Columbia network users, LAN network engineers supporting Columbia's end-user sites, and network security personnel, to implement and utilize data transfer solutions that maximize network performance of individual user network and workstation environments. Furthermore, this includes exploration of new technologies capable of maximizing network performance from the Program's HEC resources—specifically InfiniBand over WAN. InfiniBand's distance-extension technology is well-suited for NASA's HEC environment, and has the potential for substantial cost-savings as it combines clustering, storage, and WAN input/output onto a single network.

User Services Support

The Program has frontline user services entities at both Ames and Goddard to assist users day or night. In addition to answering questions, the User Services support staff plays an active role in testing and anticipating user questions related to any new tools, hardware, software, or security requirements introduced into the computing environment. Shaking out problems before users encounter them and creating documentation and training to address common problems helps maximize efficiency and provides a stable computing environment for users. Over an 18-month period—from May 2005 through October 2006—NAS and NCCS successfully closed more than 10,000 HEC user-related tickets.

Application Optimization

Enhancing performance of applications and user productivity over the entire lifecycle of projects are two key objectives of the Program's performance optimization specialists. Expertise spanning both computer science and engineering applications enables the Program to provide users with several levels of application support ranging from basic scientific consulting (for example, identifying errors in users' codes and helping them port their codes onto and among HEC systems) to working closely with a user to enhance their code, sometimes requiring extensive code changes to obtain required speed-ups.

In addition to addressing application performance, the Program focuses attention on the evaluation of tools and architectures to identify the optimal technology for enhancing user productivity in NASA's HEC environment. Part of this effort is keeping track of, and measuring performance of the current architecture landscape, which is important for optimizing performance of applications on existing systems, and for selecting systems required to meet the Agency's future high-end computing needs.

Advanced Visualization

It is important for users to be able to understand and process the science and engineering behind the massive amounts of data generated on NASA's HEC resources. In some cases, the amount or complexity of the data is too great for commercially available tools—this is where the HEC Program's advanced visualization experts play a significant role. Working closely with users, visualization experts apply, and in some cases, create new techniques to expose the intricate temporal and spatial details of the computational models, shedding more light on the science they are meant to describe. With each of these challenging applications, visualization specialists become more familiar with the issues related to both the science and the code, and are able to employ more sophisticated techniques with future applications.

As data management and movement become increasingly challenging, and the need for higher-fidelity models escalates, the Program's visualization experts have pushed the envelope in developing special techniques for concurrent visualization—moving large datasets as they are generated to graphics hardware so that they can be manipulated and analyzed on the fly.

FUTURE

A Unified HEC Environment

NAS and NCCS are joining to create a unified HEC environment built on a standardized set of services. Users will be able to seamlessly move from one computer—or one computing center—to another. The base of this environment is a common interface to HEC resources, including a single process that handles all account applications, one NASA-wide username, and a shared method for secure dual-authentication.

Once logged in, users already encounter the same mass storage software at both centers. Additionally, finding the same operating systems, accessing compilers and libraries in the same logical locations, and seeing identical conventions for accessing scratch space and storage will enable users to take advantage of different architectures with minimal code changes. A long-term goal is to develop a layer of transparency that will automatically shepherd user jobs to the most appropriate system. This transparency will include the ability to easily transfer data between centers.

Besides fostering transcontinental collaboration, routine high-speed data transfer between centers will support a robust back-up capability in case of a power failure, natural disaster, or other event. Code portability and a shared data archive will, at minimum, allow users to access data they have already generated and restart computing. Ultimately, jobs will be transferred to the other center immediately after a failure; with their data ready and available, users would simply pick up where they left off.

The efficiency of the unified HEC environment stems from relying on each center's strengths: sharing best practices and sometimes assigning joint functions to the center that does them better. A common environment also helps HEC staff track system utilization and make decisions about future allocations and acquisitions. Furthermore, a program-wide configuration clarifies the path to adding new systems.

Next-Generation Systems

In acquiring its next-generation computing systems, the HEC Program is emphasizing price-performance and stability. The Program is leveraging the commodity market but collaborating with vendors to focus that market on meeting NASA's unique mission requirements. This approach also avoids taking drastic steps from one architecture to another so users will not struggle with a new environment. Extending the current trend, the Program will manage the computing resources toward increasing utilization while optimizing job turn-around.

Figure 6: *A Linux Networx Custom Supersystem called Discover will be the NASA Center for Computational Sciences' next-generation supercomputer. Shown above, the "base unit" of the cluster provides 3.3 teraflops of peak computing power in five closet-sized cabinets.*

A Linux Networx Custom Supersystem will be the NCCS' next-generation supercomputer, called Discover. As shown in Figure 6, the "base unit" of the cluster provides 3.3 teraflops of peak computing power in five closet-sized cabinets.

Partners on the cluster include Intel, SilverStorm Technologies, IBM, DataDirect Networks, Altair Engineering, and Computer Sciences Corporation. A 512-processor "base unit" arrived this summer, and the NCCS staff is evaluating the addition of several 1,024-processor "scalable units." The system could scale to nearly 40 teraflops in its full configuration. Discover will mainly provide capacity computing for Earth and space scientists. Users will have access to the same set of tools, modules, and home file systems on the new cluster as on the existing 1,152-processor SGI Altix 3700 BX2 system (Explore).

Now that the Altix-based 10,240-processor Columbia is 2 years old, NAS is developing the requirements for a follow-on system. One goal is maintaining Columbia's current capacity while meeting users' growing computational requirements, which translates to an estimated four-fold increase in workload by 2009. A more capable leadership-class system may also be a feature. Multi-year phased replacement of Columbia will be based on comprehensive market research and architecture system evaluation, including acquisition of testbeds. It is likely that a new multi-vendor partnership will build the Columbia follow-on.

Next-Generation Applications

The HEC Program's computing systems will be critical resources in fulfilling NASA's missions.

For Aeronautics Research, Columbia will be in demand for NASA's hypersonics, supersonics, subsonic fixed-wing, and rotary-wing projects. These fundamental research efforts need to resolve basic phenomena in acoustics, integrated flight-propulsion controls, and aerothermodynamics effects into complex-geometry computational tools for design and development of advanced air vehicle concepts. Columbia also will enable creation of tools to evaluate emerging technologies such as inflatable hypersonic decelerators that could improve entry, descent, and landing systems for spacecraft. For aviation safety programs, research in integrated resilient aircraft control will push the state-of-the-art in physics-based modeling of fluid flow, while modeling of atmospheric disturbances (for example, icing and turbulence) will support development of an intelligent flight deck.

For Exploration Systems, HEC resources will play a role in system design, engineering, and mission planning. The centerpieces of NASA's exploration efforts are the next-generation space vehicles. Orion will be the Crew Exploration Vehicle that carries astronauts back to the moon and later to Mars. The Ares I rocket will be the new Crew Launch Vehicle that takes Orion into space. The larger Ares V rocket will carry heavy cargo and components into orbit for rendezvous with Orion. The Columbia supercomputer is supporting the development of all three vehicles, including simulations of aerodynamic flow during flights and stage separation of Orion from Ares I. The system is also enabling designs for the Ares launch pads.

For Science, HEC resources will need to manage increasingly vast quantities of data, especially as models and observations become more interconnected. For example, Goddard's Global Modeling and Assimilation Office combines terabytes' worth of Earth observations with coupled models to better understand past climate and research ways to improve weather and climate forecasts. The HEC Program is moving towards a data-centric computing model incorporating a variety of data management services. The new NCCS Data Portal provides a platform for sharing, searching, and visualizing model datasets. Another planned service is concurrent and interactive visualization during simulations, which will be enabled by visualization "nodes" on the Discover cluster and a next-generation hyperwall node on the Columbia follow-on system. For handling data from multiple locations, the unified HEC environment will support distributed computing, where portions of a model system—and its associated data—are run at different centers in a coordinated and coupled fashion. NASA's approach is likely to include frameworks-based modeling services.

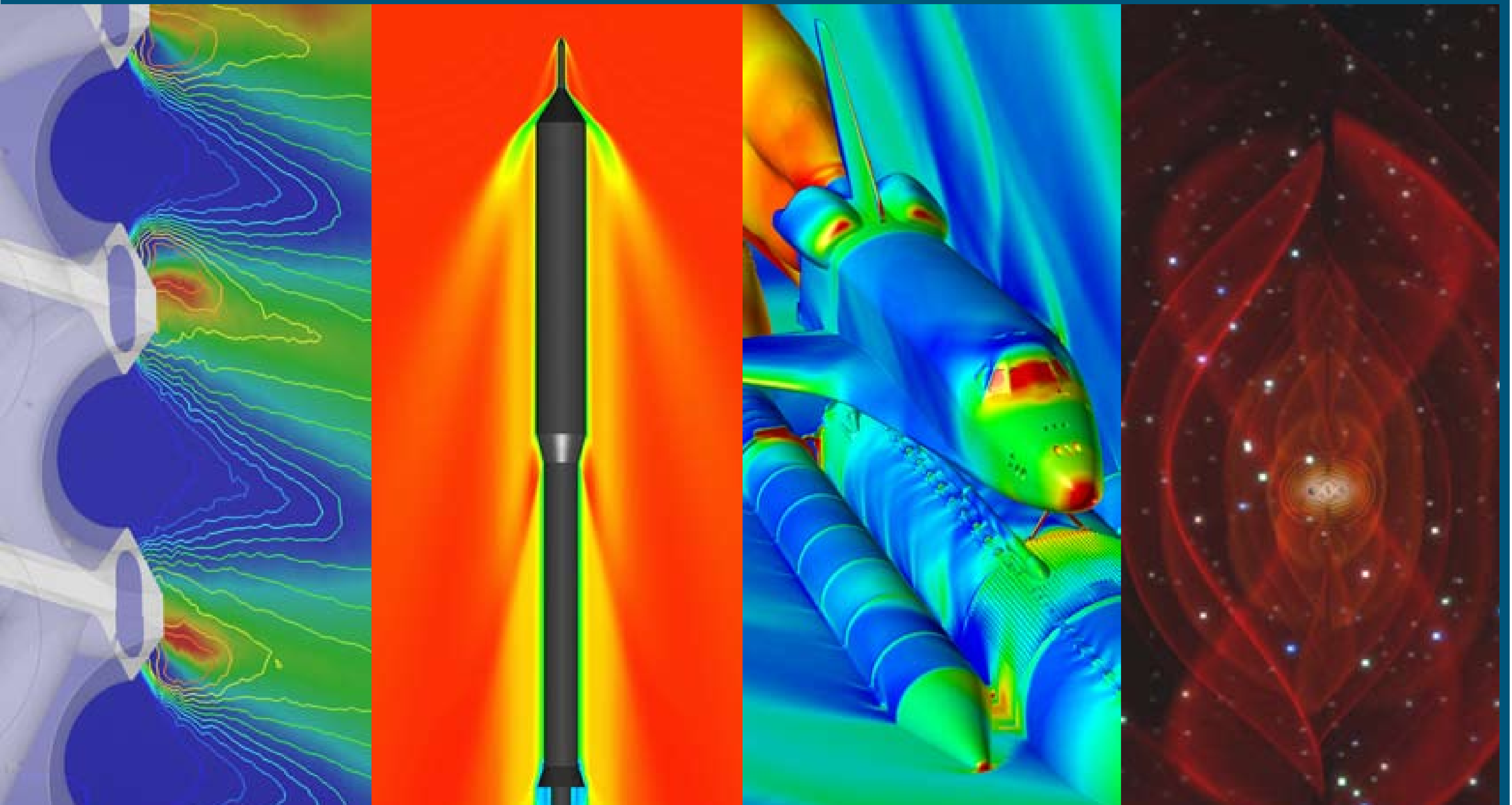
For Space Operations, Columbia must be on-call from launch to landing during the remaining Space Shuttle missions planned through 2010. Columbia's responsibilities include evaluating potential threats from ice formation and foam debris, assessing heating on the protective thermal tiles and bond lines, and analyzing design changes for components such as the external tank's ice/frost ramps. A mirrored Return to Flight data warehouse, co-located at Ames and Langley Research Centers, supports these on-the-fly analyses with rapid transfer and dissemination of data. The Hubble Space Telescope Servicing Mission 4 planned for late 2007 or early 2008, will require computational support, as it will necessitate the unprecedented launch of two Shuttles almost simultaneously.

Technology Pathfinding

During the 1990s, the computational science community began a paradigm shift—from primarily single-processor computing to routine parallel processing. The decade to come will witness another shift in which the supercomputer processor becomes only one component in a distributed collection of technologies and services. In addition to developing data management services, NASA is engaged in pathfinding activities for technologies that could significantly enhance simulation and data analysis capabilities.

NASA, the Department of Defense, and the Department of Energy are partners in the Data Intensive Computing Environment (DICE). This industry testbed provides the means to fund and try out information technology offerings and offer feedback to companies before placing new technologies into a production environment. Through DICE, NASA is gaining access to field-programmable gate arrays, specialized chips that work as accelerators alongside traditional processors, and the Cell processor, which was developed for the Sony PlayStation 3 game console but has shown some promise on scientific applications.

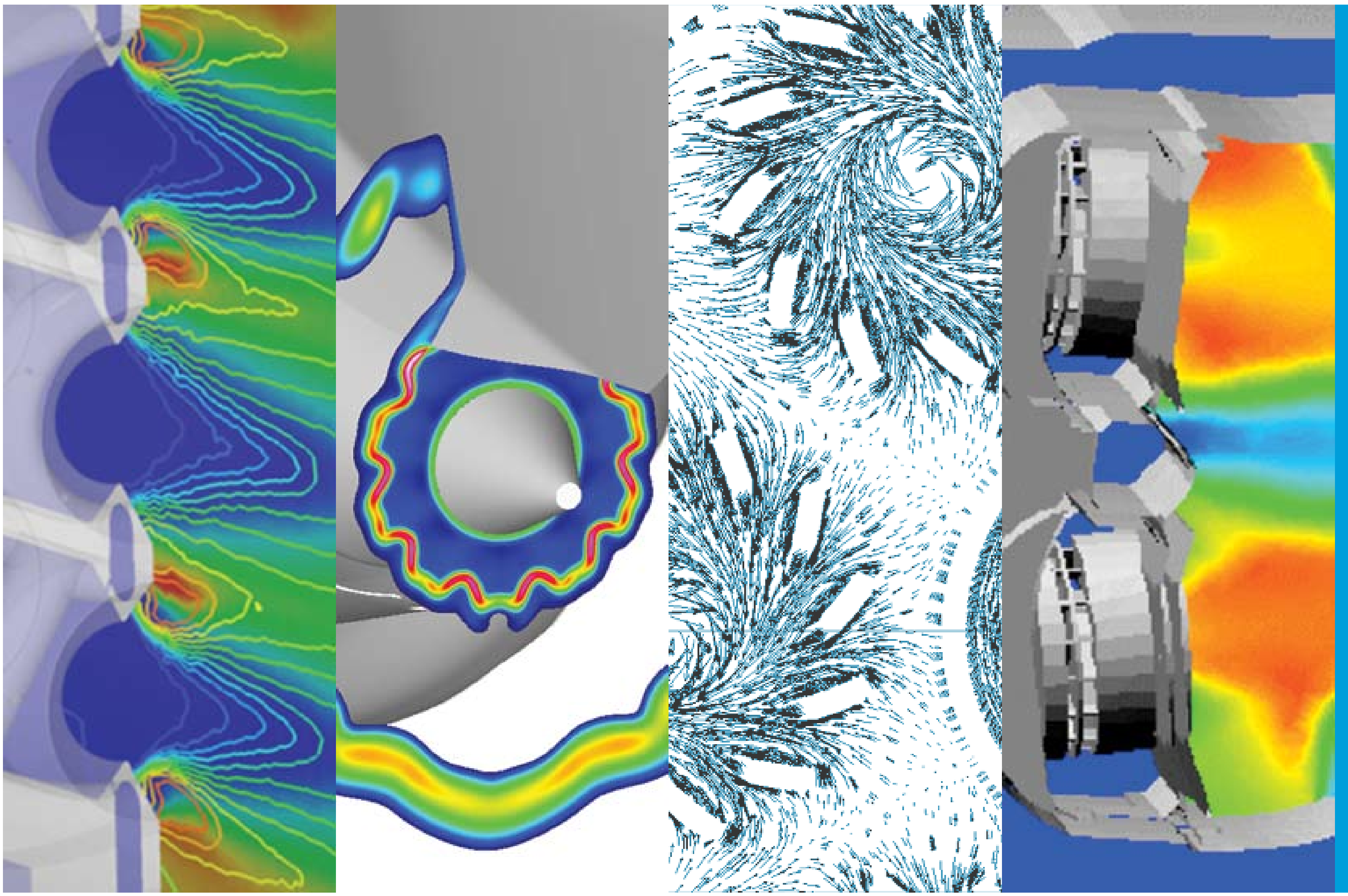
New technologies will be evaluated based on their ability to serve the HEC user community and the NASA missions they support. Undoubtedly, requirements will escalate, and priorities will be adjusted. Within this dynamic environment, NASA's HEC Program will evolve its mix of technologies and services while maintaining a steady focus on ensuring mission success.



HIGHLIGHTS

SCIENCE AND ENGINEERING

This section presents 40 user projects from NASA's Aeronautics Research, Exploration Systems, Science, and Space Operations Mission Directorates, and the National Leadership Computing System, chosen because of their importance to the Agency, their impact during the reporting period (past 18 months), and their technical maturity.



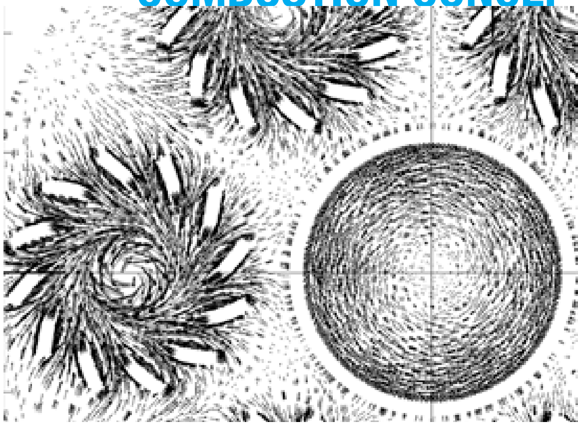
MISSION DIRECTORATE

AERONAUTICS RESEARCH

The Aeronautics Research Mission Directorate's efforts are directed toward the transformation of our Nation's air transportation system, and developing the knowledge, tools, and technologies to support future air and space vehicles. Our focus is on cutting-edge, fundamental research in traditional aeronautical disciplines. We are investing in research for the long-term in areas that are appropriate to NASA's unique capabilities, and meeting our charter of addressing national needs. We are advancing the science of aeronautics as a resource for our Nation, as well as advancing technologies, tools, and system concepts that can be drawn upon by civilian and military communities, and other government agencies.

DR. LISA J. PORTER
Associate Administrator
http://www.aeronautics.nasa.gov

CFD ANALYSIS OF ADVANCED LEAN DIRECT INJECTION COMBUSTION CONCEPTS USING THE NATIONAL COMBUSTION CODE



AERONAUTICS RESEARCH MISSION DIRECTORATE

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Figure 1: *A close-up view of the flow in the outer swirler vanes of a Smart Integrated SiC Multi-Point Lean-Direct-Injection Combustor, via an X slice. The arrows point in the direction of the fluid flow, while vector length indicates the velocity magnitude (speed). Since the mesh is unstructured, placement of the vectors' arrows is non-uniform, the swirling motion created by the vanes is evident.*

Project Goals and Objectives: The original goal of this project was to study actively controlled Lean Direct Injection (LDI) combustion concepts, currently called the Smart Integrated SiC Multi-Point Lean Direct Injection (SIMPL-DI) Combustor. However, advanced low-emissions Hydrogen LDI combustor concepts were added because of changing programmatic directions at NASA.

Project Description: The Combustion Branch at NASA Glenn Research Center is currently working on LDI, a promising low-emissions combustion concept for gas turbines (jet engines, for example). In LDI, a fuel (Jet-A, hydrogen, or natural gas, for example) is sprayed (if a liquid), or injected as a gas, directly in the engine's combustor using multiple fuel injector modules—the goal being to violently mix the fuel and air so the resulting flame is mostly "premixed." A premixed flame burns at a lower temperature, resulting in fewer nitrogen oxide and hydrocarbon emissions (if a fossil fuel is used) being released into the environment. While this combustion concept works well at full power conditions, the overall air-fuel ratio is too lean to sustain stable combustion at low power conditions. To remedy this, NASA researchers are currently focused on an active control design, SIMPL-DI, which allows operation at all ranges. While hydrogen combustion does not produce carbon monoxide or hydrocarbons, it does produce large amounts of nitrogen oxides. If a hydrogen combustor is operating at globally lean conditions, a locally turbulent non-premixed flame will still produce large amounts of nitrogen oxide emissions, because high flame temperatures still occur at the local level. We use LDI to reduce these hot spots by violently mixing the hydrogen and air, resulting in a nearly premixed flame, which dramatically reduces the amount of nitrogen oxides produced.

Relevance of Work to NASA: NASA's Aeronautics Research Mission Directorate (ARMD) is committed to aircraft emissions reduction goals at subsonic and supersonic flight conditions.

Numerical Approach: The National Combustion Code (NCC) is a state-of-the-art computational fluid dynamics (CFD) program specifically designed for combustion processes. A short summary of the features of NCC pertaining to this project are: use of unstructured grids, massively parallel computing with almost perfectly linear scalability, a dynamic wall function with the effect of adverse pressure gradient, low Reynolds number wall treatment, a cubic non-linear k-epsilon turbulence model, the well-validated Magnussen Eddy Dissipation Concept (along with Marek's fuel curve fits), a fast chemical kinetics solver, and a lagrangian liquid phase spray model. Recently, viscous low-speed pre-conditioning has been added to improve the low-speed convergence of the NCC in viscous regions, and the ability to handle multiple sets of periodic boundary conditions has been added. The combination of these features is usually not available in other CFD codes, and gives the NCC an advantage when computing re-circulating, turbulent reacting spray flows.

Computational Approach: The solid geometry models were created using Pro Engineer, while computational grids were generated using the Gridgen mesh generation program. Originally, all tetrahedral meshes were used, however, hybrid meshes were used in later cases for both the SIMPL-DI and hydrogen concepts to increase accuracy. The Pro Engineer models were then translated into Initial Graphics Exchange Specification format, for use as surface models within Gridgen. During the start of this study, computational grids with 250,000 cells were used. The grids were refined until acceptable results were obtained, and the final computational grids contained approximately 2–5 million elements. The NCC then performed a CFD combustion analysis. MPI was used for parallel processing, and Metis was used for domain decomposition (load balancing). For the SIMPL-DI concept, 128 processors were used for 3 wall-clock days on the Columbia supercomputer. Because of the numerical stiffness (in both geometrical and chemical time scales), the hydrogen combustion concept was much more computationally challenging, taking approximately 2 weeks to complete a case using 256 processors.

Results: In the past, it was assumed that a complete combustion model would address the inaccuracies in combustion CFD calculations. With this work, it is now clear that a full geometric representation of the actual combustor is needed, along with a consistent turbulent combustion model. A paper titled "National Combustion Code Calculations of a NASA Low-NOx Hydrogen Injector Concept" will be presented at the 2007 AIAA Aerospace Sciences Meeting.

Role of High-End Computing: Without the extensive supercomputing capabilities such as those afforded by Columbia, this project would not have progressed. Access to large, parallel systems have enabled the project to evolve from looking at a single injector in an array, to nearly the entire combustor geometry. Understanding of a successful combustion concept is dependent on looking at the entire geometry, because small geometric changes can drastically change the mixing process, which determines whether a combustor decreases emissions or not.

Future: Combustion CFD analysis with the NCC is included in future Subsonic Fixed Wing and Supersonic Fixed Wing ARMD goals. Hydrogen combustion will be de-emphasized, while work will continue for the SIMPL-DI concept. Exploration Systems Mission Directorate projects utilizing "green" propellants are extensions of this work.

Collaborating Organizations

- Ohio Aerospace Institute

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4. Quealy, A., Ryder, R., Norris, A., and Liu, N.-S., "National Combustion Code: Parallel Implementation and Performance," *NASA TM-2000-209801*, 2000.
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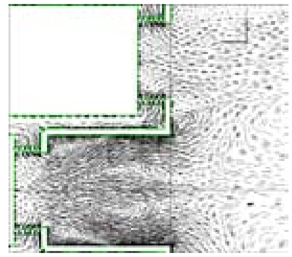

Figure 2: A close-up view of the flow in the "cup region" of a Smart Integrated SiC Multi-Point Lean-Direct-Injection Combustor, via a slice at the Z mid-plane. The arrows point in the direction of the fluid flow, while vector length indicates the velocity magnitude (speed). Since the mesh is unstructured, placement of the vector arrows is non-uniform. Multiple regions of re-circulating flow inside and outside the cup are shown.

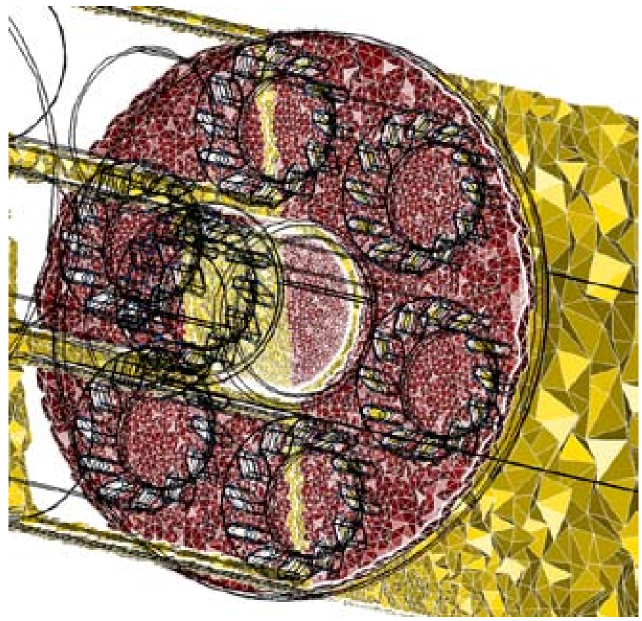

Figure 3: Computational grid of a Smart Integrated SiC Multi-Point Lean-Direct-Injection Combustor concept. The volume mesh is visualized by slices in the axial and longitudinal coordinates. This particular grid has about three-million tetrahedral and prism elements.

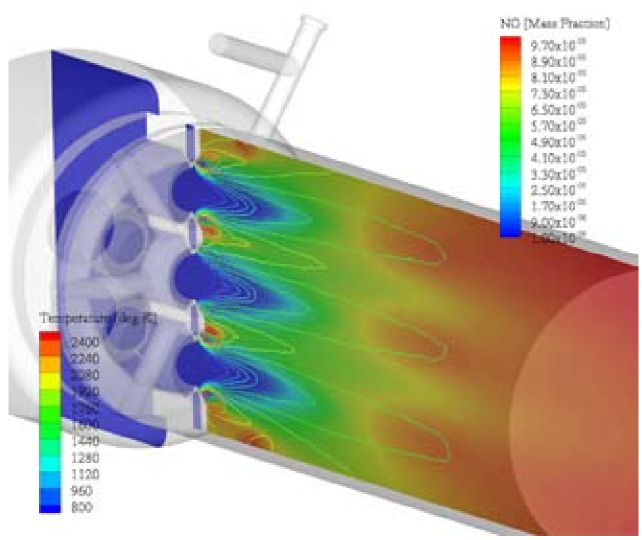

Figure 4: The translucent white shows the injector geometry. Hydrogen travels through the long tube at the top, through the manifold "ring" in the center left, and is injected through the set of four very small tubes inside the venturies. A longitudinal mid plane slice shows two sets of contours: 1) Line contours show temperature, 2) Flooded contours show nitrogen oxides (NO). As shown by the temperature contours, hot spots are minimized, and therefore the nitrogen oxides created in the flame zone are minimized. This CFD analysis confirms experimental results: the NASA Hydrogen LDI concept produces low amounts of nitrogen oxide.

COMPREHENSIVE COMBUSTION MODELING AND SIMULATION: EMISSIONS REDUCTION AND PERFORMANCE IMPROVEMENT

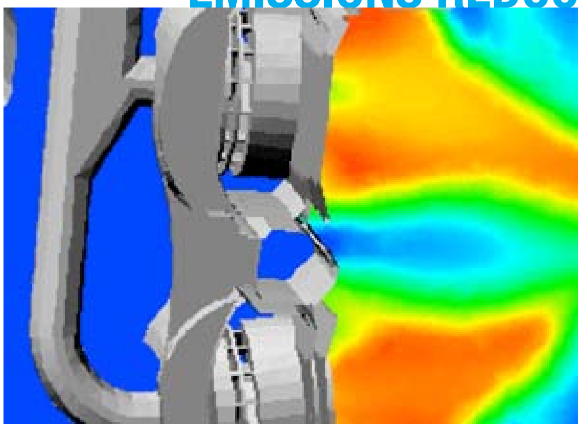

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Figure 1: *Close-up of modern turbo fan jet engine simulation seen in Figure 2.*

Project Goals and Objectives: Recent advancements in the areas of combustion modeling, numerical simulation, and high-end computing have greatly facilitated the use of computational fluid dynamics (CFD) in the development of combustion technology. However, for these CFD-based tools to play a more reliable and practical role in the design and analysis of advanced, low-emission, high-performance combustion systems, significant improvements in their abilities to predict the interacting chemical and multi-physics phenomena are needed. The aim of this project is, through the development/validation/application of the National Combustion Code (NCC), to push the state-of-the-art in comprehensive combustion modeling and simulation, and together with experimentalists and designers, establish an integrated approach using combustion CFD, diagnostics, and rig testing to advance the combustion technology for emissions reduction and performance improvement.

Project Description: Combustion operates at the intersection of fluid dynamics, fuel chemistry, and multi-phase physics. Modeling of these highly non-linear and intrinsically unsteady processes calls for a comprehensive approach. Specifically, all pertinent components and models are integrated into a simulation framework via an overall solution procedure and algorithm that can robustly and consistently account for the overall physical-chemical process occurring in the practical system of interest. In practice, not all of the temporal, as well as spatial scales, can be computationally resolved—physics-based models are used to account for the effects of unresolved scales on the directly computed scales. To model and simulate the combustion system as accurately as possible, it is imperative to make the computationally, directly resolved scales as small as possible. Our research and development of comprehensive combustion modeling and simulation is embodied in the development, validation, and application of NCC. We have been prudently using NCC within its current limitations for technology program support while concurrently improving its fidelity and extending its capability.

Relevance of Work to NASA: Researchers and engineers have been using NCC to provide analysis and design support for various aerospace propulsion technology projects such as fuel injectors for emissions reduction, revolutionary turbine accelerator and turbine-based combined-cycle engines, rocket-based combined-cycle engines, advanced rocket combustor concepts, and compressor-combustor-turbine integration (Figure 2 shows the temperature field inside the combustor). NCC is also being used as a testbed for assessing and developing combustion models and computational technologies in an engineering environment. In addition, technology transfer to external organizations has been conducted through non-exclusive Space Act Agreements.

Numerical Approach: NCC features high-fidelity representation of complex geometry, advanced models for two-phase turbulent combustion, conjugate heat transfer, and massively parallel computing. The interacting multi-phase, multi-physics processes are emulated via a hybrid Eulerian-Lagrangian-Monte Carlo algorithm. Major modeling enhancements currently in progress are liquid fuel atomization, particle and aerosol emissions, Very Large Eddy/Large Eddy Simulation (VLES/LES), and radiation heat transfer.

Results: References 1–3 summarize our most recent activity in the validation of NCC. In particular, [1] covers the comparison of NCC results with measured data and the LES results for a single-element lean-direct injection combustor aimed at low emissions. The use of NCC to provide design and analysis support for aerospace propulsion technology development is reported in [4] for a revolutionary turbine accelerator, and [5] for a pulsed detonation engine. Further, development of modeling capabilities is in progress. Implementation of the liquid fuel atomization is described in [6]. The development of directly computing the unsteady, large-scale flow structures in the context of VLES is reported in [7–9]. The use of a transport equation for the joint probability density function of the scalars to model the turbulent combustion is demonstrated in [10]. Implementation of the chemical and microphysical modeling capability for particulate emissions from jet engines is described in [11].

Role of High-End Computing: High-fidelity simulation of multi-phase turbulent combustion in a practical device requires adequate resolution of a wide dynamic range of temporal and spatial scales. This entails intense computations, which in practice, can only be carried out on massively parallel systems such as the Columbia supercomputer. To take full advantage of Columbia's parallel architecture, High-End Computing Program application specialists are assisting with optimizing the parallel performance of NCC. To date, our typical Reynolds Averaged Navier-Stokes Simulation is routinely performed on 128–256 processors. For better prediction of emissions and/or flame stability, VLES/LES will be carried out, which will require a greater amount of Columbia's parallel computing resources.

Future: Under the Fundamental Aeronautics Program, we will conduct systematic and rigorous validation simulations—first to baseline the overall fidelity of the current version of the NCC, and then to guide and measure its further development/enhancement. The ultimate goal is to have a predictive capability for providing quantitatively accurate information, accompanied by estimated uncertainties, on emissions and performance of practical combustion systems.

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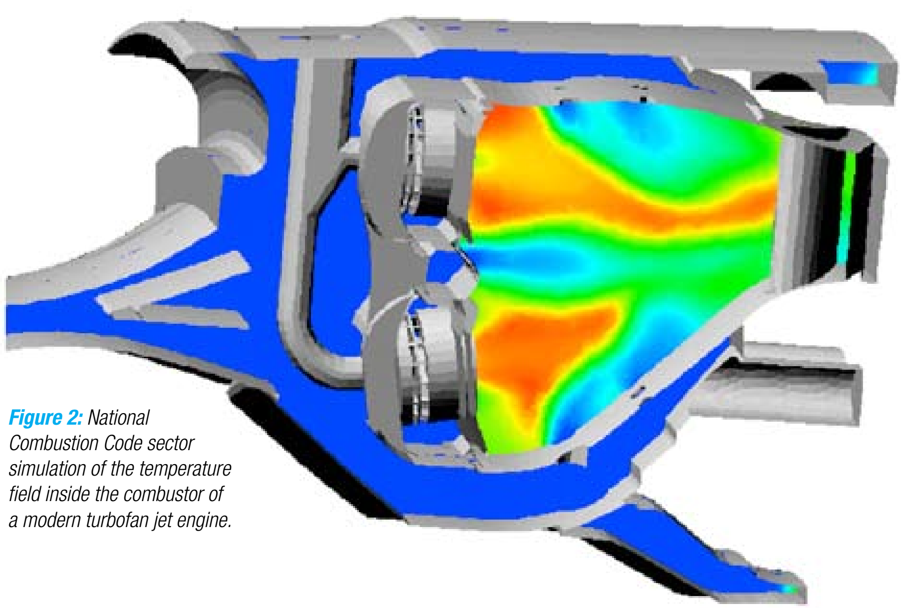

Figure 2: *National Combustion Code sector simulation of the temperature field inside the combustor of a modern turbofan jet engine.*

COMPUTATION OF HIGH-LIFT FLOWS USING A NAVIER-STOKES UNSTRUCTURED-GRID METHOD

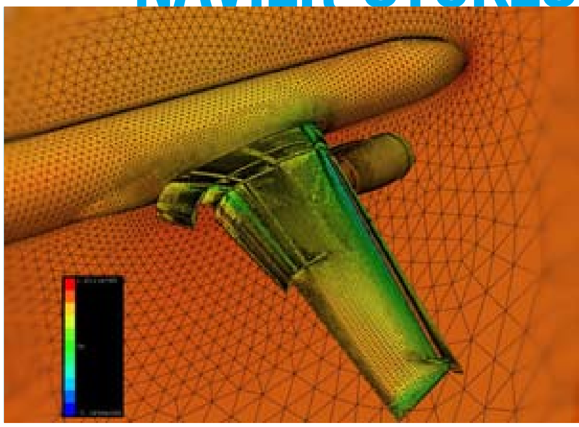

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***Figure 1:** Boeing 777 landing configuration: grid and pressure contours.*

Project Goals and Objectives: The goal of this project was to demonstrate and improve the capabilities of a computational method for predicting flowfields associated with high-lift configurations, particularly near the maximum lift (C_{Lmax}). The objective was part of a longer-range goal of improving the understanding of Reynolds number scaling and semi-span wind tunnel testing at flight Reynolds numbers.

Project Description: Accurate prediction of high-lift aerodynamics is one of the intractable problems in computational fluid dynamics (CFD). The combined complexity of geometry and flow physics associated with the high-lift problems pushes the limits of current computational methodologies and resources. Numerous attempts to solve this problem have indicated that finer grid resolutions are required in key flow regions that, in turn, signify the need for larger computing resources. Past investigations suggest that computation of high-lift problems requires grid resolutions on the order of hundreds of millions of grid points running on thousands of processors. Proper guidelines for strategic refinement of grids in dominant flow regions are critical and require further investigation.

Relevance of Work to NASA: The work presented was carried out as part of the High-Reynolds Number High-Lift task under the Efficient Aerodynamic Shapes and Integration Project of the NASA Vehicle Systems Program.

Computational Approach: Due to the geometric complexity of high-lift problems, an unstructured grid methodology was selected for this research. Unstructured grids are more flexible than their structured counterparts and adapt to complex configurations with relative ease. The Tetrahedral Unstructured Software System (TetrUSS), developed at NASA Langley Research Center, was used for the present study. The package consists of an unstructured grid generator VGRID, and a Navier-Stokes solver, USM3D. Advances were made in the generation and refinement of unstructured grids for high-lift complex configurations during the course of this study. A new octree-based surface-source concept was developed which enables strategic refinement of the grid in the wake regions of the control surfaces—this was not previously possible. The resulting capability leads to increased accuracy of high-lift solutions.

Results: Earlier study of a high-lift flowfield on a trapezoidal wing configuration identified regions of the computational domain that were critical for accurate prediction of specific portions of the lift curve. In general, proper grid resolution at the wake regions of the control surfaces was shown to have a positive effect on the quality of the predicted lift. At the time of that study, the only technique in the VGRID code for defining the grid resolution was the use of a set of "point" and "line" sources. This method, while simple and effective for refining a grid locally, is not appropriate for controlling the grid density in a large section in three-dimensional space such as extended areas in the wake regions. For example, about 2,000 line sources were previously used to refine the grid for the trapezoidal wing, which required a substantial amount of time and effort. The new octree-based surface-source technique has facilitated the process of generating good quality grids for the high-lift applications.

Figure 2 shows a tetrahedral "viscous" grid generated on the trapezoidal wing configuration using the new method. Only a handful of sources (including two surface sources) were used for this grid as opposed to more than 2,000 line sources employed before (Figure 2a). As illustrated in Figure 2b, the grid is appropriately resolved in the areas of interest. The new method was also applied to a Boeing 777 landing configuration. It consists of a wing, fuselage, leading-edge slats, trailing-edge flaps, pylon, and a "chined" nacelle. The configuration features complexities such as tight corners and very narrow gaps between various components that usually pose a challenge for grid generation. The generated "viscous" grid, containing about 108 million cells, was generated using several surface sources prescribed on the geometry and in the wake regions. Flow solutions were obtained with USM3D using the Spalart-Almaras turbulence model at a Reynolds number of 5.9 million and a Mach number of 0.21. Solutions were obtained at three different angles of attack (AOA): 12, 14, and 16 degrees. However, the focus of the study was mainly on the 16-degree case because it represented a critical near C_{Lmax} problem, which involved massively separated flows and introduced a challenge for predicting the lift accurately. Although the main features of the flow were developed and the solution appeared converged, the separation lines on the flaps remained unsettled, and the accuracy of the predicted lift was below the expected range after 15,000 iterations.

Role of High-End Computing: The computations for the Boeing 777 at 16 degrees AOA took about 17 days of continuous jobs running on the Columbia supercomputer using 140 processors. A complete lift-polar consists of about thirteen AOAs and would have required access to a much larger computational resource. Columbia was critical in reaching the level of grid density and extensive flow computations needed for the present high-lift solutions.

Future: High-lift flows involving large separated flow regions are inherently unsteady and require time-accurate solutions. In addition, better turbulence models are needed to handle such flows more accurately. Generation of larger, more efficient grids requires parallel and adaptive grid generation techniques. And finally, access to more processors is crucial to reducing the solution time for large grids of hundreds of millions of elements.

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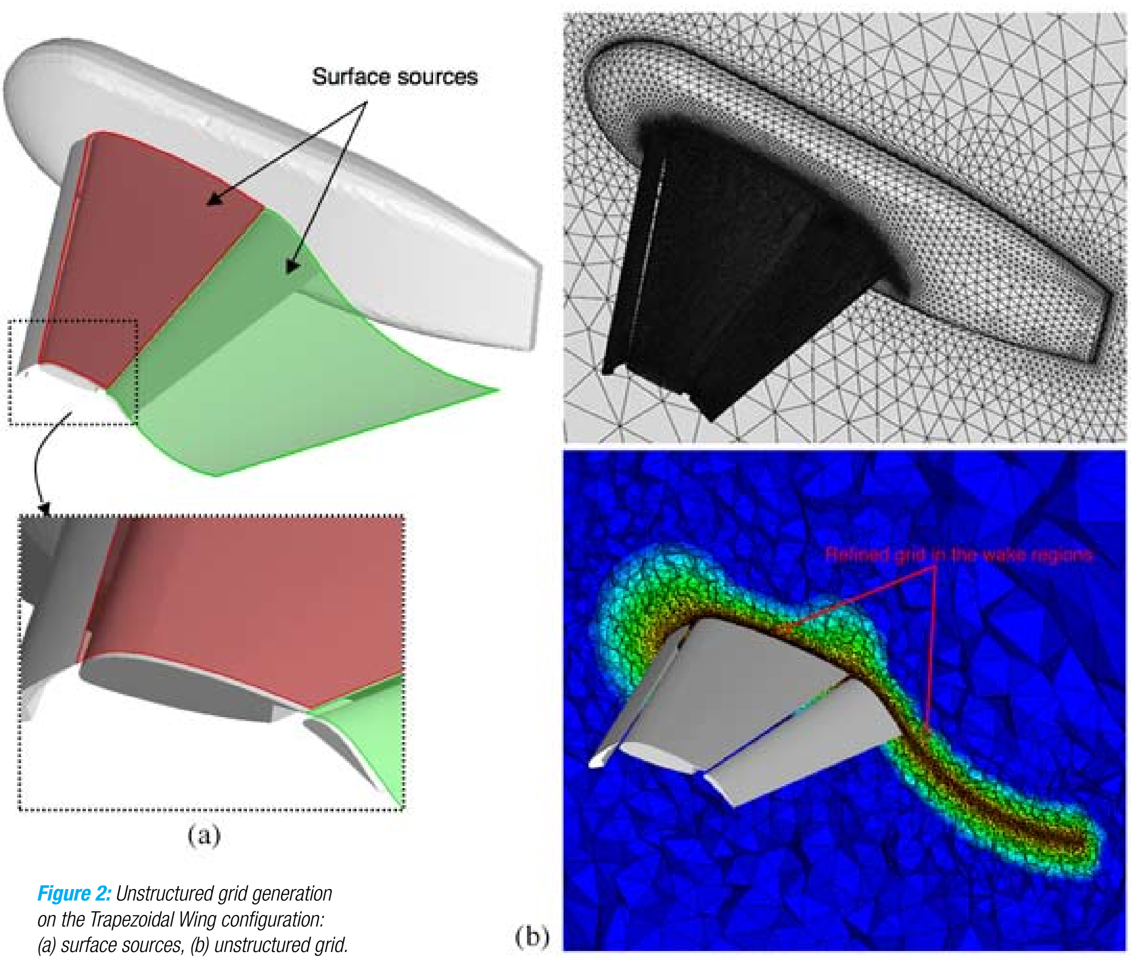

Figure 2: *Unstructured grid generation on the Trapezoidal Wing configuration: (a) surface sources, (b) unstructured grid.*

DETONATIVE COMBUSTOR MODELING: TOWARDS A HIGH-EFFICIENCY CONSTANT VOLUME COMBUSTOR

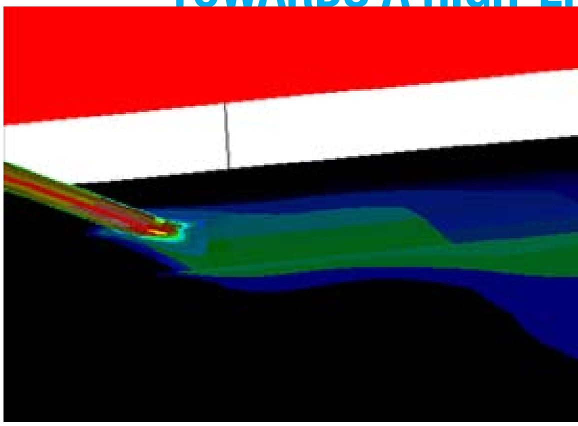

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Figure 1: *Detonation initiation in annular combustor geometry, as shown in Figure 2.*

Project Goals and Objectives: The NASA Constant Volume Combustion Cycle Engine (CVCCE) Program sought to replace the constant pressure combustor in typical gas turbine engines with a constant volume combustor. A constant volume combustion process is thermodynamically more efficient than constant pressure combustion, and a gas turbine engine with a constant volume combustor could improve its specific fuel consumption by 7–11%. The computations performed under this project aided in the development of these more efficient combustors.

Project Description: There are potentially significant performance improvements to be realized by utilizing a detonative combustor to achieve constant volume combustion in a gas turbine engine. However, there are also numerous, serious technical obstacles to making constant volume combustion cycle engines practical. Among the technical challenges to be overcome are the ability to detonate jet fuels, combustor emissions, combustor and turbomachinery durability, and obtaining a reasonable length for the transition from deflagration to detonation. To gain insight into these technical challenges, computations of Nitrogen Oxide (NOx) emissions, film (Figure 2) and ejector cooling schemes, and the affects of obstacle geometries on detonation transition length in detonative combustors were performed. Computations of advanced detonative combustor concepts (Figure 3) were also performed.

Relevance of Work to NASA: This work is a part of NASA's continuing effort to increase national aeronautics knowledge and capabilities. Successful development of a CVCCE with its large reduction in fuel consumption would provide significant commercial and national security benefits.

Computational Approach: The National Combustor Code (NCC) and an in-house upwind computational fluid dynamics code were used in this project. NCC is a three-dimensional, parallelized, unstructured grid code with reacting flow and two-phase flow capability. Second-order accurate central differences are used for the inviscid and viscous flux characterizations, and a Jameson operator is used to maintain numerical stability. Dual time stepping is used to obtain second-order accuracy for transient simulations. Turbulence closure is obtained by a low Reynolds number k-e model. A finite rate chemistry model is used to compute the species source terms for Jet-A/air chemistry. The upwind code solves the axisymmetric Navier-Stokes equations, the Spallart-Allmaras turbulence model, and a detailed kinetics mechanism for Jet-A. This equation set is solved using a fully implicit, first-order accurate-in-time, variable-step backward differention method, while the numerical fluxes are evaluated using a second-order, spatially accurate total variation-diminishing scheme. The resulting equations are then linearized in a conservative manner and solved iteratively allowing relatively large time steps to minimize computational cost.

Results: Computations were performed to aid in the design of a Jet-A/air-fueled detonative combustor test rig. This test rig was the first to demonstrate Jet-A/air detonability at gas turbine operating conditions—the critical piece of technology for CVCCE. Computations were performed with the upwind code to simulate the NOx emissions formation processes in a detonative combustor. Subsequent comparisons with NOx emissions measurements from the test rig provided excellent agreement. The NOx emissions calculations demonstrated that emissions would be a significant issue with these combustors. Strategies to lessen NOx emissions such as low stoichiometry operation or stratified charges were explored computationally. A detonative combustor would create a severe thermal and stress environment at the combustor walls. A computational study was performed to determine which cooling techniques would be effective in a detonative environment. Detailed computations of the film coolant flow in a detonative combustor were performed, along with thermal and stress computations, which were used to design a film-cooled test article. This test article was used to demonstrate that a cooling film could be maintained on the walls of a detonative combustor, and to quantify its effectiveness. Computations were also performed to aid in the design of an ejector cooling concept. Proof-of-concept tests using an ejector cooling test article were successfully completed. Chemical kinetics models for Jet-A/air detonations anchored to experimental data were developed as part of this effort. These kinetics packages would prove useful in optimizing obstacle geometry to minimize length of the transition from deflagration to detonation. These kinetics packages are being transferred to industry as requested.

Role of High-End Computing: Studying of the dynamics of detonations in these devices necessitates calculating time histories for reacting flows with fine-grid resolution. These demanding computations require a massively parallel cluster with efficient inter-processor communication such as that afforded by the Columbia supercomputer. All of the transient combustion studies performed under CVCCE consumed approximately 750,000 processor-hours on Columbia.

Future: Detonative combustor technology development efforts continue in industry.

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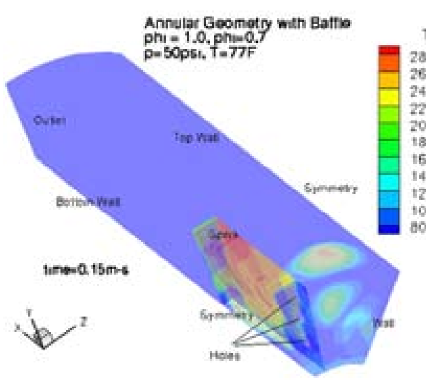

Figure 2: Film coolant dynamics as a detonation wave passes.

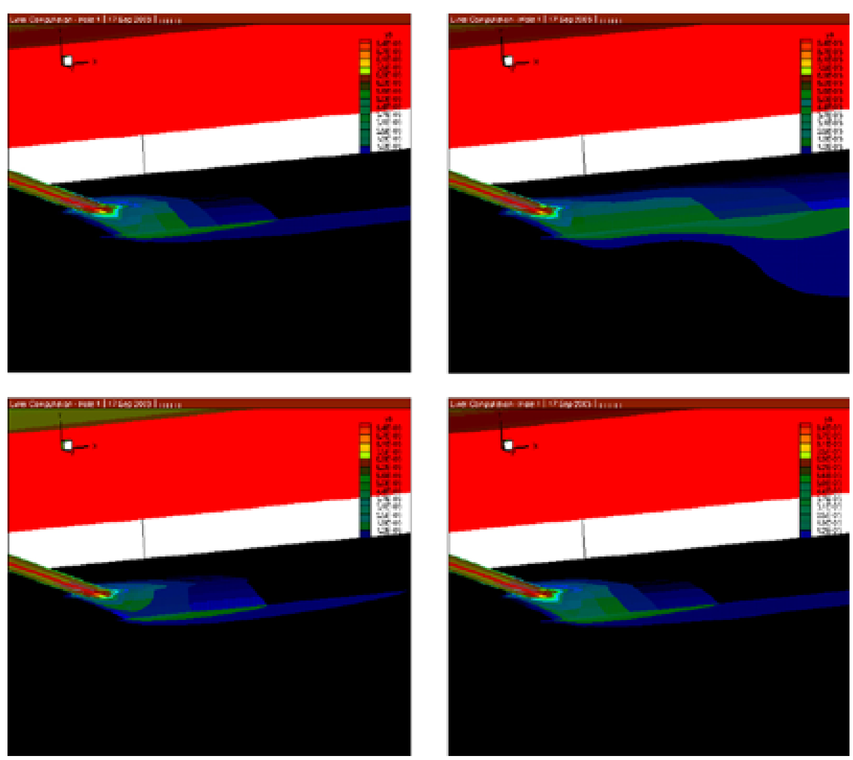

Figure 3: Detonation initiation in annular combustor geometry.

POST-FLIGHT CFD ANALYSIS OF TRANSONIC DRAG ON THE X-43 HYPER-X LAUNCH VEHICLE

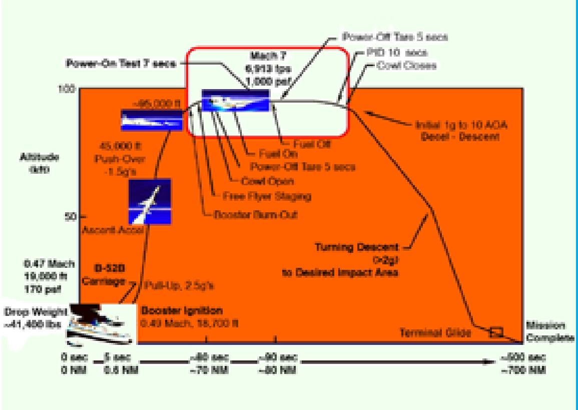

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Figure 1: *Hyper-X trajectory.*

Project Goals and Objectives: The goal of this work is to reconcile the discrepancies between preflight estimations from wind tunnel testing and computational fluid dynamics (CFD) analyses of an X43-A vehicle drag at transonic conditions, with those from flight tests. Figure 1 shows the transonic condition occurs approximately 10 seconds after drop from a B-52 aircraft.

Project Description: The aerodynamics of transonic conditions are the most difficult portion of flight to predict and test, as transonic drag values can vary widely with the slightest changes. Following successful completion of the second flight of the Hyper-X/X-43A scramjet propulsion experiment in March 2004, it was determined that the measured drag at transonic conditions on the Hyper-X Launch Vehicle was approximately 50% higher than the preflight predicted values based on wind tunnel test data and CFD results. Figure 2 shows the discrepancies observed among the 6-degree-of-freedom and flight data. To help reconcile discrepancies in preflight estimations of vehicle drag at transonic conditions, a CFD investigation of the Hyper-X Launch Vehicle configuration was conducted. This study examined a number of areas viewed as potential contributors to the transonic drag prediction discrepancies including an extensive review of the geometric modeling and CFD grids generated for the wind tunnel model and flight vehicle configurations; differences between the wind tunnel and flight Reynolds number conditions; and fluid-structure interactions resulting in aeroelastic deformations. The analytical efforts in search of the additional drag observed during the transonic portion of the flight resulted in a value within approximately 1% of the flight data.

Relevance of Work to NASA: This work is closely aligned with one of the Aeronautics Research Mission Directorate's primary aims: to pursue research and technology development that increases mobility and pioneers revolutionary aeronautical concepts for science and exploration. During its two successful flight tests in 2004, the X-43A vehicle demonstrated an advanced form of an air-breathing jet engine that could power an aircraft nearly 10 times the speed of sound.

Computational Approach: Three areas were investigated to resolve the preflight versus flight drag estimates using the results from the CFD analysis (to reconcile the transonic drag discrepancy):

- All of the computer-aided design (CAD) and GridTool models were compared with the flight and test article configurations. After conducting thorough comparisons, it was discovered that a cable raceway on the fuselage of the launch vehicle was inadvertently eliminated from the CAD and GridTool models. Furthermore, a full circumferential gap (backward-stepping surface) on the fuselage of the launch vehicle was also discovered missing from the CAD and GridTool models. To fully represent the geometry of the launch vehicle, the rim of the propulsion nozzle, as well as the internal surfaces of the propulsion nozzle up to the throat section, were added to the CAD and GridTool models.

- The second area of investigation for correction to the CFD models involved an examination of using the flight Reynolds number values for generating the CFD grid viscous layer. Prior to building a flight-quality CFD model using the flight Reynolds number, however, a grid sensitivity was performed to determine the drag as a function of number of elements in the CFD mesh. Then, attempts were made to use the same grid sourcing that resulted in a drag value for the flight-quality CFD model.

- The last area of investigation was to bring the aeroelasticity effects into the CFD model of the flight configuration. This area of investigation required identification of the most flexible portion of the Stack—the composite wing structure of the launch vehicle. For this effort, the finite element model of the wing was isolated and coupled with a representative CFD model of the wing, which was built for this exercise. Then, the pressure loads from the CFD analysis were applied to the finite element model, and the resulting deflections were used to stretch the CFD mesh. Finally, the stretched CFD mesh was used to predict the final drag. The difference between the drag values from the rigid and stretched CFD models were then added to the overall drag prediction.

Results: The results of this project show that the current aerodynamic and coupled fluid-structure interaction software codes are mature and accurate enough for predicting the vehicle aerodynamic performance under transonic conditions. Furthermore, NASA and U.S. industry can use these software codes, DDTBDM and USM3D [1,2] to predict the aerodynamic performance of new flight vehicles with higher levels of confidence. Accurate prediction of flight vehicles allows the U.S. to keep its edge over foreign competitors.

This project also proved that single disciplines cannot, and should not fully address all questions pertaining to flight hardware development—even though each discipline (for example, aerodynamics) is fully mature, integration of all pertinent areas can truly reveal the vehicle performance.

Role of High-End Computing: The fast processing power afforded by the Columbia supercomputer, coupled with the 24x7 availability was crucial to the timely completion of this work. For a period of two months, two to three runs were conducted on Columbia daily, each consuming 64 processors for an 8-hour period. Each run ranged from flight conditions between Mach 0.92 and 1.1.

Future: While these methods are now considered a viable means for predicting transonic drag at various flight conditions, and the technology has been transferred to U.S. industry and U.S. military, basic research efforts in the development of hypersonic vehicle design are ongoing at NASA Langley Research Center.

Co-Investigators

- Luis Bermudez, Orbital Sciences Corporation

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2. Frink, N.T., Pirzadeh, S., Parikh, P., Pandya, M.J., and Bhat, M.K., "The NASA Tetrahedral Unstructured Software System (TetrUSS)," *The Aeronautical Journal*, Vol. 104, No. 1040, October 2000, pp. 491–499.

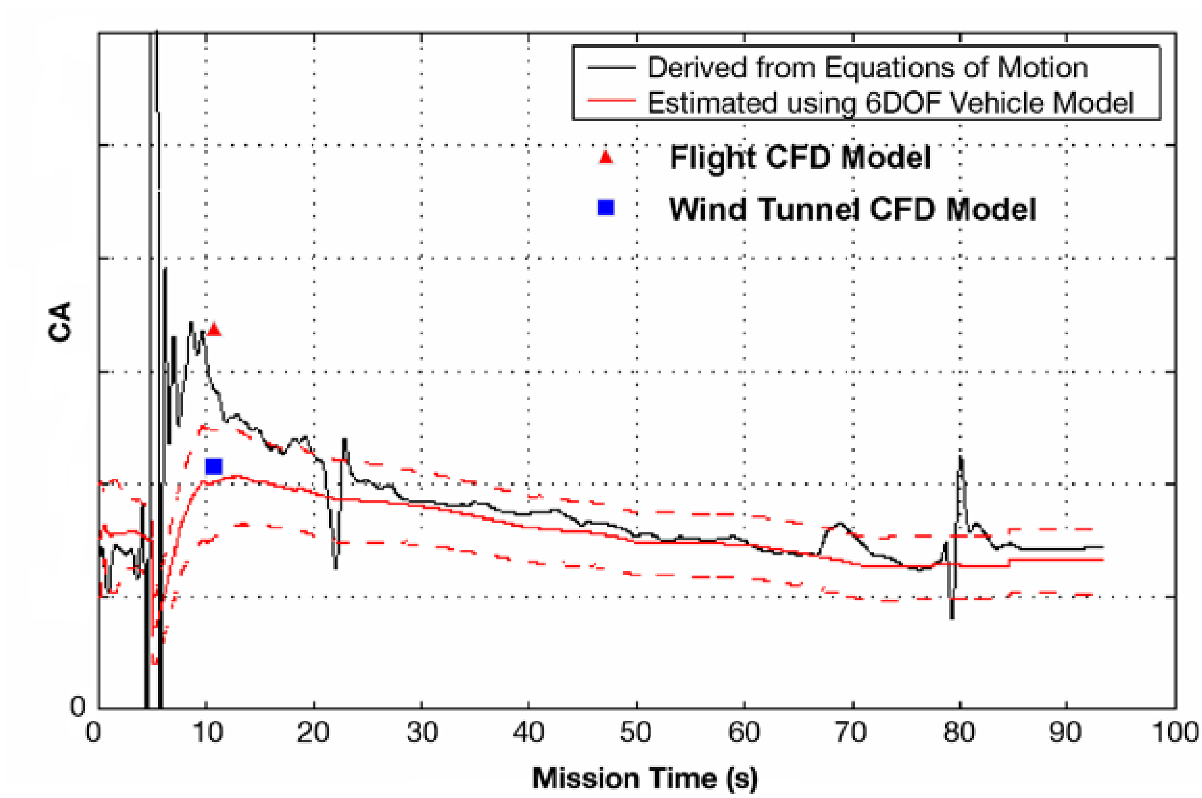

Figure 2: *Post-flight drag versus mission time.*

POST-FLIGHT CFD ANALYSIS OF X-43A RESEARCH VEHICLE AT HYPERSONIC CONDITIONS

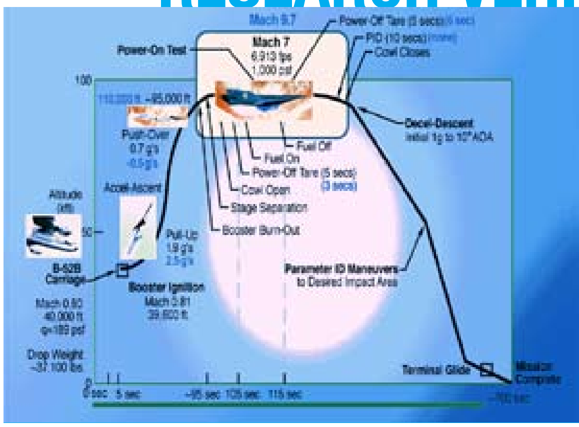

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Figure 1: *A representative flight trajectory for the X-43A Mach 7 and 9.7 experiment.*

Project Goals and Objectives: The aim of this work was to conduct studies to determine the performance of the X-43A Research Vehicle (RV) at hypersonic conditions using available flight data obtained during a flight test in November 2004. Of paramount importance was to first compare the drag values from a test-validated computational fluid dynamics (CFD) model of the vehicle against the measured flight data. Upon confirming the validity and accuracy of the methods, CFD models were once more applied to validate the results against the flight data at a designated point in the flight regime. Figure 1 shows the trajectory of the X-43A after being dropped from a B-52 aircraft.

Project Description: While predicting drag at transonic conditions is very difficult, it is not so challenging at hypersonic conditions. On the flip side, however, it is extremely difficult to accurately predict aero heating under hypersonic conditions due to the higher velocities (more than ten times the speed of sound). An aerodynamic study of the X-43A RV configuration was conducted in two different environments: a wind tunnel and a live flight-test at free-stream Mach 10. The study at flight conditions was conducted at the release of the RV from the Pegasus Launch Vehicle (Pegasus is used both commercially and by the U.S. government to deploy small satellites), and before the propulsion cowl door opens. Two areas of interests were investigated, namely validation of the aerodynamic coefficients and pressure mapping based on the flight instrumentation readings.

Relevance of Work to NASA: The objective of NASA's Aeronautics Research Mission Directorate is to pioneer and validate high-value technologies that enable new exploration and discovery, and improve quality of life through practical applications. This work focused on evaluating the performance of the X-43A RV is closely aligned with that objective, as the vehicle is part of NASA's "Hyper-X" Program, which was established to explore scramjet-powered airplanes at hypersonic speeds (speeds greater than Mach 5). Unlike a rocket-powered vehicle such as the Shuttle, scramjet-powered vehicles operate more like airplanes, promising increased affordability, flexibility, and safety for ultra-fast travel in the future.

Computational Approach: Three CFD models of increasing fidelity using three CFD software codes (FUN3D, USM3D, and HEFSS), and two flow conditions (laminar and turbulent) were employed for this work. The idea was to identify the combination of CFD models and software codes yielding the closest match between predicted drag and values measured during flight tests. The use of software in this case proved that all software codes used for the study (developed at NASA Langley Research Center) are equally good.

Results: Examination of the results against the wind tunnel test data and flight made it possible to show the accuracy of all methodologies used in this study: the drag values from flight data and CFD results were within 3% (Figure 3). The analytical efforts in mapping the flight pressure readings to those from CFD results showed an outstanding match (Figure 2, [1]).

The results of this project demonstrate that the current aerodynamic software codes (FUN3D, USM3D and HEFSS) are mature and accurate enough for predicting vehicle performance under hypersonic conditions [1]. Furthermore, NASA and U.S. industries can now use these software codes to predict the aerodynamic performance of new flight vehicles with higher levels of confidence. Accurate prediction of flight vehicles also allows U.S. industry to keep its edge over foreign competition.

Role of High-End Computing: Runs of the test-validated CFD model of the X-43A RV configuration were conducted on the Columbia supercomputer under flight conditions up to Mach 10. A total of 40 runs were done, each consuming

64 processors and 8 hours on Columbia. The fast processing power afforded by Columbia, coupled with the 24x7 availability, was crucial to the completion of this work. Since the number of species (gas-air dissociation) entailed is a function of temperature, the extreme temperatures at Mach 10 make the CFD highly complex, and thus required run-times are approximately five times longer to handle the additional equations.

Future: These particular methods have been deemed a practical means for accurately predicting vehicle performance under hypersonic conditions, however, there is still much work to be done in the area of hypersonic vehicle design and development. Ultimate applications of this technology include hypersonic airplanes, the first stage of two-stage-to-orbit reusable launch vehicles, and single-stage-to-orbit reusable launch vehicles.

Collaborating Organizations

- NASA Dryden Flight Research Center

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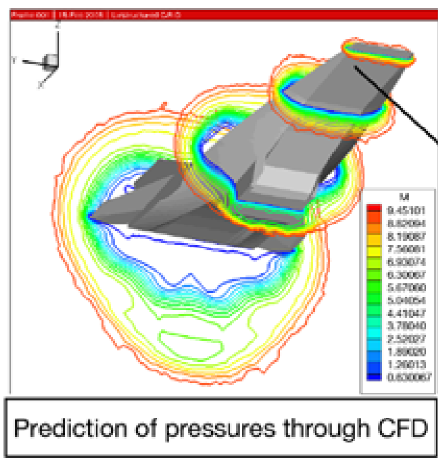

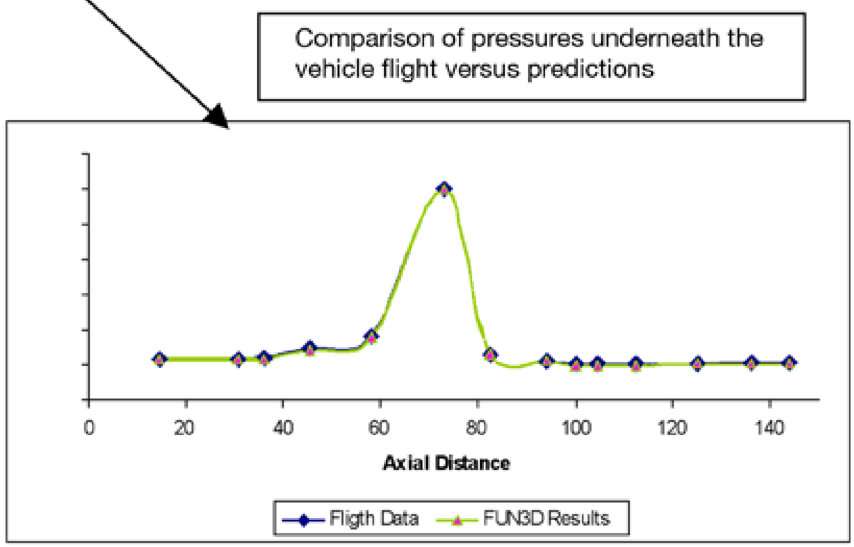

Figure 2: Post-flight validation pressure mapping of the X-43A Research Vehicle configuration at Mach 10.

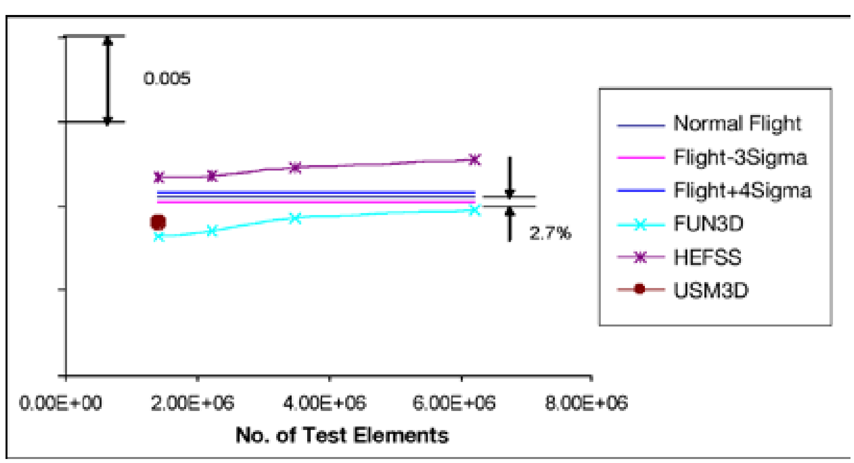

Figure 3: Drag comparison: prediction versus flight.

PROPULSION AIRFRAME AEROACOUSTIC COMPUTATIONAL ANALYSIS

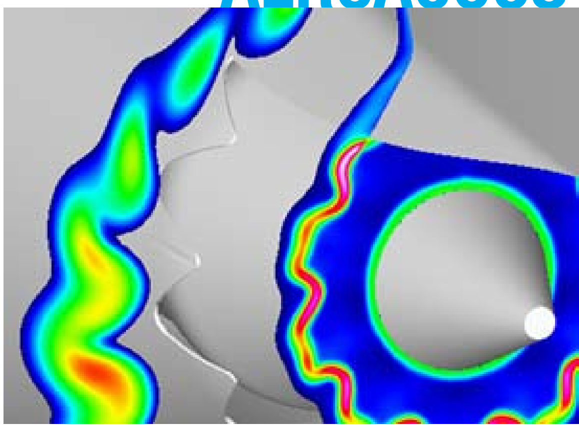

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Figure 1: *Close-up of the simulation seen in Figure 2.*

Project Goals and Objectives: With the dramatic progress in commercial aircraft noise reduction over the last few decades, and with the increasing demands of economy, developing additional increments of noise reduction is requiring increasingly sophisticated approaches, physical understanding, and predictive methods. One new approach has focused specifically on the aeroacoustic effects of propulsion airframe integration known as propulsion airframe aeroacoustics (PAA). This method includes both reducing the noise sources that arise specifically from integration of propulsion and airframe, and the use of the installation itself as a means to reduce noise sources from a particular airframe or propulsion source. PAA was largely undeveloped until a few years ago due to limited prediction method capabilities and computational resources, and the more complex experimental approaches required for intricate, fully integrated systems. The aim of this project is to make increasingly complex predictions of integrated propulsion and airframe systems.

Project Description: Realistic PAA configurations are highly three-dimensional and have many detailed features that can have a significant impact on the flowfield and noise. Large computational grids and the ability to compute many conditions are also required to develop an understanding of an individual effect. The same is required when studying a proposed noise reduction approach. Several PAA noise reduction concepts were investigated recently in a partnership between The Boeing Company, General Electric Company, Goodrich Corporation, All Nippon Airways, and NASA on the Quiet Technology Demonstrator 2 flight-test project. Large computational studies were conducted to investigate the potential design of PAA concepts for realistic and complex geometries and flight conditions involved. Additional studies were performed to successfully use predictions for improving understanding of the complex PAA phenomena observed.

Relevance of Work to NASA: This work is an important part of NASA's Aeronautics Program, specifically with regards to system-level capabilities. PAA is a multi-disciplinary approach to both aeroacoustics and aerodynamics, integrating increased fidelity physics-based prediction methods and noise reduction technology development.

Numerical Approach: Flowfield computations are performed using the Reynolds-Averaged Navier-Stokes structured code PAB3D [1] and unstructured code USM3D [2]. Noise source maps are computed with the Jet3D [3], which has been developed to handle complex three-dimensional turbulent flows and installed jet configurations. Average grid sizes in this study are approximately 30-million cells. Typical runtimes for the fully converged solution at the fine grid level on a 31-million cell grid required 24 wall-clock hours on 42 of the Columbia supercomputer's processors, with the solver running in parallel at a speed on the order of one-quarter of a microsecond per iteration.

Results: The PAA computations are breaking new ground in terms of numerical accuracy and high grid resolution to resolve the spatial and time scales for noise prediction. Both structured mesh (PAB3D) and unstructured mesh required careful tailoring of grid density and cell aspect ratio near the nozzle exit, pylon, and throughout the engine exhaust plume regions to meet the accuracy and resolution requirements for PAA. Extensive tools and application practices were developed during the past year, and the end results of accurate flow and acoustic simulations have proven that the efforts carried out under this high-end computing project met the objectives, and that the results contributed significantly to the noise reduction technology goals of the agency. The technical accomplishments were presented in a trio of AIAA papers at the 12th American Institute of Aeronautics and Astronautics/

Confederation of European Aerospace Societies Aeroacoustics Conference in Cambridge, Massachusetts, May 2006 [4–6]. Figure 2 shows an example of a simulation done using Columbia, and describes the complex interaction of an asymmetrical fan chevron nozzle with the asymmetrical effect of a jet-pylon interaction as visualized by the computation of turbulent kinetic energy.

Role of High-End Computing: Columbia's architecture and software environment has allowed us to seamlessly transition our codes, which were previously used primarily on commodity clusters. Columbia's large number of processors and high-speed interconnects have allowed us to routinely solve many more cases and expand our computations into unsteady flows and unstructured solvers—both of which are critical to increasing fidelity of the flow simulations, and capturing the complexity of propulsion and airframe interactions. Hundreds of simulations were performed during the last year, consuming a total of 800,000 processor-hours on Columbia.

Future: Computational developments continue to be driven by more challenging application opportunities. Particularly, unstructured grid generation and refinement tools will continue to be developed and validated. Turbulence models and unsteady flow methods will be researched to improve the simulation of important physics to PAA applications. In addition, new PAA noise reduction concepts will be developed for future experimental and flight test opportunities.

Co-Investigators

- Russ Thomas, Craig Hunter, both of NASA Langley Research Center
- Steven Massey, Eagle Aeronautics, Inc.
- Alaa Elmilligui, Analytical Services & Materials, Inc.

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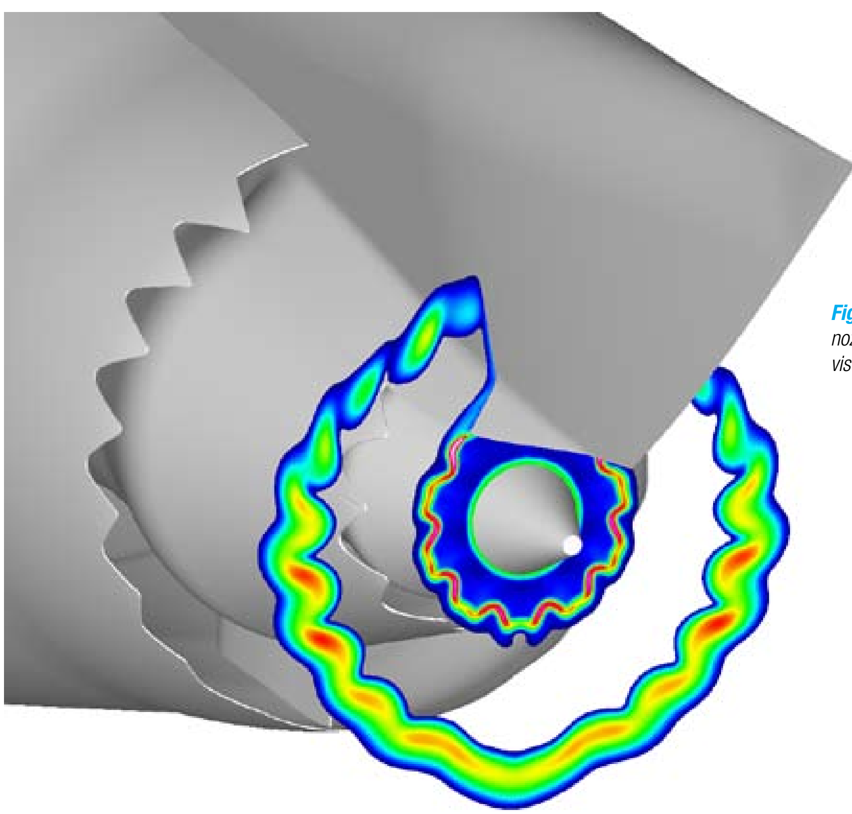
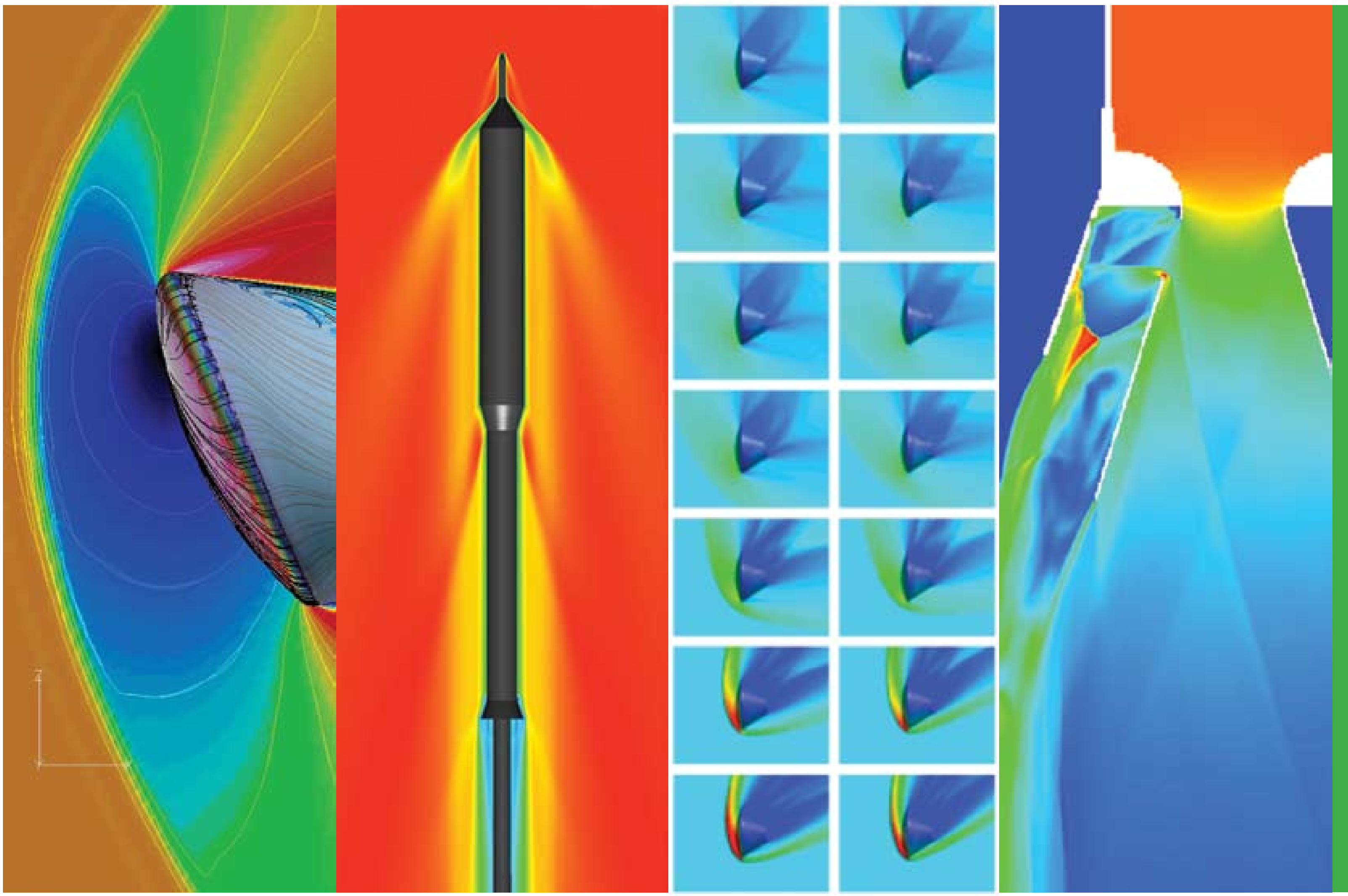


Figure 2: *The complex interaction of an asymmetrical fan chevron nozzle with the asymmetrical effect of a jet-pylon interaction as visualized by the computation of turbulent kinetic energy.*



MISSION DIRECTORATE

EXPLORATION SYSTEMS

The Exploration Systems Mission Directorate is developing a constellation of new capabilities, supporting technologies, and foundational research that enables sustained and affordable human and robotic exploration of the moon and later Mars. Key research areas include: development of Orion, the new crew exploration vehicle for astronaut travel in space; health and safety assurance of crews on long-duration space missions; development of the Ares I, the launch vehicle that will carry the Orion and its astronaut crew into space, and the Ares V, the heavy-lift cargo launch vehicle that will carry the equipment astronauts need to explore the moon and beyond.

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AUTOMATED AERO-DATABASE CREATION FOR LAUNCH VEHICLES

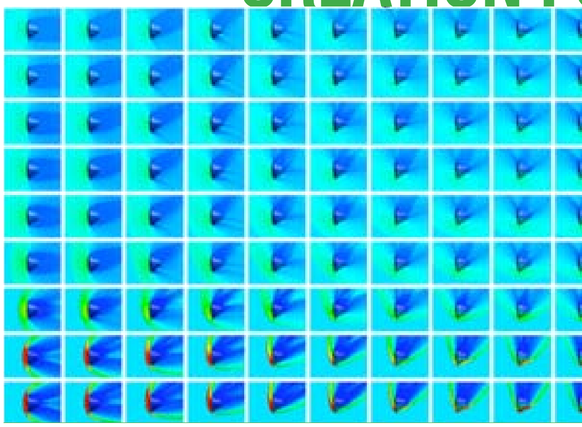

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Figure 1: *Two-dimensional slice of simulations in an aerodynamic database for SSLV showing the variation of Mach number with gimbal of both the center SSME and SRB nozzles.*

Project Goals and Objectives: Recent progress in automated methods for numerical simulation of vehicle aerodynamics now enables complete simulations to be performed with little to no human intervention. This progress coincides with an unprecedented increase in NASA's high-performance computing capacity afforded by the Columbia supercomputer. These two concurrent developments put NASA in a unique position to explore the viability of developing fully automated aerodynamic performance databases for new aerospace vehicles. Such databases describe the aerodynamic performance of new vehicles throughout their entire flight envelope, and enable vehicles to be "flown" through this database to quantify their performance for any candidate mission profile. The aim of this project is to develop and deploy a prototype system for rapid aerodynamic performance database generation, and to use it on real-world problems faced by the Exploration Systems and Space Operations Mission Directorates.

Project Description: Computational fluid dynamics (CFD) is routinely used to analyze vehicle performance at isolated design points by performing computations at fixed flight conditions (Mach number and angle of attack, for example), for a particular vehicle configuration. This isolated-point analysis is typically performed using high-fidelity methods at only a handful of critical design points—cardinal Mach number or a sample of points along a flight trajectory, for example. Current research is aimed at extending the point analysis to the entire performance envelope with high-fidelity tools, including the variation of both flight conditions and all permissible control surface deflections. This database, which opens up radical new possibilities for the designer, gives a much broader picture of aerodynamic performance and is used both in preliminary design to quickly estimate performance, and in final design to augment traditional methods such as wind tunnel tests and aerodynamic modeling. The performance database can be used with six-degree-of-freedom trajectory simulations coupled with guidance and control (G&C) systems. "Flying" a design through an aerodynamic database in faster-than-real-time enables rapid evaluation of performance estimates for prototypes, in addition to supporting the rapid development of novel G&C systems.

Relevance of Work to NASA: NASA's Exploration Systems Mission Directorate is currently faced with the challenge of developing the Crew Exploration Vehicle (CEV), Crew Launch Vehicle (CLV), and related exploration architecture systems to replace the Space Shuttle Transportation System for providing the nation's access to space. During development, NASA continues to fly and modify its fleet of Space Shuttle Launch Vehicles operated by the Space Operations Mission Directorate. With these challenges ahead, our need for advanced simulation technology has never been greater.

Computational Approach: A typical CFD aerodynamic database currently contains on the order of 10^4–10^6 simulations, depending on the problem requirements. Cart3D is a massively parallel, automated aerodynamic simulation package which scales linearly to thousands of processors. Automated tools drive this package to manipulate the geometry for control surface deflections, produce surface and volume grids, and manage the massive numbers of simulations that populate such large datasets. Further automation is used to harvest meaningful results and capture them in a performance database.

Results: Since Cart3D's development, over a dozen designs have been evaluated using this system. The accompanying figures show some snapshots extracted from simulations in performance databases for an early CEV design and the Space Shuttle Launch Vehicle (SSLV). Figure 1 shows part of the CEV study—performance databases were computed for several capsule shapes from the computer-aided design models of various CEV designs. A matrix of cases showing the flowfield surrounding the capsule for variations of Mach number and angle-of-attack are also shown. These simulations facilitated a study of the stability characteristics of various CEV designs and were compared against those of the Apollo capsule. Figure 2 shows a database slice for the SSLV examining the nozzle-gimbal of the main engines, as well as the gimbal of the solid-rocket motors. Such simulations quantify the control authority provided by nozzle gimbal that is necessary for rolling and pitching the full launch vehicle during ascent. Other examples include quantification of risk (to both crew and vehicle) due to the abort of potential CEV/CLV designs during launch and ascent.

Role of High-End Computing: This unprecedented simulation capability is contingent upon high-end computing. Each simulation in a database typically has 15–50 million degrees-of-freedom, and a performance database usually consists of 5–100 thousand simulations. Such computationally intense calculations can only be carried out on a massively parallel system such as Columbia, which has the capacity to provide a large set of dedicated processors with a high bandwidth interconnect. Using Cart3D and the prototype system, a dedicated 512-processor node of Columbia can perform 10–20,000 simulations per hour. Given the low cost-per-processor hour on this system, this is, by far, the cheapest method available to obtain high-quality aerodynamic data.

Future: As NASA continues to develop Project Constellation, our simulation requirements continue to grow. Not only are there increasing numbers of designs to analyze, but error-estimation and validation due diligence mandates that we recreate wind tunnel test databases as well. As Constellation evolves, these tools offer NASA an unprecedented ability to "fly" candidate vehicle designs through various mission profiles to gain insight into vehicle performance and perform trade studies.

Collaborating Organizations

- NASA Ames Research Center
- NASA Johnson Space Center
- New York University
- University of Wyoming

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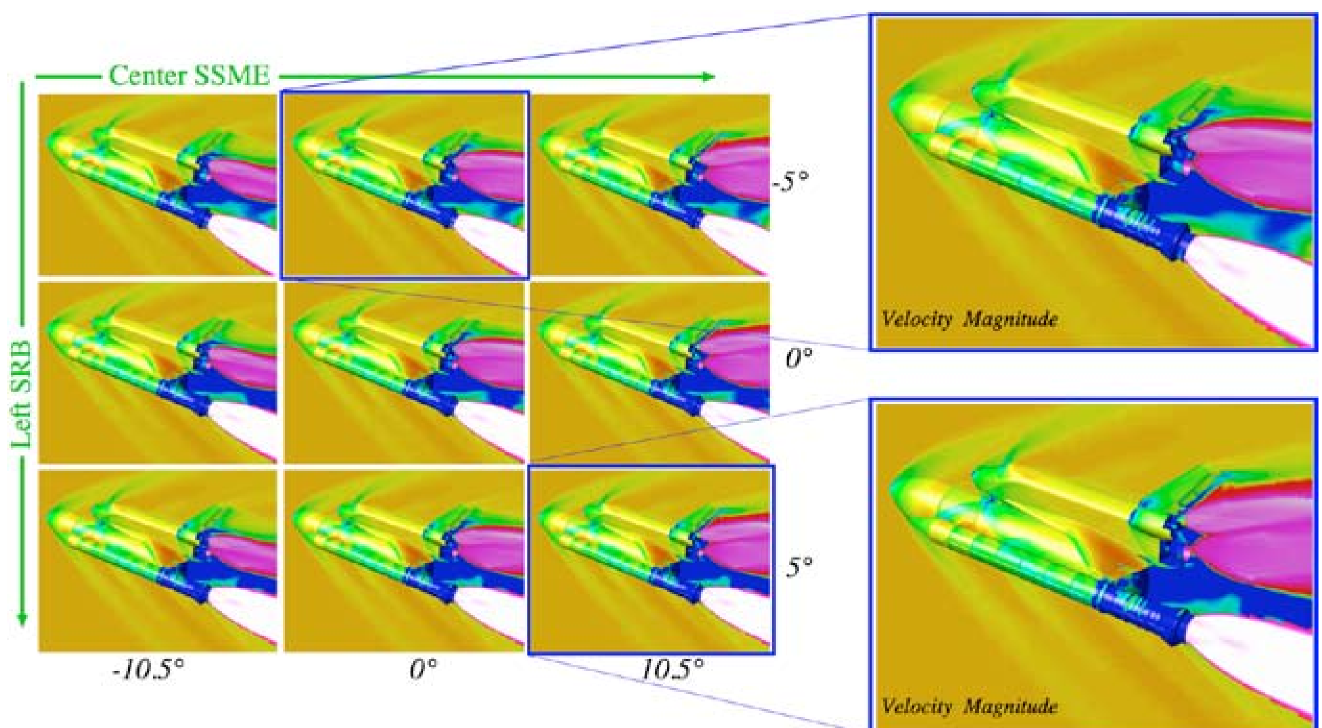

Figure 2: Two-dimensional slice of simulations in an aerodynamic database for Space Shuttle Launch Vehicle showing variation of Mach number with gimbal of both the center Space Shuttle Main Engine and Solid Rocket Booster nozzles.

CREW EXPLORATION VEHICLE AEROSCIENCES PROGRAM

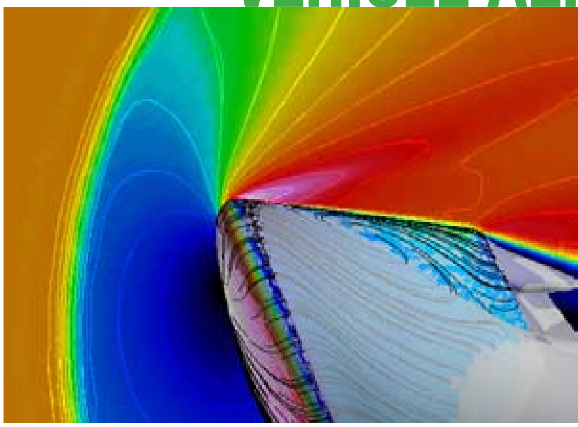

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Figure 1: *Close-up of blunt-bodied Crew Exploration Vehicle shown in a supersonic OVERFLOW solution.*

Project Goals and Objectives: The Crew Exploration Vehicle (CEV) Aerosciences Program (CAP) is responsible for developing the complete aerodynamic and aerothermodynamic databases for the CEV, covering the range of all possible angles-of-attack and freestream conditions. These databases will be developed primarily using computational tools, and supporting wind tunnel tests will provide code validation data and help quantify uncertainties in the numerical quantities. Database development will require thousands of high-fidelity numerical solutions modeling flowfield surrounding the CEV for all flight regimes. The databases will be provided to the CEV prime contractor and used to support both design and operation of the vehicle.

Project Description: CAP is part of the Vehicle Integration Office of the CEV Project, and is managed from NASA Johnson Space Center with over 35 aerodynamicists and aerothermodynamicists from NASA Ames Research Center, NASA Johnson, and NASA Langley Research Center.

Accurate aerodynamic data such as lift, drag, pitching moment, and dynamic stability derivatives are required to design the flight control system and ensure the pinpoint landing requirement can be met. The aerodynamic database covers the entire CEV operational envelope including nominal ascent, ascent abort scenarios, on-orbit plume environments, re-entry flight from the hypersonic through subsonic regimes, and the terminal landing approach including heatshield jettison and parachute deployment.

The aerothermodynamic database covers the portion of atmospheric flight that produces significant aeroheating on the vehicle. While the heating environment during ascent is relatively benign, it must be quantified to ensure vehicle integrity during nominal and off-nominal ascent conditions. Specialized thermal protection system (TPS) material is required to protect the vehicle from the extreme heating rates experienced during re-entry. Design of the TPS requires convective and radiative heating environments for the entire vehicle surface, including localized heating rates on penetrations and protuberances.

Relevance of Work to NASA: The CEV is a key component of NASA's mission to return to the Moon—one of the primary objectives of the agency's Exploration initiative. The CEV will initially be used to carry astronauts to and from the International Space Station. Later, it will be used to transport astronauts to and from the Moon. The aerodynamic and aerothermodynamic databases are critical to the design and operation of the CEV.

Computational Approach: We use a number of high-fidelity codes to compute the flowfield surrounding the CEV. Using multiple, independent codes for the same flight conditions increases our confidence in the computed results. The Data-Parallel Line Relaxation and Langley Aerothermodynamic Upwind Relaxation Algorithm codes are reacting Navier-Stokes solvers that include thermochemical nonequilibrium. They are used to compute aerothermodynamic heating rates and aerodynamic coefficients in the hypersonic regime. The Nonequilibrium Air Radiation solver is a first-principles physics code that computes the production of radiation by gas in the hot shock layer, transport of the photons through the shock layer, and radiative heating to the CEV surface. Aerodynamic coefficients in the subsonic, transonic, and supersonic regimes are computed using four different computational fluid dynamics (CFD) tools: OVERFLOW, which solves the Reynolds-Averaged Navier-Stokes equations using multiple overset structured grids; Cart3D, which is an inviscid, compressible flow analysis package that uses Cartesian grids to solve flow problems over complex geometries such as the CEV with Launch Abort System attached; the unstructured Euler CFD package, Finite Element Langley Imperial Swansea Ames; and the tetrahedral, cell-centered

Navier-Stokes flow solver, Unstructured Method 3D are also being used.

Results: We have generated hundreds of full-body, three-dimensional CFD solutions on the baseline CEV Command Module geometry covering the range of angle-of-attack and freestream conditions. This aerodynamic and aerothermodynamic heating data is already being used for CEV design work.

Figure 2 shows the computed normalized surface convective heat transfer rate contours. The upper-left image shows half of the symmetric forebody, the upper-right image shows the side, the lower-left image the windward surface, and the lower-right image the leeward surface. Accurate heat transfer rate calculations require modeling the nonequilibrium chemistry, ionization, and nonequilibrium distribution of internal energy of the hot gas in the shock layer.

Figure 3 shows a supersonic OVERFLOW solution. For blunt bodies such as the CEV, the computed lift, drag, and pitching moment coefficients are sensitive to the extent of the wake region behind the capsule. The computed size of the wake region is highly sensitive to the choice of turbulence model. For this calculation, the Lag Turbulence Model was used. Comparisons of the CFD results and recent wind tunnel data at these conditions are ongoing, and results will be used to select a baseline turbulence model.

Role of High-End Computing: While each individual solution may only take a few hundred to a few thousand node-hours depending on the analysis code and geometric complexity modeled, the thousands of high-fidelity CFD solutions needed to populate the CEV databases could not be completed without access to a supercomputer such as Columbia. The availability Columbia affords, coupled with the advancements in CFD fidelity, have allowed the CEV Project to create databases using computational results—as opposed to having to conduct wind tunnel tests, which would consume thousands of hours and tens of millions of dollars.

Future: Over the next few years, CAP will compute thousands of high-fidelity numerical solutions to populate the aerodynamic and aerothermodynamic databases. The geometric models of the CEV will become increasingly more complex, and the computations more memory-intensive and time-consuming—as detailed design work is completed on the various cavities, penetrations, and protuberances of the basic CEV shape. Terabytes of data consisting of the complete flowfield information will also have to be analyzed and stored for future use.

Publications

1. K. Bibb, et al., "Numerical Uncertainty Estimates for computed CEV Hypersonic Aerodynamics," *AIAA Paper* to be presented at Reno, 2007.
2. S. Lawrence, et al., "Computational Fluid Dynamics Simulations in Support of CEV Aerodynamics Wind Tunnel Testing," *AIAA Paper* to be presented at Reno, 2007.
3. R. Lilliard, et al., "CEV Crew Module Shape Selection Analysis and CEV Aeroscience Project Overview," *AIAA Paper* to be presented at Reno, 2007.
4. J. Olejniczak, et al., "An Experimental and Computational Study of High Enthalpy Convective Heating for the NASA CEV," *AIAA Paper* to be presented at Reno, 2007.

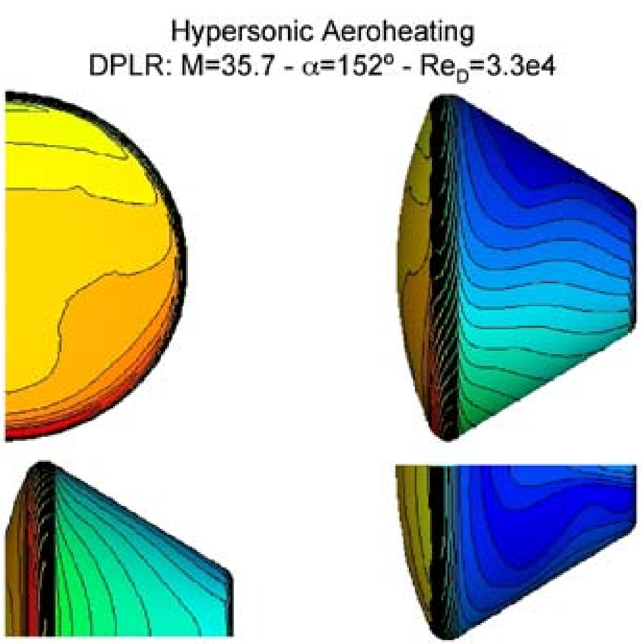

Figure 2: Data Parallel Line Relaxation code solution of chemically reacting hypersonic flow over the Crew Exploration Vehicle showing surface heat flux.

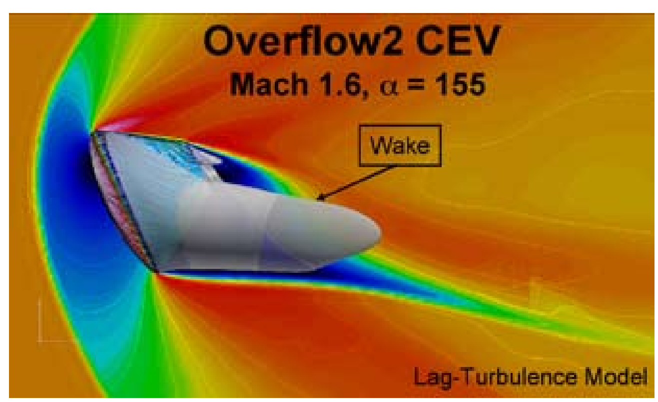

Figure 3: OVERFLOW2 solution of the Crew Exploration Vehicle capsule showing the extent of the wake region.

HIGH-FIDELITY SIMULATIONS SUPPORTING CREW ABORT RISK

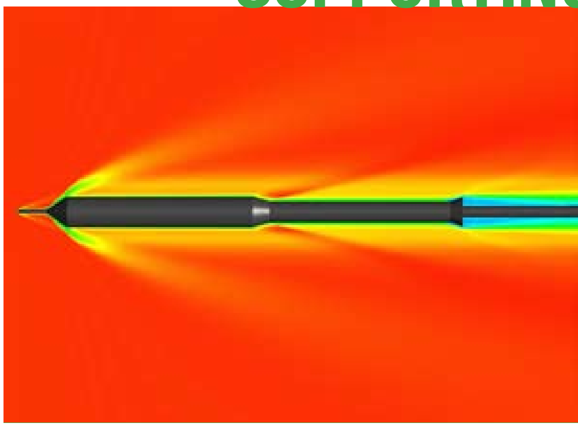

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Figure 1: *Flowfield surrounding a Crew Launch Vehicle concept computed using OVERFLOW-2, showing Mach contours in a plane of symmetry for supersonic flow.*

Project Goals and Objectives: The objective of the Simulation Assisted Risk Assessment (SARA) Project is to develop tools and processes for integrating phenomenological simulation and analysis methods of various levels of fidelity with probabilistic risk assessment methods—to understand the impact of various physical phenomena on system-level risk. This year, specific objectives included developing an understanding of the effects of Crew Launch Vehicle (CLV) failure modes on the ability of the Launch Abort System (LAS) to successfully perform its mission, in addition to assisting in the general aerodynamic characterization of the launch vehicle.

Project Description: Existing risk analysis is based on sparse flight, test, and/or simulation data from legacy vehicles. SARA is using risk assessment methods to identify gaps in our understanding that could play an important role in our ability to design and develop a launch vehicle system significantly safer than existing systems. Appropriate physics-based modeling is then applied in an effort to provide the information/data most useful in closing the gaps. Using vehicle models integrated with risk analysis tools, we can generate higher confidence data through targeted modeling and simulation applied to solutions that effectively reduce overall system risk.

Relevance of Work to NASA: This project, along with a similar project through NASA Langley Research Center, is primarily responsible for providing the computational aerodynamic characterization of the CLV concepts in support of Project Constellation. Results from these projects have played a significant role in decision-making regarding the outer mold line shape of the upper stage, as well as the LAS configuration size and shape. In addition, results of failure mode analyses have provided insights into the failure consequences, including sizes and time scales of failure environments.

Computational Approach: Aero Panel support was provided through the application of computational fluid dynamics (CFD) codes such as OVERFLOW2 and Cart3D. Failure mode analyses have been performed using a multi-fidelity, multi-disciplinary set of tools including blast modeling, trajectory, and structural analysis tools, in addition to the aforementioned CFD applications.

Results: Results were obtained by characterizing several failure modes of the launch and escape systems, including: 1st stage case breach, 1st stage nozzle burn-through (Figure 2), and 2nd stage explosion. In addition, aerodynamic characterization of various aspects of the launch vehicle was performed, including the full launch stack (Figure 1) and several abort concepts. Simulations of various LAS concepts have contributed significantly to the evolution of the current LAS baseline configuration.

Role of High-End Computing: The volume of compute cycles afforded by the Columbia supercomputer enabled the exploration of a wide range of failure situations at moderate levels of complexity, as well as targeted simulations of high complexity. Aerodynamic characterization of the launch vehicle was particularly demanding of compute resources due to the large number of cases required, the varying spatial scales associated with the vehicle (for example, a long slender vehicle with several abrupt diameter changes), and the relative complexity of the resulting flowfields. In addition, the hyperwall visualization system, connected to Columbia, was a highly effective method for communicating the breadth and depth of the crew abort analyses to various customers and stakeholders.

Future: SARA will continue to support the CLV (Ares) project in 2007. As more design details are specified, and as the design matures, it is expected that the trend will be toward more focused sets of higher fidelity simulations. For the Aero Panel support, this may include additional geometric details (the reaction control system and cable trays, for example), in addition to looking at separation dynamics. Risk assessment work is expected to bring in data from a broader range of failure mode physics-based analyses.

Co-Investigators

- Jerry Yan, Goetz Klopfer, Jeff Onufer, Shishir Pandya, Mike Olsen, William Chan, all of NASA Ames Research Center

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2. Mathias, D. and Lawrence, S., "Launch Architecture Impact on Ascent Abort and Crew Survival," presented at the 8th Probabilistic Safety and Management Conference, New Orleans, LA, May 2006.
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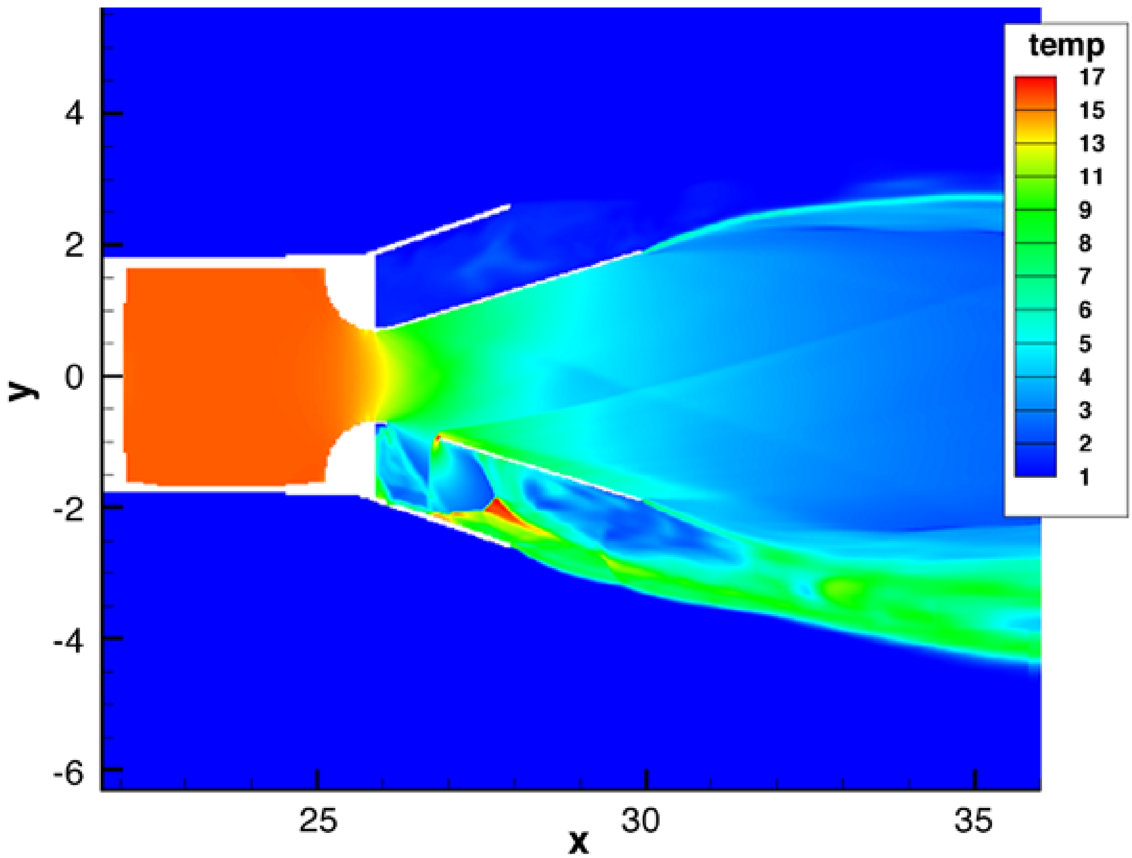

Figure 2: *Temperature contours for a nozzle burn-through scenario computed using Cart3D. Hole is located upstream of the nozzle skirt on the lower side.*

INTEGRATED MODELING & SIMULATION ENTRY DESCENT AND LANDING

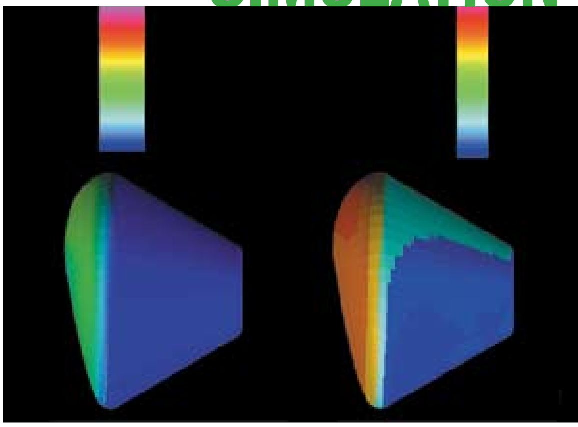

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Figure 1: *Close-up of proposed capsule shape for Exploration Systems Architecture Study.*

Project Goals and Objectives: The primary goals of NASA's Integrated Modeling and Simulation (IMS) Project are to support design decisions in a schedule-driven manner, and to provide detailed technical assessments throughout the lifecycle of a given exploration mission.

Project Description: To support the Entry Descent and Landing (EDL) phases of an exploration mission, NASA Ames Research Center was tasked with leading and integrating multiple disciplines—from trajectory analysis to aerothermodynamics to thermal protection system (TPS) analyses (Figure 2)—into a single environment to perform design trades, which lead to design decisions. One example of this is the IMS-EDL team's support of the recent NASA Exploration Systems Architecture Study (ESAS) during which they provided rapid design decisions for NASA's Crew Exploration Vehicle (CEV).

Relevance of Work to NASA: A clear need for this technology exists within NASA's Space Exploration Initiative, which calls for development of a single mission architecture to replace the aging Space Shuttle, and to develop an architecture to return humans to the Moon and eventually to Mars. The CEV (Orion Project) and CLV (Ares Project) are two elements of this architecture.

Computational Approach: Traditionally, analytical tools applied in the early phases of vehicle design rely on engineering methods because of the rapid turnaround time, ease of use, and robustness associated with these methods. The drawbacks of engineering methods are that they approximate the physics governing the process to be modeled, and have potential for being used outside their limitations.

Unlike engineering methods, high-fidelity methods are based on solutions to basic physics equations, and yield more accurate results if used within their limitations. These high-fidelity methods tend to be difficult to set up, and computationally expensive (typically hundreds of times more processor-intensive than engineering methods). However, if crew safety is a driving requirement, the design must consider off-nominal system/vehicle operations—it is in these conditions where the governing physics likely become more complex and, consequently, the engineering methods are more prone to fail.

Given the long-term impact of decisions made during conceptual design, it would seem that the effective design of a truly crew-safe vehicle, meaning one in which safety is designed into the system rather than added on, will require the introduction of higher-fidelity analyses in the conceptual phase. To address the deficiency in engineering and high-fidelity methods, we turn to a hybrid approach, leveraging high-fidelity analyses with engineering methods using both sophisticated data fusion (also known as anchoring) and interpolation techniques. This approach allows us to generate data rapidly and at better-than-engineering fidelity levels—it essentially becomes a "smart" engineering-based interpolation method.

Results: A prototype multi-fidelity, multi-discipline integrated analysis process has been developed to perform planetary re-entry for vehicle designs. In addition, this integrated process has been applied to entry vehicle shape optimization for the recent NASA ESAS and to providing rapid analysis and TPS sizing trade-off studies for selection of the CEV's TPS materials (Figure 3). The ESAS shape optimization study also demonstrated that the use of high-fidelity aero/aerothermaldynamic simulations were crucial in identifying critical vehicle design issues that would otherwise have gone undetected.

Role of High-End Computing: The ESAS shape optimization study demonstrated how the combination of engineering methods and high-fidelity, physics-based methods allowed engineers to quickly and accurately analyze numerous design options. Due to the use of the Columbia supercomputer, it is becoming feasible to perform high-fidelity analyses, such as computational aerothermodynamics to influence early design decisions. Specifically, the large number of processors afforded by Columbia reduced turnaround time for running the high-fidelity aerothermodynamics simulations by a factor of five.

Future: With advancement in high-end computing and the proven benefits of introducing high-fidelity analysis earlier in the space vehicle design process, it is crucial that we continue pursuing the use of high-fidelity simulations in the early conceptual design stage. By doing so, we can integrate safety into the system rather than try to incorporate it later.

Collaborating Organizations

- Launch and Ascent Mission Segment Simulator team, NASA Langley Research Center
- Rendezvous and Docking team, NASA Johnson Space Center
- Validation, Verification, and Accreditation team, NASA Marshall Space Flight Center
- Ground Operations team, NASA Kennedy Space Center

Co-Investigators

- Ted Manning, Dinesh Prabhu, James Brown, Chun Tang, Grant Palmer, Loc Huynh, Gary Allen, Kathy McGuire, Peter Gage, all of NASA Ames Research Center

Publications

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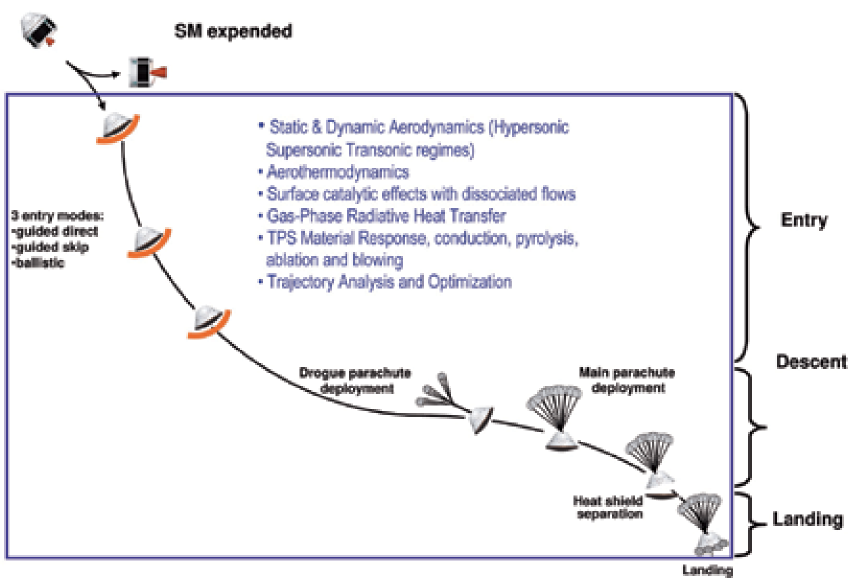


Figure 2: Typical mission profile for planetary entry.

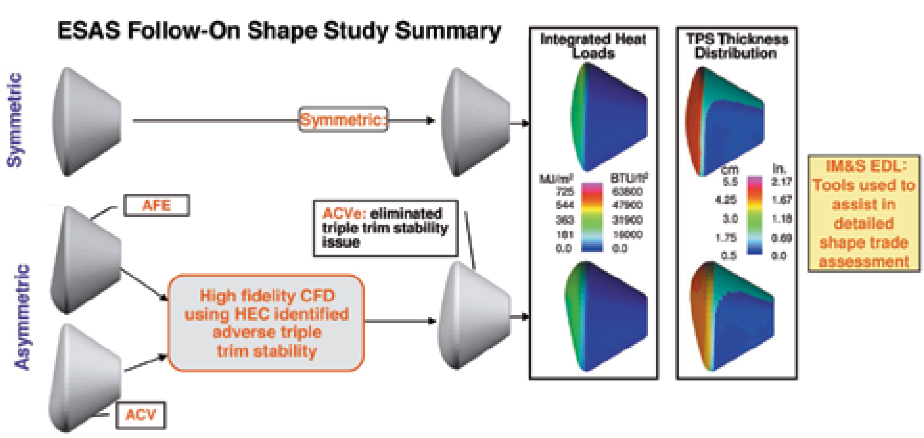
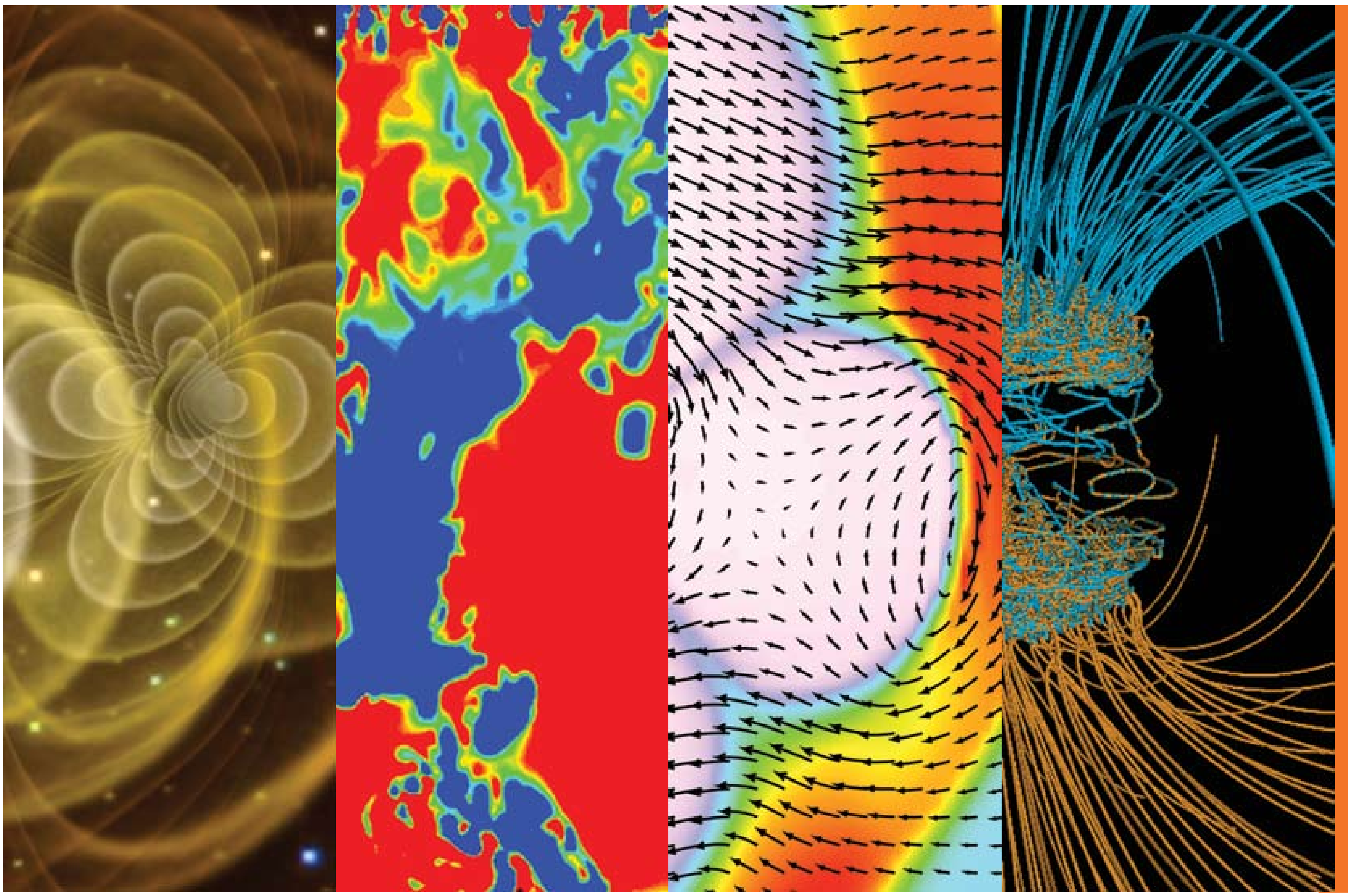


Figure 3: Exploration Systems Architecture Study (ESAS) follow-on shape study summary.



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APPLICATIONS, EVALUATION, AND IMPROVEMENT OF MULTI-SCALE MODELING SYSTEMS

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***Figure 1:** Three-dimensional visualization of a simulated convective cloud system that occurred on February 23,1999 over Amazonia in western Brazil. The simulation was made using the Goddard Cumulus Ensemble model with improved cloud microphysics. The visualization shows a rendering of the modeled cloud field, which consists of the sum of the simulated cloud water and cloud ice.*

Project Goals and Objectives: The foremost challenge in parameterizing cloud systems in climate models is the proper representation of the many coupled processes that interact over a wide range of scales, from microphysical to planetary. This makes the comprehension and representation of clouds and convective cloud systems one of the most complex scientific problems in Earth science. The goals of this project are (1) to develop and improve better numerical models to advance our understanding of the global energy and water cycle, (2) to produce multi-dimensional cloud datasets to improve NASA satellite rain retrievals and the representation of cloud processes in climate models, and (3) to use high-resolution NASA satellite cloud data to validate and improve models.

Project Description: The hydrological cycle distinguishes Earth from the other planets. A key component of this cycle is rainfall, which is also the primary heat source for the atmosphere. Present large-scale weather and climate models simulate cloud processes only crudely, reducing confidence in their predictions on both global and regional scales. Multi-scale modeling systems (coupled global model-cloud resolving model and land surface model) were developed and used in a wide range of studies, including investigations of the dynamic and thermodynamic processes associated with hurricanes, surface effects on atmospheric convection, and cloud-chemistry-aerosol interactions from local to regional to global scales.

Relevance of Work to NASA: These efforts (primarily supported by the NASA Headquarters Atmospheric Dynamics and Thermodynamics Program and the NASA Precipitation Measuring Mission, in addition to the NASA Cloud Modeling and Analysis Initiative Program) are an important part of NASA's continuing quest to improve long-range forecasts and climate prediction capability. By combining the NASA satellite programs (for example, TRMM, Terra, Aura, Aqua, and CloudSat) and numerical models, we can provide cloud, precipitation, aerosol, land characteristics, and other data at very fine spatial and temporal scales to improve our understanding of the roles of cloud and precipitation processes on global energy and the water cycle.

Computational Approach: A hybrid parallelism, which uses both distributed-memory Message Passing Interface (MPI) and shared-memory multithreading (OpenMP) is implemented to efficiently solve fluid dynamics, cloud processes, surface (land and ocean) processes, and solar and infrared irradiance radiation in atmospheric models. The simulation code employs both finite-volume dynamic and finite-difference numerical schemes. To improve the performance and scalability, two-dimensional horizontal domain decomposition is necessary to yield the high degree of parallelization required.

Results: We were able to use the new multi-scale modeling systems to produce better and more realistic three-dimensional clouds and cloud systems over different geographic locations (Figures 1,2). These clouds and cloud systems were used to improve the performance of diabatic and rainfall retrieval algorithms for the NASA Tropical Rainfall Measuring Mission (TRMM) Program. We were also able to use the new modeling system for simulating the vertical structure of an intensive hurricane. A realistic simulation of a hurricane allows us to understand the impact of microphysical processes upon the hurricane track forecast and its intensity prediction. In addition, we were able to apply the new modeling system to simulate many weather features/climate phenomena that cannot be simulated with traditional global circulation models and/or climate models. These features include the timing of diurnal variation over land and ocean, a single Intertropical Convergence Zone over the Pacific, and the direction of the propagation of convective systems in the tropics.

Role of High-End Computing: The new multi-scale modeling systems require a substantial amount of computing resources, two to three orders of magnitude more expensive than current climate models. Only supercomputers with thousands of processors such as the Columbia supercomputer are able to achieve results in a timely fashion. In addition, a vast amount of data will be generated by the modeling systems. Storing and retrieving this immense dataset poses a real challenge. However, the aggregate memory available on Columbia, in combination with new tools and methodologies, enable us to manage and display the model-generated cloud datasets. The Columbia modeling projects consumed approximately 95,000 processor-hours on 32–256 processors.

Future: We will continually use multi-scale modeling systems to improve our understanding of the cloud and precipitation processes and their interactions with radiation and land surface. The fine spatial and temporal cloud and precipitation data from the NASA TRMM and A-Train satellites, and NASA field campaigns will be used to validate and improve model performance. We plan to use multi-scale modeling systems in real-time forecasts for NASA's Modeling, Analysis, and Prediction Program (MAP '06) and NASA field campaigns. Approximately 25–30 cases will be performed using the multi-scale modeling systems each year. Each simulation will utilize 32–2,048 processors, and will require approximately 50 gigabytes of temporary disk space. Overall, the total annual resource requirements will be approximately 1,000,000 processor-hours and 10 terabytes of long-term disk storage.

Co-Investigators

- William Lau, Jiun-Dar Chern, Steve Lang, Bo-Wen Shen, Christa Peters-Lidard, Roger Shi, Xiaowen Li, Xiping Zeng, Sujay Kumar, Chung-Lin Shie, all of NASA Goddard Space Flight Center

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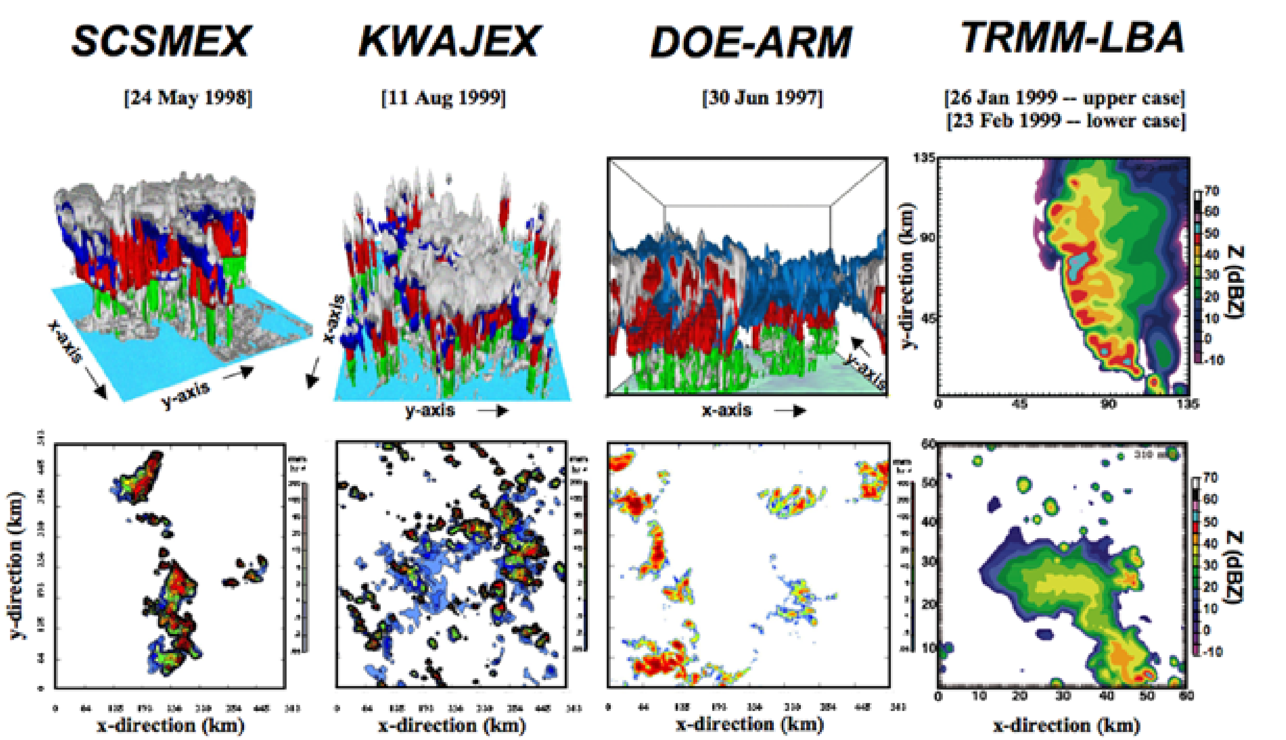

Figure 2: Isometric projections of volume hydrometeor distributions (three left-most upper panels) and plan-view near-surface rain rates (corresponding three left-most lower panels) for instantaneous realizations of three-dimensional Goddard Cumulus Ensemble simulations of NASA South China Sea Monsoon Experiment (SCSMEX), NASA Kwajalein Experiment (KWAJEX), and Department of Energy-Atmospheric Radiation Measurement (DOE-ARM) Mesoscale Convective Systems (MCS) cases. Upper panel isosurface color scheme assigns: (i) white for cloud droplets and ice crystals, (ii) blue for snow, (iii) red for graupel and hail, and (iv) green for rain. Right-most diagram pair shows mid-level simulated radar reflectivity for the Tropical Rainfall Measuring Mission-Large-Scale Biosphere-Atmosphere Experiment (TRMM-LBA) easterly (upper panel) and westerly (lower panel) regime MCS cases.

BINARY BLACK HOLE MERGER DYNAMICS AND WAVEFORMS

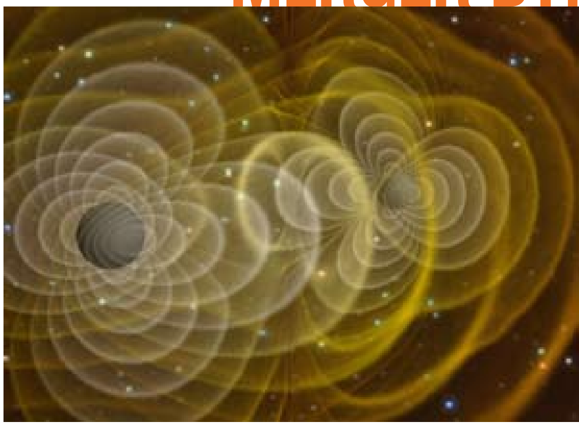

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Figure 1: *Two black holes prepare to merge in a three-dimensional simulation solving Einstein's general relativity equations.*

Project Goals and Objectives: The Laser Interferometer Space Antenna (LISA), selected as an integral part of NASA's Beyond Einstein Program, is scheduled to launch in 2015. The Laser Interferometer Gravitational-Wave Observatory (LIGO) is currently operational and is scheduled to have a sensitivity upgrade in the near future. These gravitational wave detectors not only promise to verify Einstein's general theory of relativity to greater precision than previously possible, but also open up a new window for astronomy. In order to discern signals from noise, data analysis for these detectors will require matched filtering based on numerically generated templates of predicted gravitational waves. Towards this end, our aim is to model binary black holes, the most promising sources for LISA, through inspiral, merger, and ringdown.

Project Description: Although the inspiral and ringdown phases of binary black hole evolution can be modeled to some extent via analytic perturbative techniques, the merger phase admits no such approximations and requires numerical solution of Einstein's full nonlinear field equations. We are simulating all three phases numerically and developing techniques to do so efficiently and accurately. We are modeling the full range of astrophysically relevant configurations, including various mass ratios and spins, with initial separations far enough apart to overlap with post-Newtonian approximations. Our simulated domain includes the wave zone, where we are extracting accurate waveforms from these simulations.

Relevance of Work to NASA: We are laying the groundwork for data analysis that will be critical to NASA's LISA mission. This research is directly responsive to NASA's Strategic Sub-goal 3D: "Discover the origin, structure, evolution, and destiny of the universe, and search for Earth-like planets." Gravitational wave observations with LISA will give us a new means of exploring the universe, and merging binary black holes constitute one of the strongest and most important classes of sources for LISA. This work will also make a significant contribution to NASA Science Outcome 3D.1: "Progress in understanding the origin and destiny of the universe, phenomena near black holes, and the nature of gravity." Since LISA will detect binary black hole mergers at high signal-to-noise ratios, these calculations of the merger waveforms provide a means of testing Einstein's general theory of relativity in the strong-field, nonlinear regime.

Numerical Approach: We are integrating a 3+1 formulation of Einstein's field equations with a massively parallel, finite-differencing code equipped with adaptive mesh refinement (AMR). Our initial data is typically obtained with the aid of a multi-grid elliptic equation solver, which guarantees accurate satisfaction of the constraints, and then evolved, unconstrained, using 4th-order Runge-Kutta integration and 4th-order accurate spatial differencing stencils. Our exact formulation of Einstein's equations and coordinate conditions (including our groundbreaking "moving puncture" approach [4,6]) have been fine-tuned for stability. AMR is imposed dynamically according to the strength of curvature, to ensure sufficient accuracy at the black hole sources.

Results: The various technologies we have developed [1–3], including AMR, and, in particular, new coordinate conditions for Einstein's equations [7], have made it possible to simulate inspiraling binaries, with stability and accuracy, for longer durations than ever before [4,5]. These efforts (funded by NASA's Beyond Einstein Foundation Science Program, the LISA Project, and the Goddard Internal Research and Development Program) led to a recent breakthrough simulation of four and a half orbits (Figures 1,3)—a world record at the time (featured in *The New York Times* on May 3, 2006). The resulting waveforms, the first of their kind for such widely separated initial black holes, have given every indication of being physically accurate. Not only do the merger parts of the waveforms from our equal-mass binary simulations agree with each other for different initial separations (Figure 2), as they should, but they also agree with results recently obtained by other numerical relativity groups. Further, our results are consistent with that of post-Newtonian calculations, in their domain of validity. We have also successfully simulated unequal mass binaries and obtained predictions for the "kicks" due to radiative recoil [6]. These latter computations have direct astrophysical relevance for predictions regarding the likelihood of black holes being ejected from galactic nuclei.

Role of High-End Computing: Accurate waveform computation requires very high resolution in the vicinity of the sources in order to resolve the strong gradients there, as well as sufficient resolution in the wave zone to resolve the waves. Further, the computational boundary must be far enough away to minimize the influence of spurious wave reflections during the course of the evolution. And the simulation must run long enough to evolve from wide initial separations through multiple orbits, in order to permit overlap of the earlier part of the inspiral with post-Newtonian predictions. Such simulations, we have found, can take over 100,000 processor-hours, and are only made practical by the copious memory and 500- to 2,000-processor jobs afforded by the powerhouse Columbia supercomputer. The four-and-a-half-orbit simulation consumed 18 processor-years on Columbia. To visualize 200 gigabytes of data sampled from the calculation (Figures 1,3), NASA High-End Computing Program visualization experts developed a programmable graphics processing unit-enabled volume renderer that could handle the AMR data without resampling, and used a mini-hyperwall display to process the simulation time series in parallel. For more modest simulations, in particular test runs for code development, 100- to 200-processor jobs available on systems such as Explore are critical. As our simulations are also data-intensive, the disk memory, coupled with ease of data transfer on these machines, has proven essential.

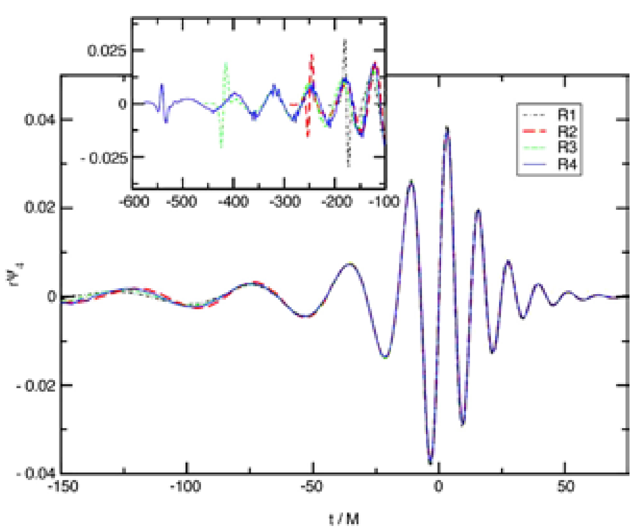

Figure 2: Characteristic waveforms of the amplitude of emitted gravitational wave radiation from the merging black holes.

Future: We plan longer runs of equal-mass binaries in the future in order to further probe our agreement with post-Newtonian predictions. We also intend to investigate additional mass ratios to pin down the overall dependence of the recoil kick on that parameter. Finally, we will explore spinning black holes, the various possible orientations of which open up a much larger frontier of parameter space. Throughout, we intend to further improve our accuracy and efficiency.

Co-Investigators

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Publications

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Figure 3: Gravitational waves radiate from inspiraling black holes.

CONVECTION AND MAGNETIC FIELD GENERATION IN GIANT PLANETS

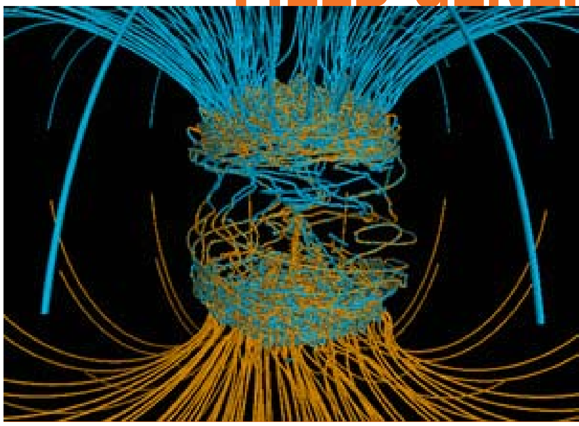

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Figure 1: *Close-up view of the simulated magnetic field in a model of Saturn illustrated with magnetic lines of force.*

Project Goals and Objectives: The purpose of this work is to explain how the observed banded zonal winds and dipolar magnetic fields are maintained on giant gas planets like Saturn and Jupiter, and to predict the flow and field structures in the deep interiors of these and other planets.

Project Description: Theses studies are conducted using computer simulations generated by codes developed at the University of California, Santa Cruz. The models solve a coupled nonlinear system of equations that describes conservation of mass, momentum, and energy, and the induction of a magnetic field [1, 2]. The solution is the time-dependent fluid velocity, magnetic field, density, pressure, and entropy within the modeled rotating fluid sphere. Each simulation requires these variables to be updated millions of times on typically tens of millions of grid points to capture the turbulent dynamics that maintain zonal flows and fields similar to those observed. Snapshots and movies of the simulations are analyzed to understand the physics of these problems, and to predict what types of planets exist in orbit about other stars.

Relevance of Work to NASA: These studies, funded by the Outer Planets Research and the Solar Heliospheric Programs, improve our physical understanding of the observations of atmospheric winds and magnetic fields made on NASA missions to other planets. They also predict the unobserved winds and fields deep below the surfaces to provide a more complete picture of these planets. The predictions and improved explanations will also help in choosing and planning future missions.

Numerical Approach: The model uses a spectral solution method, meaning the variables are expanded in spherical harmonics to represent their horizontal structures, and in Chebyshev polynomials to describe their radial structures. This method is very accurate; the challenge is to make the required global communication among hundreds of processors efficient on massively parallel machines. A spectral transform method, using fast Fourier transforms, is used to compute the nonlinear terms. The solution is evolved in time, treating the linear terms implicitly and the nonlinear terms explicitly. This model was validated by simulating a rotating convection experiment flown on board a past Shuttle mission [3]. Now, the model runs on 256 of the Columbia supercomputer's processors, advancing the solution about 1,000 numerical time-steps per wall-clock hour.

Results: We have produced the first dynamically consistent three-dimensional computer simulation of turbulent convection and magnetic field generation in a giant planet, with a realistic density stratification [6]. The resulting banded pattern of surface zonal winds and dipolar magnetic field are very similar to those observed on Saturn (Figure 2). The surface winds are manifestations of the differential rotation in radius and latitude deep within the liquid interior. The mechanism for maintaining this differential rotation is based on the local generation of vorticity as rising fluid expands, and sinking fluid contracts.

Role of High-End Computing: The NASA Advanced Supercomputing facility at NASA Ames Research Center provided extensive supercomputing cycles on Columbia, and the data storage needed to carry out this work. NASA's High-End Computing (HEC) Program network engineers established partnerships with the Corporation for Education Network Initiatives in California to carry high-speed network traffic between Columbia and the California university system. Additionally, HEC Program application optimization specialists provided expert assistance with troubleshooting issues associated with parallelizing Dynamo (a dynamic geodynamo model based on the anelastic magnetohydrodynamic equations), identifying a workaround, and then performing the necessary recoding to enable successful parallelization.

Future: Although this simulation was run for over three-million numerical time-steps, representing approximately six simulated years, the zonal wind bands are still slowly developing at high latitude, and the magnetic field has not fully evolved in the deep interior. We also need to increase the spatial resolution to reduce the model's viscosity and obtain more turbulent convection, which will yield an even more realistic simulation.

Co-Investigators

- Martha Evonuk, ETH, Zurich
- Tamara Rogers, National Center for Atmospheric Research

Collaborating Organizations

- University of California, Santa Cruz

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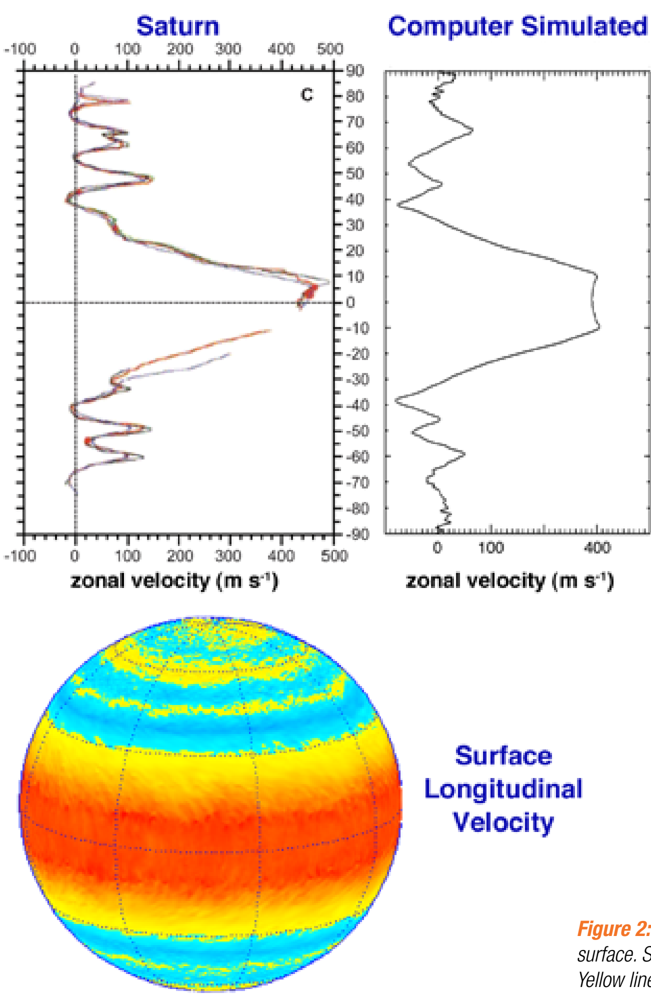

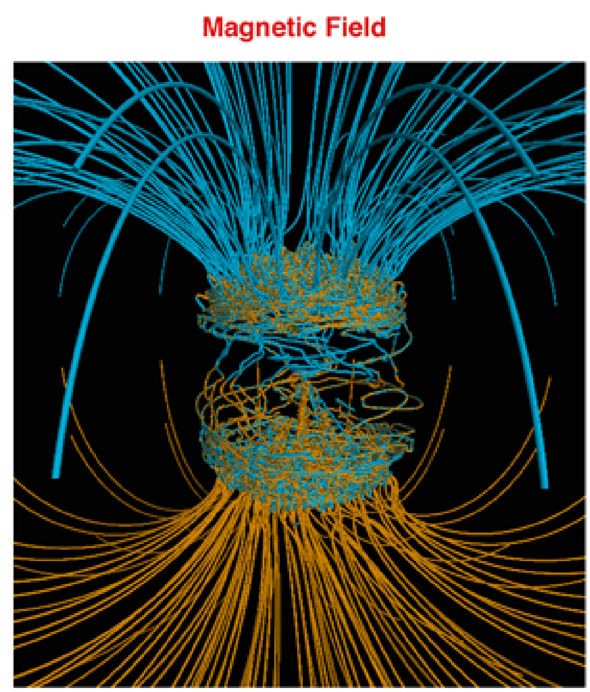

Figure 2: Simulated zonal winds (differential rotation) compared to that measured on Saturn's surface. Simulated magnetic field in a model of Saturn illustrated with magnetic lines of force. Yellow lines represent outward-directed field, and blue lines represent inward-directed field.

A COSMOLOGY-BASED BENCHMARK FOR CHARACTERIZING SYSTEM BALANCE ON HEC SYSTEMS

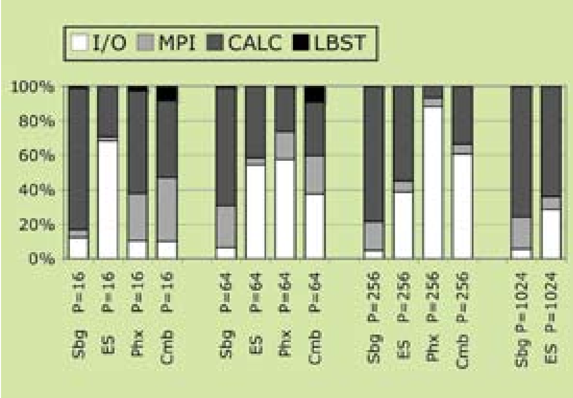

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Figure 1: *Relative timings for MADbench.*

Project Goals and Objectives: The aim of this work is to accurately measure the detailed statistical properties of the Cosmic Microwave Background (CMB) using the Microwave Anisotropy Dataset Computational Analysis Package (MADCAP) on several high-end computing (HEC) platforms including the Columbia supercomputer.

Project Description: Measuring the detailed statistical properties of the CMB has been a high priority ever since its serendipitous discovery in 1965. The challenge lies in the fact that the continued expansion of the universe has reduced the mean temperature of the CMB from around 3,000 Kelvin (K) at last-scattering to only 3 K today, and the anisotropies whose statistics we want to determine are at the 10^{-5} level in temperature, and anticipated to be at the 10^{-6} to 10^{-8} level in polarization.

Realizing the extraordinary scientific potential of the CMB requires making precise measurements of the microwave sky temperature over a significant fraction of the sky at very high resolution. Such measurements are made by scanning the sky for as long as possible with a cryogenically cooled telescope and as many microwave detectors as possible. The reduction of the resulting datasets—first to a pixelized sky map, and then to an angular power spectrum—is a serious computational challenge, and one which is only getting worse with increasing dataset sizes, as we try to make ever more precise measurements. It is therefore critical to choose the optimal algorithmic approach and supercomputing platform; one approach is MADCAP [1], which has been widely used on a variety of supercomputers.

Relevance of Work to NASA: This work, funded by NASA's Planck Mission, is closely in line with the Science Mission Directorate's pursuit to better understand and answer looming questions about the nature of our universe. The CMB, an image of the universe only 400,000 years after the Big Bang, provides an exquisitely sensitive probe of the fundamental parameters of cosmology.

Numerical Approach: The analysis of a CMB dataset typically starts from the noise-dominated time-ordered data, constructs a pixelized map of the observed region (typically with signal-to-noise of around unity), and finally extracts the signal-dominated two-point angular correlation function, or power spectrum, of the CMB signal together with the errors on this spectral estimate (Figure 2). The MADCAP approach is to first calculate the analytic maximum likelihood map and its residual pixel-pixel noise correlations, and then iteratively estimate the maximum likelihood power spectrum and its fisher information matrix.

The full MADCAP spectral estimator code, MADspec, includes a large number of special-case features—from preliminary data checking to marginalization over foreground templates—that dramatically increase the size and complexity of the code without altering its basic operational structure. For simplicity, we have therefore developed a stripped-down version, called MADbench, expressly designed for benchmarking that preserves all the computational challenges of the problem while removing the extraneous bells and whistles.

Results: Figure 1 shows the relative performance of MADbench across four of our evaluated HEC architectures: Seaborg, Earth Simulator, Phoenix, and Columbia. In a broad sense, MADbench spends almost all of its time calculating, communicating, or reading/writing data to disk. We identify the time associated with each of these activities as CALC, Message Passing Interface, and input/output (I/O); additionally, we show LBST, which captures load balancing including synchronization time. Detailed analysis of these results [2, 3] demonstrates the complex interplay between the architectural paradigms, interconnect technology, and I/O filesystem. These design tradeoffs play a key role in algorithmic design and system acquisitions. We are using the acquired data to increase MADspec efficiency as well as relate potential architectural bottlenecks to system designers.

An overall conclusion of this work is that greater clarity in the application context and overall specificity of performance timings greatly benefit understanding of how the distinct parts of large-scale parallel applications interact with the major subsystems of HEC platforms. It is therefore insufficient to report only the total runtime for a full-blown scientific application and expect to understand its parallel performance. As witnessed in our extensive analysis [2, 3], the achieved performance will not approximate that seen in simple computational kernels, which model only the compute phase and often vastly overestimate sustained performance. Such in-depth analysis is critical in first understanding and then bridging the gap between theoretical and sustained parallel performance.

Role of High-End Computing: CMB data analyses have typically been performed on superscalar-based commodity microprocessors due to their generality, scalability, and cost effectiveness. In this work, we examine the Columbia supercomputer, which brings an unprecedented level of computational power at a fraction of the cost of typical supercomputers. In addition, we evaluate two innovative parallel-vector architectures—the Earth Simulator and the Cray X1—which promise to narrow the growing gap between sustained and peak performance for many classes of scientific applications. To characterize what these platforms offer scientists that rely on HEC, it is imperative to critically evaluate and compare them in the context of demanding scientific applications.

Future: Future work will examine higher-scalability simulations across a broad range of supercomputing systems. We also plan to investigate MADbench's data transpositions and I/O transfer requirements in more detail, with the goal of reducing the impact of these overheads. In particular, we are interested in exploring the potential of dramatically improving performance by effectively overlapping computation with asynchronously scheduled I/O. This planned work will take advantage of a high-speed (10 gigabits/sec) network between NASA and Department of Energy (DOE) sites, established by NASA's High-End Computing Program network engineers—in partnership with the DOE's Energy Sciences Network.

Co-Investigators

- Jonathan Carter, David Skinner, both of Lawrence Berkeley National Laboratory

Collaborating Organizations

- National Energy Research Scientific Computing Center, Lawrence Berkeley National Laboratory

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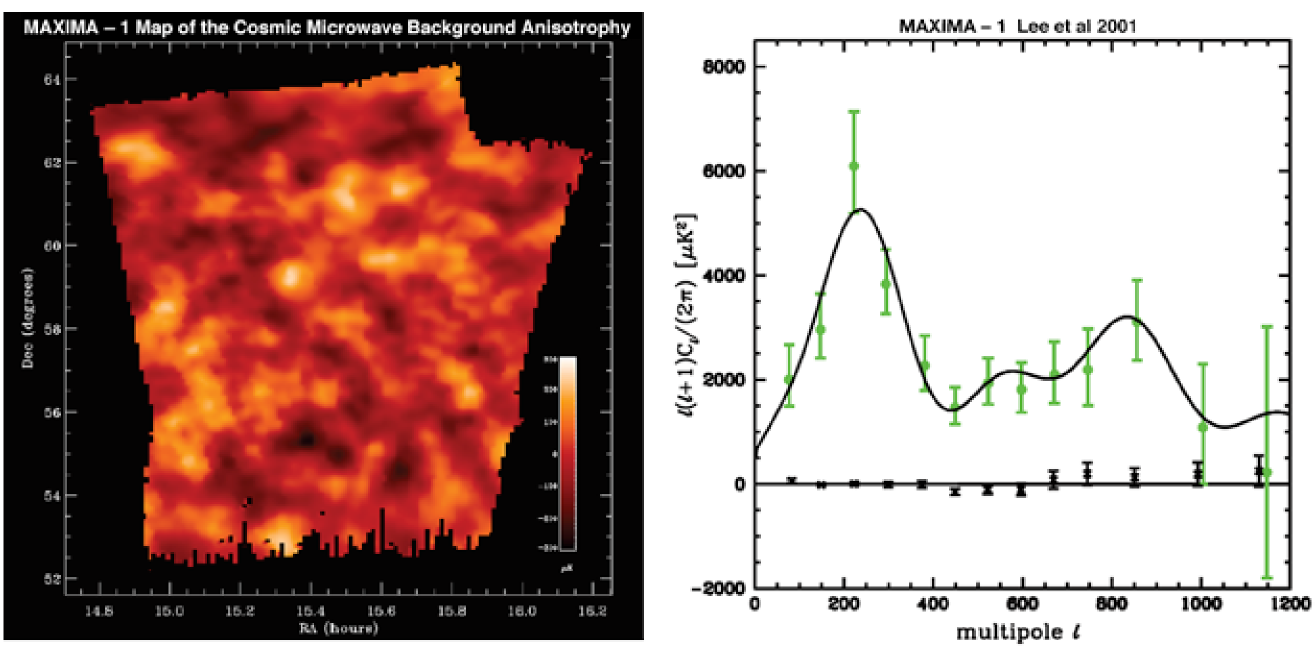

Figure 2: The map and associated angular power spectrum of the part of the Cosmic Microwave Background sky measured by the MAXIMA experiment, as calculated by the Microwave Anisotropy Dataset Computational Analysis Package.

EXPERIMENTAL HIGH-RESOLUTION WEATHER/ HURRICANE PREDICTIONS WITH THE NASA FVGCM

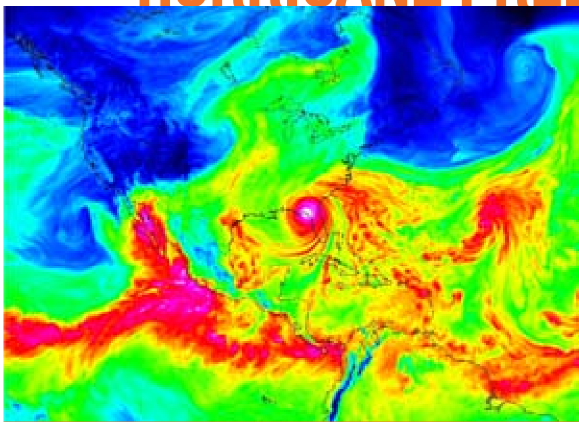

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Figure 1: *This continental-scale view shows total precipitable water from 5-day forecasts initialized at 0000 UTC September 1, 2004 with the 1/8-degree finite-volume General Circulation Model (fvGCM). The track forecast of Hurricane Frances (2004) is documented in Shen et al. (2006a).*

Project Goals and Objectives: Hurricane forecasts pose challenges for General Circulation Models (GCM), the most important being the horizontal grid spacing. The main goal of this project, supported by NASA's Weather Data Analysis and Assimilation Program, Earth Science Division, is to study the impacts of increasing resolution on numerical weather/hurricane forecasts, aimed at improving forecast accuracy.

Project Description: Previously, we had demonstrated the superior computing power of the NASA Center for Computational Science's Halem supercomputer by successfully completing high-resolution (1/2-degree) global weather predictions [2]. To further investigate the impact of high-resolution modeling on weather predictions, and to improve the model in both accuracy and efficiency, we deployed the finite-volume GCM (fvGCM) at higher (1/4- and 1/8-degree) resolutions on the Columbia supercomputer. This work was in support of our NASA-sponsored project, "Application of the High-Resolution NASA finite-volume GCM to Medium-Range Weather Predictions in Support of NASA Modeling and NOAA/NCEP Operational Weather Forecasting." The model has been running in real time to evaluate its performance on hurricane forecasts.

Relevance of Work to NASA: As accurate hurricane forecasts are important to our daily lives, this project can help address the central question of NASA's mission in hurricane research: *How can weather/hurricane forecasts be improved and made more reliable over longer periods of time using computer modeling?*

Computational Approach: With unprecedented computing resources provided by Columbia, the horizontal resolution of the fvGCM has been rapidly increased to 1/4 degree in early 2004 [1] and 1/8 degree in early 2005 [4]. Currently, the fvGCM at 1/12-degree resolution is being tested. The 1/12-degree fvGCM is the first global weather model with single-digit resolution, namely 9 kilometers (km) in the equator and 6.5 km in the mid-latitudes. A 5-day forecast of total precipitable water with the 1/12-degree fvGCM (Figure 2) clearly shows fine-scale weather events in the tropical area, which brings us to the point of overcoming the fundamental barrier between global and mesoscale models [4].

Results: As of July 2006, the team has published three important articles highlighting computations completed on Columbia since it came on-line in summer 2004. Two of them have been selected as *American Geophysical Union Journal Highlights*, and the first article about the 1/8-degree fvGCM has been cited as pioneering work (by Professor Roger Pielke, Sr. of Colorado State University). Recently, the article for the high-resolution simulations of Hurricane Katrina (2005) [5] has been highlighted in *Science* magazine [6]. These published results, along with yet more interesting results to be submitted for publication soon, are briefly summarized below.

During the 2004 hurricane season, the 1/4-degree model, which doubled the resolution adopted by most global models in operational Numerical Weather Prediction (NWP) centers at that time, was running in real time experimentally, and provided remarkable landfall predictions up to 5 days in advance for major hurricanes such as Charley, Frances, Ivan, and Jeanne [1, 4]. Moreover, the model was shown to be capable of resolving features such as erratic track, abrupt recurvature, and intense extratropical transition. In the 2005 hurricane season, a new research focus was put on validations of the 1/8-degree fvGCM's performance on hurricane forecasts, while the real-time 1/4-degree forecasts provided a baseline for comparisons. Being a global mesoscale-resolving model, the 1/8-degree model was the first global model to simulate mesoscale vortices (such as the Catalina Eddy and the Hawaiian Lee Vortex shown in [4]), which were generated by the interaction of the large-scale flows with better-resolved surface forcing. As shown in Figure 1, for 5-day forecasts, the

1/8-degree fvGCM was able to simulate detailed structures of Hurricane Frances (2004).

The 2005 Atlantic hurricane season was the most active in recorded history. There were 28 tropical storms and 15 hurricanes, four of which were rated Category 5. Accurate forecasts of these storms posed a great challenge to global and mesoscale modelers. It is especially well known that GCMs' insufficient resolutions undermine intensity predictions. Thanks to the considerable computing power of Columbia, this limitation could be overcome, as illustrated by [5], who performed six 5-day forecasts of Hurricane Katrina with the 1/8-degree fvGCM, and obtained promising intensity forecasts with small errors in center pressure of only ±12 hectopascals. It has also been shown that the notable improvement in Katrina's intensity forecasts occurred when grid spacing decreased from 1/4 degree to 1/8 degree, which is sufficient to simulate the near-eye wind distribution, and to resolve the radius of maximum winds.

Role of High-End Computing: The quantum jump in computing power at NASA provides unprecedented opportunities for advancing weather forecasting and hurricane modeling. In addition, NASA High-End Computing Program application specialists provided expert assistance with computational issues to speed up model development. While the mesoscale-resolving fvGCM has produced very promising results for the past 2 years, a great potential for further modeling advancement is still ahead of us. With the ultra-high-resolution global model, we will be able to investigate and illustrate the uncertainties of cumulus parameterizations, on which progress has been very slow during the last 40 years. We believe supercomputer power will soon enable breaking the cumulus parameterization deadlock [3] by advancing current work and inspiring related modeling research, and then open opportunities for more challenging problems, including hurricane genesis and hurricane climatology.

Future: During the past several years, substantial modeling work has been completed, and significant results have been achieved. We will document these results with a focus on illustrating the uncertainties of cumulus parameterizations with hurricane forecasts, thereby transferring our knowledge to the broader community.

Co-Investigators

- Wei-Kuo Tao, Oreste Reale, Jiun-Dar Chern, Tsengdar Lee, Johnny Chang, Christopher Henze, Jui-Lin Li, all of NASA
- Shian-Jiann Lin, NOAA Geophysical Fluid Dynamics Laboratory

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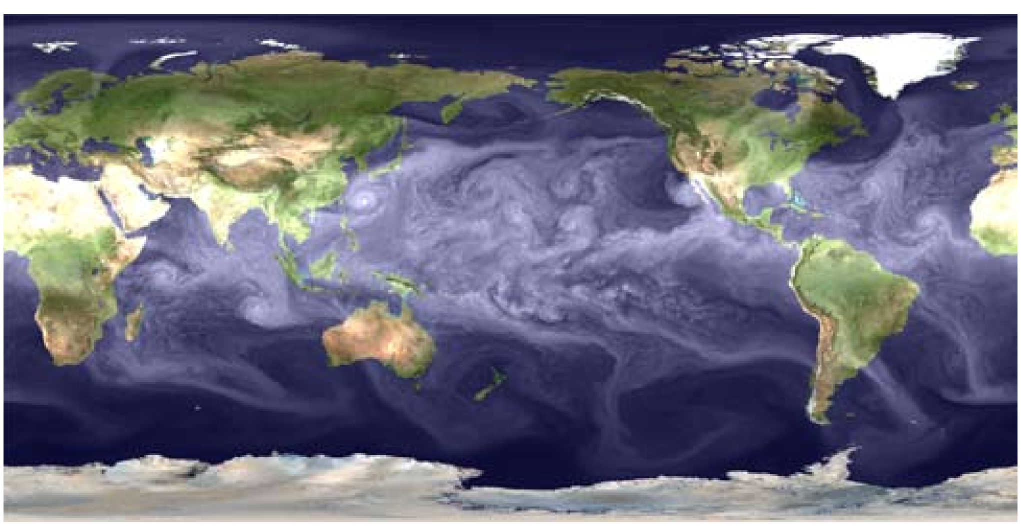

Figure 2: This global view shows total precipitable water from 5-day forecasts initialized at 0000 UTC September 1, 2004 with the 1/12-degree fvGCM, giving a grid spacing of 9 kilometers at the equator.

GEOS-5: GLOBAL MODELING AND ASSIMILATION DEVELOPMENT

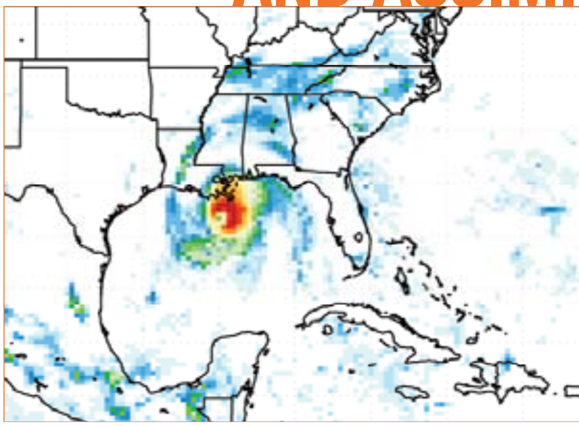

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***Figure 1:** Results from a 1/4-degree GEOS-5 atmospheric general circulation model forecast of the precipitation rate before Hurricane Katrina made landfall.*

Project Goals and Objectives: The Goddard Earth Observation System, Version 5 (GEOS-5) is being developed in the Global Modeling and Assimilation Office (GMAO) as a comprehensive model for weather and climate applications, with an associated atmospheric data assimilation system (DAS) for satellite data synthesis. The longer-term goal is to develop a next-generation atmospheric data assimilation capability to meet NASA's goals of maximizing the use of satellite observations to advance our understanding of processes related to climate variability and change, improve our modeling and prediction of the Earth system, and define future Earth observing systems. The shorter-term objective is to conduct simulations, assimilations, and forecasts to prepare a well-tuned, state-of-the-art system running at 1/2-degree resolution for the atmospheric DAS and 1-degree resolution for climate applications. Among other requirements, the DAS must support the Modern Era Retrospective-analysis for Research and Applications (MERRA) Project—a major reprocessing of all atmospheric data during the satellite era.

Project Description: The two main components of the GEOS-5 DAS are the atmospheric general circulation model (AGCM) and the analysis system. The GEOS-5 AGCM is the first major operational system built using the Earth System Modeling Framework (ESMF) and its object-oriented concepts. The analysis system is the National Oceanic and Atmospheric Administration/National Centers for Environmental Prediction's next-generation Grid-point Statistical Interpolation (GSI) system, now being developed in collaboration with the GMAO. Since GEOS-5 is intended as an assimilation, weather prediction, and climate modeling system, it must be tested and tuned in each of these configurations.

Relevance of Work to NASA: This project is a core element of NASA's Modeling, Analysis, and Prediction (MAP) Program and is primarily supported by the MAP Program, Earth Science Division. The GEOS-5 DAS supports NASA's Earth science research in the synthesis of Earth satellite observations, Earth Observing System (EOS) instrument team products, observing system modeling and design, climate and weather prediction, and chemistry-climate interactions.

Computational Approach: Both the model and the analysis are finite-difference grid-point codes, written in Fortran-90. The GCM relies heavily on the ESMF superstructure and infrastructure for its internal architecture. Parallelization is primarily Message Passing Interface (MPI). The model runs on a two-dimensional decomposition, transposing internally between horizontal and vertical layouts. Some of the physics, such as the solar radiation, which at any given time is active over only half the globe, is load balanced. The code scales well, and scalability increases linearly with problem size. At 1/2-degree and higher resolution, the code scales very well up to 480 processors on an Altix node. As part of our experimentation on the Columbia supercomputer, we have attempted to run the 1/4-degree model across nodes (up to 1,920 processors for a single image). Overall, the scaling is quite good even in this extreme use of Columbia.

Results: Using the NASA Advanced Supercomputing Division's Columbia and NASA Center for Computational Sciences' Explore supercomputers, we have run many hundreds of simulations in weather, climate, and assimilation modes. Runs were made at various resolutions, using different parameterizations, and undertaking parameter sweeps. Since there are many uncertainties in the formulations of both the model and analysis system, and since most processes being modeled are highly interdependent, we are faced with an almost infinite number of combinations to be evaluated. Comprehensive diagnostics and a validation suite assembled for evaluation of our GEOS-5 system were used to guide the parameter sweeps and minimize the number of experiments.

The initial test-production version of GEOS-5 has been run globally at various resolutions, including a 1/4-degree resolution to support hurricane forecasts as part of MAP '05. Simulations of Hurricane Katrina at 1-, 1/2-, and 1/4-degree resolution show the importance of resolution in how the model is able to simulate the details of extreme mesoscale weather events (Figures 1, 2). The performance of the model in climate simulations has been evaluated in 1-degree simulations. In this configuration, GEOS-5 has compared well with other national climate models.

The GEOS-5 DAS is still undergoing the last stages of tuning, and the final implementation of fine details needed for well-balanced analysis states. Nevertheless, the test version of the DAS has demonstrated a credible analysis capability so that it has been used for initial tests of the impact of EOS/Aqua/atmospheric infrared sounder on the statistics for global weather prediction skill.

Advanced diagnostic tools based on adjoint methods have been developed for both the AGCM dynamics with simple physics and for the GSI. Adjoints relate errors in forecasts to errors in initial conditions generated by the DAS, and then ultimately back to individual observations. Using these tools, the impact of particular observations on improving forecast skill can be evaluated. Thus far, several GMAO studies have probed the sensitivity of forecasts to specific observations. A more comprehensive view requires more experiments for statistical reliability. Such results also need to be investigated with our updated, tuned system and compared with other operational systems to evaluate the robustness of our results.

Role of High-End Computing: Models and assimilation systems are integrating tools that expand the usefulness of satellite observations. However, these systems have to be tuned to make optimal use of the data. Earth system models are not simply theoretical tools. The confrontation with data not only readily exposes deficiencies in the system, but also provides a powerful potential for rectifying those deficiencies. To do so requires experimentation at high resolution. These sorts of experiments, both numerous and computationally intense, can only be carried out on massively parallel systems such as Columbia and Explore.

Future: The experimentation required to improve the model and analysis system is unending; the societal benefit to be gained by improved weather and climate prediction provides the imperative. In addition, the information to be gained about the existing observing system and the potential impact of planned new observations is invaluable. Thus, we plan to continue to improve the GEOS-5 system to generate meteorological products in support of NASA instrument teams, to conduct high-resolution simulations in support of hurricane prediction during 2006, and to prepare for the next-generation comprehensive Earth system model and analysis system.

Co-Investigators

- Ron Gelaro, Julio Bacmeister, Larry Takacs, Ricardo Todling, all of NASA Goddard Space Flight Center

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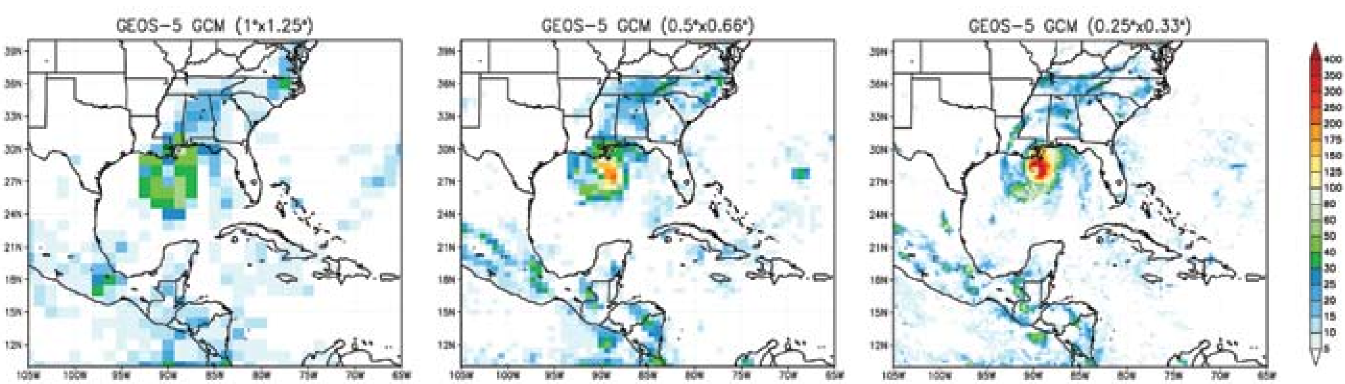

Figure 2: Forecast precipitation rate from a 2-day forecast before Hurricane Katrina made landfall, from the version of GEOS-5 used during MAP '05. From left to right, the forecasts are 1-, 1/2-, and 1/4-degree resolution. All forecasts are initialized from the National Oceanic and Atmospheric Administration/National Centers for Environmental Prediction operational forecast at 35-kilometers (slightly coarser than 1/4-degree) resolution.

GLOBAL CLIMATE MODELING: THE FUTURE OF OUR PLANET

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Figure 1: *Close-up of the percent deviation from the mean in specific humidity as calculated by Goddard Institute for Space Studies ModelE.*

Project Goals and Objectives: Earth's climate is changing, and it has become clear that humans are a major factor in driving this change. It is important to develop a good understanding of climate change, to minimize negative effects, and optimize adaptation. This project aims to develop global models that can predict changes in the composition of the Earth's atmosphere that result from human-made and natural factors, and in turn, the changes in climate that result from changes in atmospheric composition.

Project Description: The composition of Earth's atmosphere is changing rapidly. In the past 200 years, atmospheric carbon dioxide has increased from 280 parts per million (ppm) to 380 ppm. Other gases, such as methane, have changed by even greater fractions. The atmospheric amounts of carbon dioxide and methane are larger than at any time in the past million years, and the Earth's history shows that these changes will drive global climate change with consequences for all life on the planet. To model and understand climate change, we must simulate the complex Earth system, including the carbon cycle—which distributes carbon-containing molecules among the atmosphere, ocean, and land—and the weather and climate variables that define Earth's environment.

The new Goddard Institute for Space Studies (GISS) ModelE is designed to provide a unified approach to Earth system modeling, with the same model framework used for simulations of atmospheric composition as for studies of climate change. This allows the complete system to be as fully interactive as desired, and also to be simplified so that the effects of each component can be analyzed.

Relevance of Work to NASA: Primary funding for GISS work comes from NASA Goddard Space Flight Center's Earth Science Division, and is central to NASA's Earth Science Program. It helps to define the satellite and other observations that are needed to understand global and climate change. It is central to NASA's contributions to the U.S. Climate Change Science Program and the Intergovernmental Panel on Climate Change (IPCC) global assessments.

Computational Approach: We use the high-end computers at NASA Goddard for a large number of atmosphere, ocean, and climate simulations focused on a variety of time- and space-scales (Figures 1–3). The best tests of model capabilities are made on paleoclimate time-scales, which can cover thousands of years and thus use a relatively coarse spatial resolution. At the other extreme, simulations using very high spatial resolution, with the atmosphere divided into 100 or more vertical layers, are carried out to analyze the role of chemical, dynamical, and radiative processes in global change.

Results: We completed many global simulations that contributed insights about how the Earth system works, including relevance to policy making. A large number of climate simulation ensembles were carried out for 20th and 21st century climate change as input to the 2007 IPCC climate assessment. These simulations begin to address fundamental issues such as the question of how much greenhouse gas emissions would need to be reduced to avoid dangerous human-made interference with the global climate.

The model has also been stretched in different ways, for example, via simulations of the Earth's climate 8,200 years ago, when a massive flood of meltwater into the North Atlantic Ocean altered the global ocean circulation and global climate—providing a check on how well the model can simulate possible future changes. Another way that the model has been stretched is via simulations that include reasonably comprehensive atmospheric chemistry in the climate model. An application of this model shows that, despite expected global warming from increasing atmospheric carbon dioxide, it may still be possible to "save the Arctic" from drastic changes including the loss of all sea ice, if tropospheric pollutants such as ozone, methane, and soot aerosols are reduced.

Role of High-End Computing: The climate applications demand a flexible computing capability, which includes the possibility of running large ensembles with moderately high resolution for long periods, as well as the possibility of a smaller number of runs with high spatial resolution, these latter runs requiring good parallel computing capability. The model generates a large amount of data, which need to be stored and made available for diagnostic studies.

Future: Global Earth system models will continue to get more complex as additional components are made interactive. At the same time, higher spatial resolution is needed to improve the fidelity with which the climate system is represented. These requirements increase the demand for number of processors, processor speed, and data storage capabilities.

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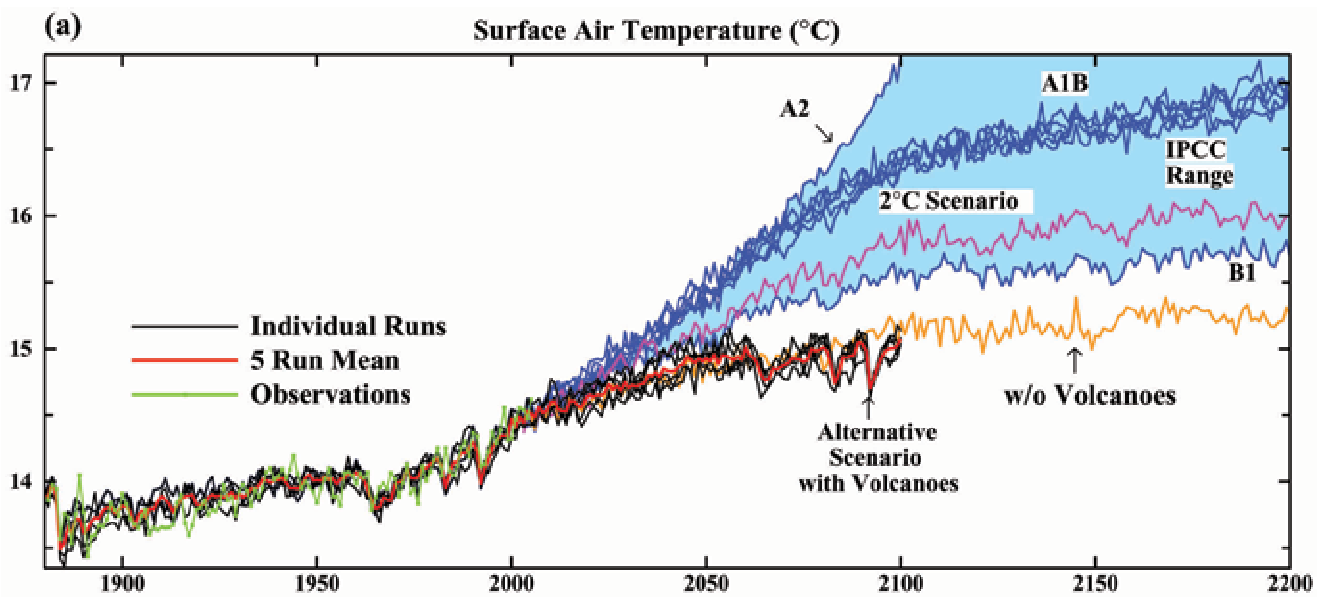

Figure 2: The global mean surface air temperature for several scenarios calculated by the Goddard Institute for Space Studies (GISS) ModelE coupled climate model as extensions of earlier 1880–2003 simulations for "all forcings." Climate forcings include the effects of increasing atmospheric carbon dioxide and other gases, volcanic and human-made aerosols (small particles), solar variations, and land use changes.

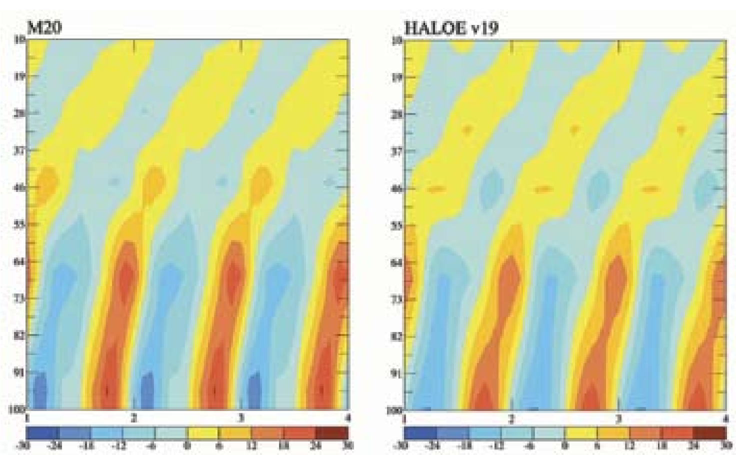

Figure 3: The percent deviation from the mean in specific humidity as calculated by Goddard Institute for Space Studies ModelE compared to the Halogen Occultation Experiment (HALOE) data in the tropical upper troposphere/lower stratosphere (12°S–12°N). Each picture is a climatology, repeated 3 times to allow a stratospheric tape recorder effect—which shows how water vapor is pumped into Earth's stratosphere at low latitudes—to be made clearer.

THE GLOBAL MODELING INITIATIVE

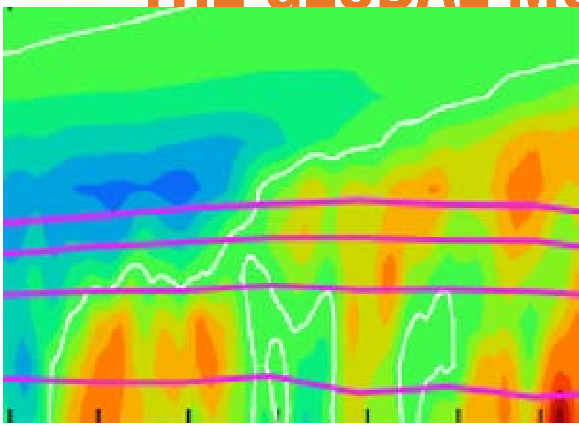

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Figure 1: *Close-up of Global Modeling Initiative model carbon monoxide transport.*

Project Goals and Objectives: The Global Modeling Initiative (GMI), supported by the NASA Modeling, Analysis, and Prediction Program, Earth Science Division, has developed modular three-dimensional chemistry and transport models (CTMs) for the stratosphere and troposphere that incorporate different components and inputs into a common computational framework. A goal of the GMI effort is to reduce uncertainties in model results and predictions by understanding the processes that most contribute to the variability of results and by evaluating model results against existing observations of atmospheric composition. GMI also contributes to the assessment of the anthropogenic perturbations to the Earth system.

Project Description: The diagnosis of physical and chemical processes that determine the composition of Earth's atmosphere and the uncertainties in these processes is a necessary step towards achieving credible assessment of anthropogenic perturbations. Because of its modular architecture, the GMI has been able to test the sensitivity of model results to different adopted meteorological fields. These fields come from both free-running general circulation models (GCMs), such as those from the Goddard Institute for Space Studies, the National Center for Atmospheric Research, and the NASA Global Modeling and Assimilation Office (GMAO), as well as winds assimilated for different years, provided by the different GMAO systems. Each model is tested against a suite of observations: ground-based, aircraft, balloon, and satellite.

Relevance of Work to NASA: GMI studies are relevant to improving our understanding of Earth systems. GMI integrates modeling studies with observations to test our understanding of atmospheric processes. The process-oriented validation made possible by observations allows GMI to critically evaluate the components of climate models.

Numerical Approach: The CTM solves a series of coupled partial differential equations for 117 species. The equations express the principle of mass continuity, and explicitly represent transport by advection, convection, and small-scale diffusion. Chemical production and loss of species involves the coupling of several hundred chemical reactions. Finally, removal by wet and dry deposition is also included for the relevant species.

The different processes incorporated into the model are solved sequentially through an operator-splitting approach. Advection is solved by utilizing the flux-form semi-Lagrangian algorithm of Lin and Rood. The stiff system of coupled chemical production and loss reactions is solved by Jacobson's highly accurate Sparse Matrix Vectorized GEAR solver. Convective transport is treated with the algorithm proposed by Rasch et al. Wet and dry deposition are solved by the mechanisms of Liu et al. and Weseley.

Results: GMI simulations were contributed to the atmospheric composition assessment of the upcoming Intergovernmental Panel on Climate Change report. Simulations were also provided for the World Meteorological Office/United Nations Environment Programme assessment of stratospheric ozone. In addition, GMI results are being used to analyze and validate measurements from the Aura satellite. One of these comparisons has been accepted for publication in the *Journal of Geophysical Research* [2], where it is shown that GMI does a credible job of representing the tropospheric column ozone derived from a combination of Ozone Monitoring Instrument and Microwave Limb Sounder (MLS) measurements.

The power of the GMI model in the Upper Troposphere/Lower Stratosphere (UT/LS) has been shown in the simulation of the carbon monoxide "tape recorder" observed in the MLS data (Figures 1, 2 and [1]). This simulation gives confidence to the representation of dynamical and chemical processes in the UT/LS.

Role of High-End Computing: High-resolution meteorological datasets, combined with large numbers of species to be simulated, drive the need for very large computing memories, file systems, and tools to access the data efficiently. The demand for raw computational power is driven by the expensive calculations to solve the very stiff systems of equations that describe the chemical reactions in the atmosphere. Unlike many other disciplines, spatial resolution per se is not the sole driver for computing resources. The need to simulate a wide variety of scenarios with different available meteorological datasets produces a requirements profile intermediate between capability and capacity computing. Typical experiments require 128–256 processors, and consume 10,000–40,000 processor-hours.

Future: The GMI CTM will continue to be used in international assessment efforts. These include the Chemistry-Climate Validation sponsored by the international Stratospheric Processes and their Role in Climate Project, and the model intercomparison/assessment of long-range transport of pollutants (a multi-year international effort spearheaded by the Environmental Protection Agency, with support from NASA and other agencies).

The GMI combined stratospheric-tropospheric "Combo" model is being used in the analysis of Aura measurements of ozone, carbon monoxide, and other constituents. In addition, an aerosol component is being coupled to the model chemistry, allowing simulations of the response of aerosol concentrations to different anthropogenic emissions and the perturbation to cloud condensation nuclei.

Finally, GMI is working closely with ongoing efforts to simulate the coupled chemistry-climate system in NASA Goddard Space Flight Center's Atmospheric Chemistry and Dynamics Branch and GMAO. GMI is testing and providing the chemistry and deposition modules for this effort. These modules have been modified to be compatible with the Earth System Modeling Framework, and will also be incorporated into GMAO's GEOS-5 model.

Co-Investigators

- Bryan Duncan, University of Maryland, Baltimore County

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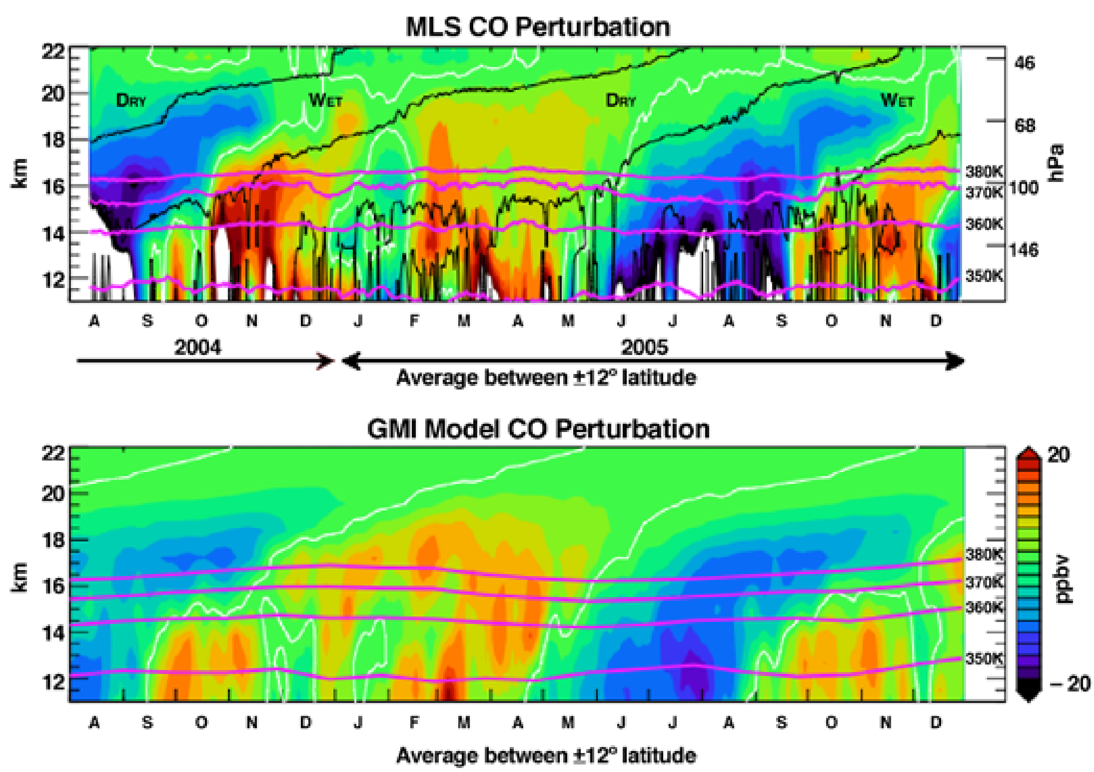

Figure 2: Top panel: Zonal mean Aura Microwave Limb Sounder (MLS) carbon monoxide (CO) data with the annual average removed versus time (months). Altitude scale is 7 kilometers log(1000/p) where p is pressure. Black lines show the zero contour for MLS water vapor tape recorder with 'wet' and 'dry' labels indicating the sign of the perturbation. White contours are zero lines for CO data. The right-hand scale shows pressure levels for MLS level 2 data. Pink lines show the zonal mean potential temperature surfaces (350–380 Kelvin). Bottom panel: Global Modeling Initiative model CO with transport driven by Global Modeling and Assimilation Office GEOS-4 meteorology with 1994–5 observed sea-surface temperature forcing.

HALLOWEEN STORM SIMULATIONS WITH THE SPACE WEATHER MODELING FRAMEWORK

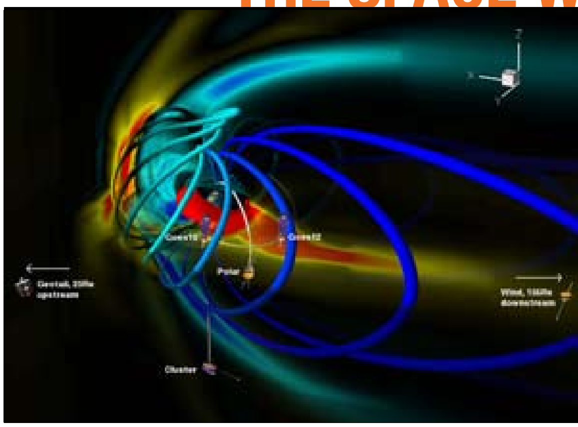

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Figure 1: *A reduced image of the simulated Earth magnetosphere during the Halloween storm.*

Project Goals and Objectives: Our goal was to simulate the effects of solar storms on the space environment.

Project Description: On the Columbia supercomputer, we carried out an end-to-end simulation of the Sun-Earth environment during the solar storm of October 28–29, 2003—widely nicknamed the "Halloween" storm. Past magnetosphere simulations attempted to match the observation of a single satellite. Even these single-point comparisons were often not very good.

Relevance of Work to NASA: Primary support for this research comes from the Living with a Star Program, Heliophysics Division. The objective of this work specifically addresses the goals of the Geospace Science program Goal II SEC 1.c to identify and understand the response of the magnetosphere to external and internal drivers such as intense solar coronal mass ejection events like the Halloween storm.

Computational Approach: Our simulations were carried out with the high-performance Space Weather Modeling Framework (SWMF) that was developed with NASA Earth Science Technology Office-Computational Technologies Project funding and the essential availability of Columbia. The SWMF is made up of nine interoperating models of physics domains, ranging from the surface of the sun to the upper atmosphere of the Earth.

We achieved a parallel scale-up of the SWMF from an SGI Origin 3000 to the NASA Center for Computational Sciences' Halem supercomputer and then to Columbia (Figure 2). This parallel scaling was achieved by using several innovative new technologies:

- Concurrent/mixed execution of components.
- Adaptive grids in the BATSRUS code, which incorporates the Solar Corona, Inner Heliosphere, and Global Magnetosphere (GM) models.
- Implicit time-stepping in GM/BATSRUS.
- Efficient field line tracing between the GM and Inner Magnetosphere models.

A scaling curve for several computing systems is shown in Figure 2.

Results: SWMF and its components are currently running in production mode. The Halloween storm represents an extremely computationally challenging simulation, and we are very pleased that the codes are flawlessly able to handle the challenge. For the first time, we achieved faster than real-time performance of all the different components coupled together and operating efficiently on a large sun-to-Earth simulation. Such capability is essential if we want to be able to predict conditions in the near-Earth space environment.

Role of High-End Computing: For the first time, we attempted to match the simultaneous observations of six satellites located at very different regions of the magnetosphere (Figure 3). This is a big qualitative leap in magnetospheric physics, made possible by Columbia. Because we were able to explore the parameter space in the simulations, we obtained excellent agreement with all six magnetospheric satellites.

Future: We are planning to finish the simulations as soon as time on Columbia becomes available.

Co-Investigators

- Darren De Zeeuw, Ward Manchester, Igor Sokolov, Gabor Toth, all of University of Michigan
- Ilia Roussev, University of Hawaii

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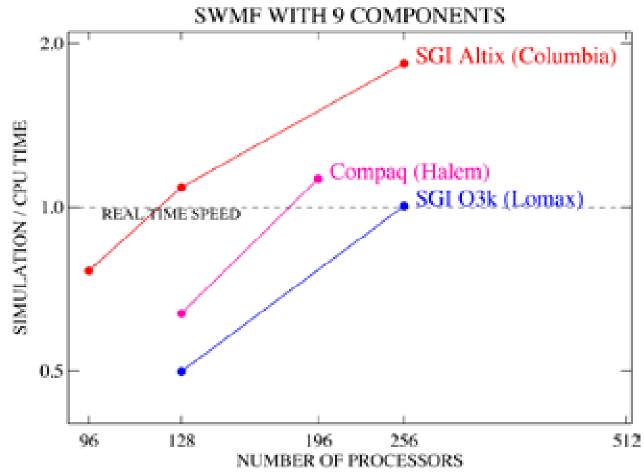

Figure 2: *Parallel scale-up of the Space Weather Modeling Framework (SWMF) on various platforms.*

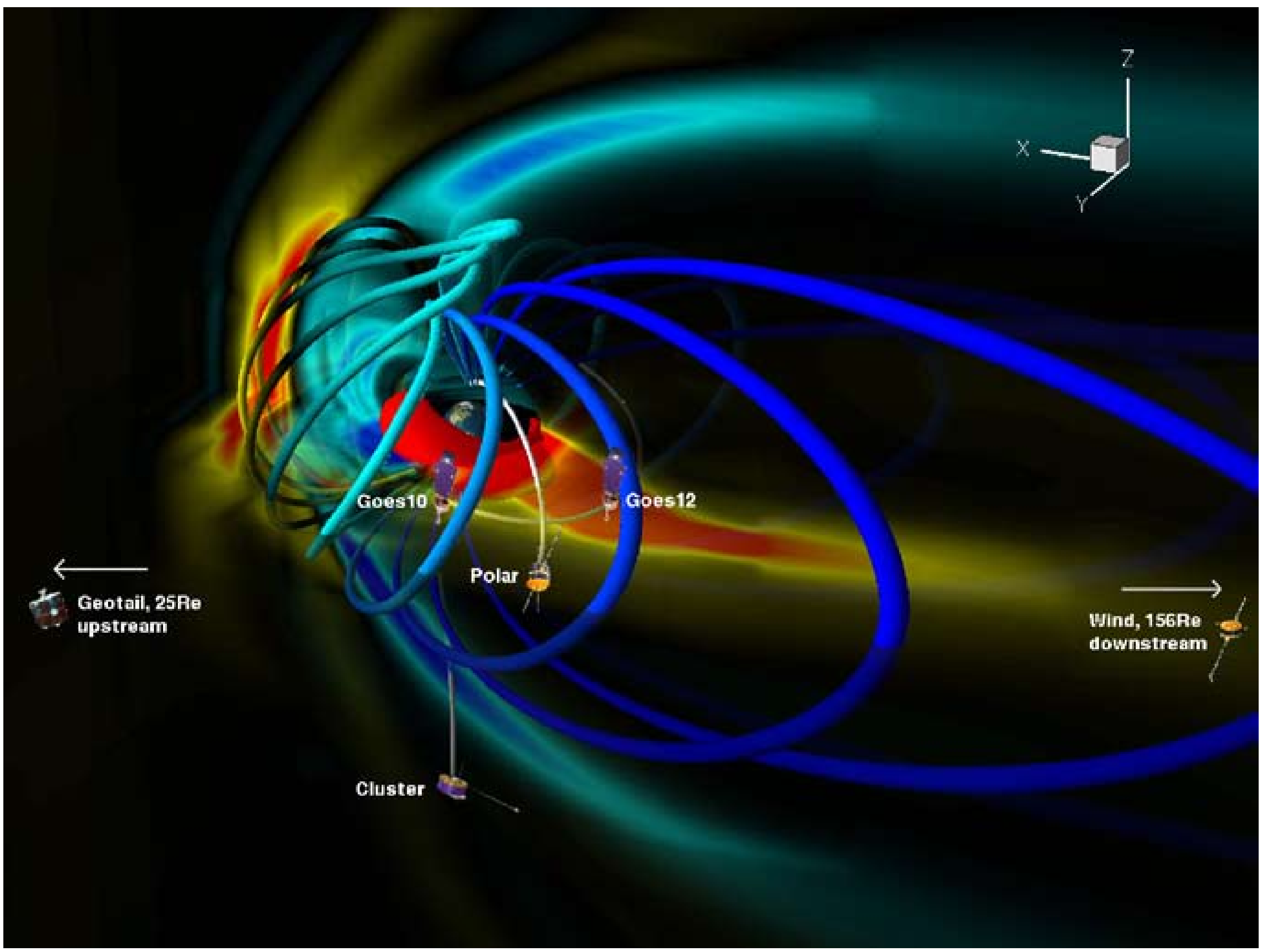

Figure 3: *Simulated Earth magnetosphere during the Halloween storm. The tubes represent the last closed magnetic field lines color-coded with the thermal plasma pressure. The pressure is also shown on several cut planes. The positions of satellites with magnetospheric instrumentation are also shown.*

HIGH-PERFORMANCE SIMULATION & DATA ASSIMILATION WITH LAND & ATMOSPHERE MODELS

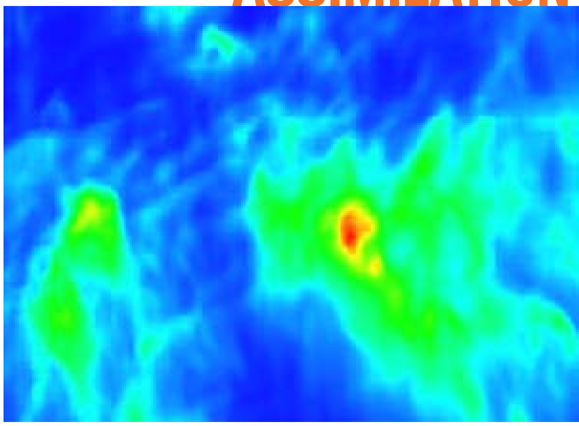

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***Figure 1:** Close-up of the control rainfall distribution (6 seconds) from a comparison with model runs using different time-step frequencies.*

Project Goals and Objectives: The advance of remote sensing technology in recent years has enabled us to monitor and measure Earth's land surface at an unprecedented scale and frequency. Such observations provide a huge volume of valuable data of Earth's land surface properties, such as vegetation, moisture, and energy fluxes. We developed both a high-resolution, off-line land surface modeling system and a coupled land-atmosphere system with the goal to fully exploit NASA's unique resource of satellite observations to improve the understanding, monitoring, and forecasting of our home planet's environment. The objective is to be able to resolve and study more important physical and dynamical processes that were not possible with low-resolution models by performing modeling and data assimilation at spatial scales comparable to that of the satellite observations.

Project Description: We combined emerging technologies and interoperable Earth system standards such as the Earth System Modeling Framework (ESMF) to couple complex Earth system model components. The code is an integration of three modeling systems: the Land Information System (LIS) Weather Research and Forecasting (WRF), and Goddard Cumulus Ensemble (GCE) atmospheric models. The advanced features of LIS and WRF are combined by integrating these modeling systems into a coupled hydrometeorological system.

The use of parameterizations to represent physical processes in numerical models is becoming more expensive as their level of sophistication increases. These parameterizations are used to represent precipitation processes, deep cumulus convection, land-surface interactions, and long- and short-wave radiation interactions, to name a few. Of these, the radiation parameterizations are clearly the most computationally expensive. The frequency of radiation updates for use in mesoscale models, such as WRF, is generally performed on the order of several minutes, even when grid spacings are reduced to the order of 1 kilometer. The assumption is that the results will not be significantly affected over the course of the simulation, thus saving computing costs.

Relevance of Work to NASA: Our land surface modeling system has implemented a strongly modular, portable, and interoperable design and built-in parallelism for both shared- and distributed-memory platforms. These technologies are critical to advancing the Science Mission Directorate's science and prediction goals to demonstrate NASA's unique capability in scientific modeling and computational technologies for Earth system studies. Further, the integrated coupled hydrometeorological modeling systems facilitate several multi-model studies of land-atmosphere coupling that can be used to advance Earth system studies.

Computational Approach: High-resolution modeling requires large amounts of memory and processing power. Coupling between the land and atmospheric models at various space and time scales, and the parallelism based on the Message Passing Interface (MPI) demand a large number of high-performance processors and high-throughput, low-latency communication. In addition, scalability is critical as we push our model toward even higher resolutions. The three modeling systems were coupled with ESMF, and they used its MPI-based virtual machine architecture. All three modeling systems have been parallelized with MPI within the code, making it possible to run on a large number of processors. This approach allows the more frequent calls to computationally expensive parameterizations, such as the radiation parameterization, which increases computational time by over 300% when it is called.

Results: In this work, supported by the NASA Earth Science Technology Office's Advanced Information Systems Technology Program, we were able to integrate at sufficiently high resolutions to explicitly resolve hydrometeors and their interaction with long and shortwave radiation, investigating the effects of calling the radiation parameterization at different model timestep intervals. The computational resources also allowed us to examine these effects using different initial conditions for the land and atmospheric states, as well as multiple land surface models.

In one set of experiments we used an ideal initialization, where the atmosphere was initialized with a single thermodynamic and momentum profile for the entire domain. This was done for dry and wet atmospheres. The study indicated a wide divergence in model solutions when the radiation parameterization was called at different timestep multiples. The effects were magnified in the wet atmospheric case (Figures 1, 2), suggesting the importance of the interaction of radiation with the microphysics. This is an important result since it questions the robustness of radiation parameterization, and the assumption that it can be called at a frequency much larger than the model timestep.

Role of High-End Computing: The ability to employ high-resolution coupled land and atmospheric numerical modeling is a valuable tool for investigating moist atmospheric processes, the effects of input data and boundary conditions, and the predictability of parameterizations. NASA computational resources, such as the Halem and Columbia supercomputers, provide the ability to perform these computationally intensive simulations through a parallel environment that enables high-bandwidth inter-processor communication.

A typical simulation requires roughly 50 gigabytes of available memory. Each 24-hour integration performed with infrequent calls to the radiation parameterization on 128 processors required nearly 3,000 processor-hours and produced roughly 160 gigabytes of output. When the radiation parameterization is called every model timestep, the processor-hours required approached 10,000.

Future: The use of the coupled LISWRF modeling system in a pseudo-operational mode will require the organization of datasets approaching several terabytes in size. In addition, high-bandwidth connections will be required for post-processing and dissemination of model forecasts. Parallel input/output techniques have already been developed by the LISWRF team, and will provide a valuable tool for future developments of the modeling system.

Co-Investigators

- Joseph Eastman, Sujay Kumar, Yudong Tian, Steve Lang, Xiping Zeng, all of NASA Goddard Space Flight Center

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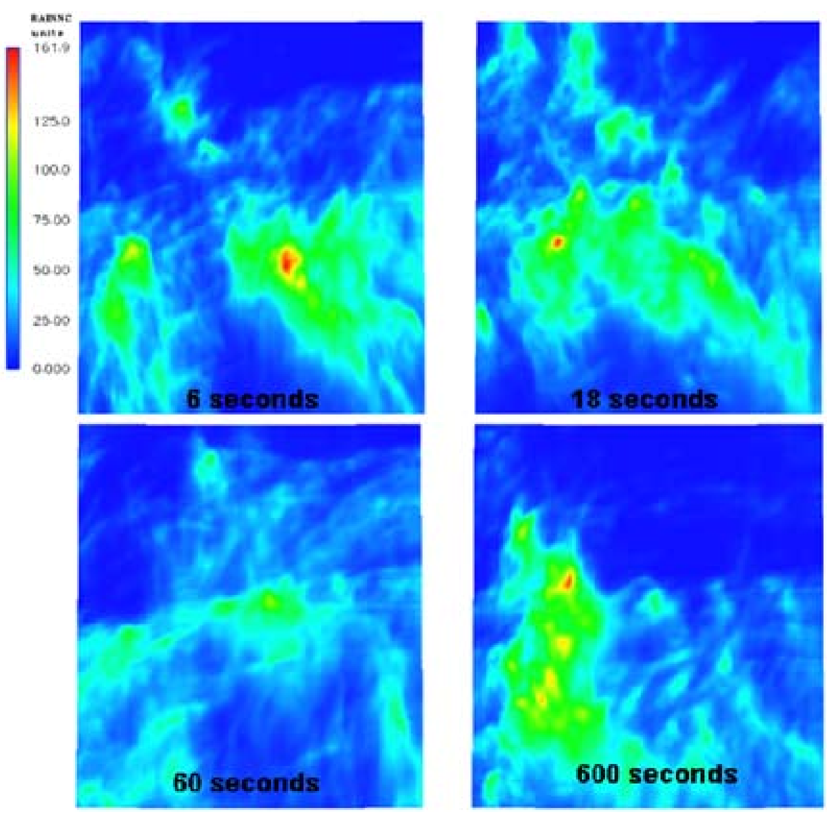

Figure 2: *Side-by-side comparison of the control rainfall distribution (6 seconds) next to the every 18, 60, and 600 seconds runs (3-, 10-, and 100-timestep frequencies, respectively). The results show significant differences. The 3-timestep pattern is the closest to the control, but diverging solutions are evident. The 100-timestep results are vastly different.*

HIGH-RESOLUTION GLOBAL-OCEAN AND SEA-ICE DATA SYNTHESIS

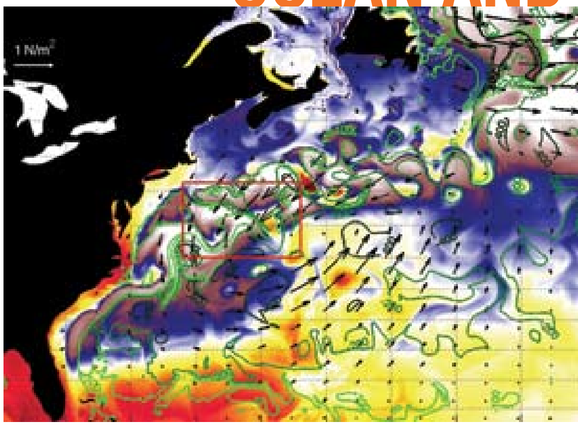

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***Figure 1:** As part of the National Science Foundation-funded CLIMODE project, G. Maze and J. Marshall at Massachusetts Institute of Technology are using ECCO2 high-resolution solutions to study the impact of ocean eddies on Mode water formation. The figure to the left shows surface heat flux (yellow-red indicates ocean warming and blue-gray indicates cooling), mixed layer depth (green contour lines), and surface wind stress (black arrows) on March 1, 2003, in the Gulf Stream region, an active region of Mode water formation.*

Project Goals and Objectives: The consortium for Estimating the Circulation and Climate of the Ocean (ECCO) aims to produce a best possible synthesis of most available global-scale oceanic data obtained during the past few decades. ECCO has demonstrated the feasibility of carrying out these challenging computations. The resulting estimates have proven useful for a wide variety of oceanographic and interdisciplinary studies. Existing solutions, however, have several shortcomings, including coarse horizontal resolution and a lacking representation of Arctic Ocean and sea-ice processes. To address these and other shortcomings, a new high-resolution ocean state estimation project, ECCO2, has been initiated under the auspices of the NASA Modeling, Analysis, and Prediction (MAP) Program.

Project Description: To increase understanding and predictive capability for the ocean's role in future climate change scenarios, the ECCO2 Project aims to produce increasingly accurate syntheses of all available global-scale ocean and sea-ice data—at resolutions that start to resolve ocean eddies and other narrow current systems, which transport heat, carbon, and other properties within the ocean [6]. ECCO2 data syntheses are needed to quantify the role of the oceans in the global carbon cycle; to understand the recent evolution of the polar oceans; to monitor time-evolving term balances within and between different components of the Earth system; and for many other science applications.

Relevance of Work to NASA: This work, funded by the MAP Program, is an important part of NASA's continuing quest to study Earth from space, to advance scientific understanding, and to meet societal needs. A better understanding and predictive capability for global ocean circulation and ocean-atmosphere exchanges of heat, freshwater, and biogeochemical tracers will lead to progress in understanding the role of oceans, atmosphere, and ice in the climate system. In turn, this will lead to improved predictive capability for the future evolution of Earth's climate system.

Computational Approach: ECCO2 data syntheses are obtained via the least-squares fit of global full-depth-ocean and sea-ice configurations of the Massachusetts Institute of Technology (MIT) general circulation model to the available satellite and in-situ data. Initially, this least-squares fit is being carried out for a small number of control variables using a Green's function approach [7]. The longer-term objective is to use an adjoint-model approach to estimate hundreds of billions of control variables [3, 9]. This is a huge technical and computational challenge.

Results: Currently, a number of projects are working with pre-release ECCO2 products. Here, we list some example applications from early users of ECCO2 products:

- *Studying the genesis of Mode waters:* This project is examining high-resolution ECCO2 solutions to help develop and validate theoretical models of the air-sea processes that drive Mode water formation (Figure 1, [5]).
- *Arctic Ocean carbon flux studies:* This project is part of a larger effort to study the Arctic region carbon cycle, including developing a better understanding of exchanges between marine and terrestrial carbon pools and of possible exchanges between these large carbon reservoirs and the atmosphere (M. Follows, MIT).
- *Eddy propagation characteristics:* This project uses correlation between successive maps of sea-surface height to estimate eddy propagation characteristics. Similarities and differences between results from observed and simulated sea-surface height variability improve understanding of model and data errors and of underlying physical processes (L.-L. Fu, NASA's Jet Propulsion Laboratory, Figure 2).
- *ICESat over Arctic sea-ice:* ECCO2 estimates of Arctic sea-surface height variability are used to estimate contribution of oceanographic circulation signal to Ice, Cloud, and land Elevation Satellite (ICESat) retrievals to help interpret altimetric and reflectivity profiles [4].

- *Estimating eddy variability and errors:* Hydrographic and altimetric data are being used in conjunction with high-resolution ECCO2 simulations to estimate global hydrographic variability and model representation errors [2, 8].

Role of High-End Computing: Carrying out, visualizing, and analyzing coupled ocean/sea-ice global data assimilation at eddy-resolving resolutions over the full ocean depth for decades or more is computationally very demanding. It requires iterating over decade-long prognostic simulations containing approximately 10^8 grid cells. The calculation footprint of a single decade of simulation is approximately 10^{17} arithmetic operations. On a modern desktop computer this computation would take several years to complete but this can be reduced to less than a week using just 512 processors of the Columbia supercomputer. NASA's High-End Computing (HEC) Program personnel are helping to meet this challenge by assisting with optimization of the ECCO2 code, with visualization of the results, including high temporal resolution concurrent or "live" visualization (Figure 3, [1]), and with support of the largest volume of data transfers in the HEC Program's history across the wide area network between Columbia and NASA's Jet Propulsion Laboratory.

Future: ECCO2 plans to release a first-generation public state estimate around mid-2007. This estimate will be obtained using a Green's function approach to estimate a small number of control variables. In the longer term, depending on available computer resources, it is planned to adopt an adjoint-model approach, which will permit estimation of hundreds of billions of control variables. ECCO2 also aims to address issues pertaining to solution convergence in forward simulation as resolution is increased.

Co-Investigators

- Lee-Lueng Fu, NASA Jet Propulsion Laboratory
- Patrick Heimbach, Massachusetts Institute of Technology
- Christopher Henze, NASA Ames Research Center
- John Marshall, Massachusetts Institute of Technology
- Carl Wunsch, Massachusetts Institute of Technology

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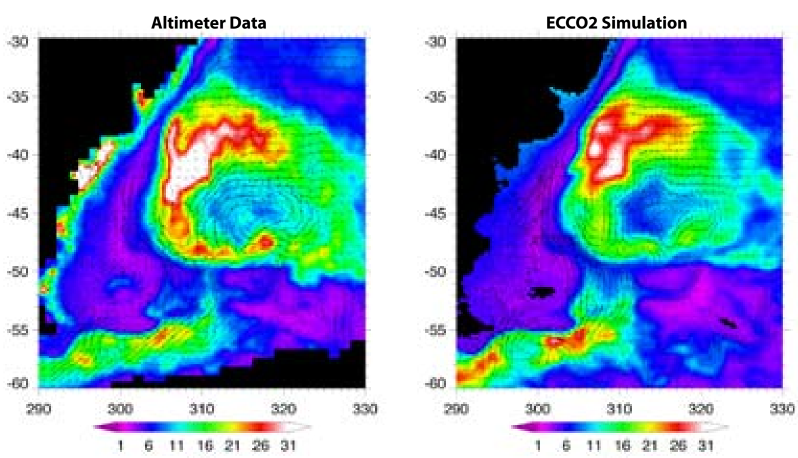

Figure 2: Containing 90% of the kinetic energy in the ocean, ocean eddies (the storms of the oceans) with scales from 10–100 kilometers, are difficult to observe and simulate. Using data from TOPEX/Poseidon, Jason, and ERS radar altimeters, the energy level and propagation velocity of eddies were estimated and compared to a high-resolution ECCO2 simulation. Shown here is an example in the Argentine Basin. The color map indicates sea-surface height standard deviation and the arrows indicate eddy propagation velocity. The large standard deviation near the coastline in the altimeter data is caused by residual tidal correction errors, which are not present in the ECCO2 simulation.

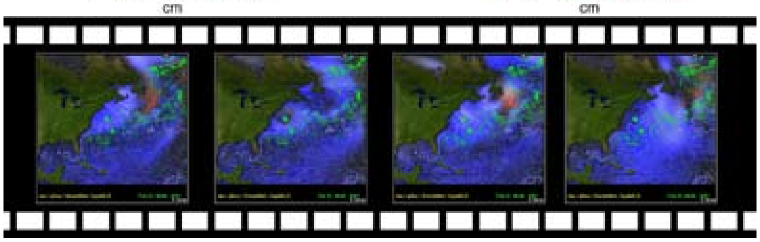

Figure 3: Snapshot images capturing air-sea exchange for the same time on four consecutive days in February 2001, taken from real-time animations made on the Columbia 2,048 system.

HIGH-RESOLUTION SIMULATIONS OF LARGE-SCALE STRUCTURE AND GALAXY FORMATION

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Figure 1: *Close-up of a simulated spiral galaxy seen in Figure 2.*

Project Goals and Objectives: Recent progress in theoretical and observational cosmology has established, for the first time, a standard model for the material content of the universe and the initial conditions for structure formation. According to this "double dark" model, the universe consists mostly of invisible "stuff"—dark matter and dark energy—with all the visible material in the universe making up only about 0.5% of the cosmic density [1]. One of the biggest challenges is to explain how the structures we see in the universe today formed within this cosmological framework, and to test these new theories against rapidly improving observational evidence.

Project Description: Initial fluctuations in dark matter, seeded by an early inflation epoch, are amplified by gravity as the universe expands and eventually collapses to form the galaxies we see today. One of our main projects is to simulate/model this process. On very large scales, gravity is the only important force, and it is possible to simulate only the behavior of the dark matter and dark energy to predict where and how we should expect to see galaxies form. We are doing some of the highest resolution simulations of this kind. Our other main project is to model "gastrophysics" both on cosmological scales, and in the formation of the stellar spheroids—elliptical galaxies and central galaxy bulges—in which both supermassive black holes and most of the stellar mass in the universe reside today.

Relevance of Work to NASA: This work, funded by the Hubble and Spitzer Space Telescope Missions, is an important part of NASA's continuing quest to increase our understanding of the origin and evolution of our universe through supporting theoretical research and simulations, and the comparison of these predictions to observational data. We are providing the main theoretical support for the Deep Extragalactic Evolutionary Probe (DEEP) Project, which has extensive data from NASA's Chandra, Hubble, and Spitzer Space Telescopes, in addition to NASA's Galaxy Evolution Explorer (GALEX) spacecraft.

Numerical Approach: We use our massively parallel N-body Adaptive Refinement Tree code for our cosmological simulations, including those involving gas physics. We use Volker Springel's GADGET code for our simulations of stellar spheroid production by galaxy mergers, including star formation and feedback. We use our new Sunrise code to predict the effects of dust in these simulations. Because the dust typically absorbs about nine-tenths of the light from bright, new stars produced in galaxy mergers and re-radiates it at longer (infrared) wavelengths, simulating the effects of dust in mergers is crucial [2]. Sunrise is the first code capable of doing this, and we have recently improved its speed by more than an order of magnitude [3]. Figures 2–3 are examples of optical images from our galaxy merger simulations, including dust effects.

Results: A dynamic range of 10^5 per dimension (three-dimensional) is routinely achieved in our dissipationless simulations—this allows for extremely accurate statistical characterizations of the large-scale structure of the universe, and provides a nearly complete inventory of all luminous galaxies above about a hundredth of the characteristic galaxy luminosity. This aspect is particularly important for constructing a new generation of theoretical mock galaxy catalogues that allow a direct comparison to observational datasets. On the basis of earlier simulations, we were the first to predict that galaxies would become more clustered on small scales, and less so on larger scales compared to nearby galaxies. This prediction has been refined using simulations run and/or analyzed on the Columbia supercomputer, and confirmed with remarkable accuracy by new data [4]. Shortly after NASA's Wilkinson Microwave Anisotropy Probe reported new values for the parameters of the standard "double dark" theory in March 2006, we ran a large simulation on Columbia with exactly those parameters—to compare with both our older simulations and observations. We are using our galaxy merger simulations including the effects of dust to interpret the Great Observatories Origins Deep Survey and DEEP galaxy images from Hubble to measure the galaxy merger rate, for example.

We are also using the infrared data from Spitzer and the X-ray data from Chandra to locate the galaxies where supermassive black holes are forming, and to see whether their galaxy hosts are as predicted [5].

Role of High-End Computing: Direct numerical simulations are an indispensable tool for the theoretical study of the galaxy formation process over the 13.7 billion-year history of the universe. Such computationally intense calculations can only be carried out on massively parallel systems such as Columbia, which have the capacity to provide a large set of dedicated processors with a high bandwidth connection—for handling significant amounts of inter-processor communication.

Future: We are comparing our theoretical predictions regarding shapes of galaxy and dark matter halos [6] with data from Chandra [7], and predictions regarding star formation and supermassive black holes in galaxy mergers with DEEP data [5] (and papers in preparation). Many more simulations will need to be compared to observational data currently being collected to fully develop and test theories regarding the formation of most stars in the universe.

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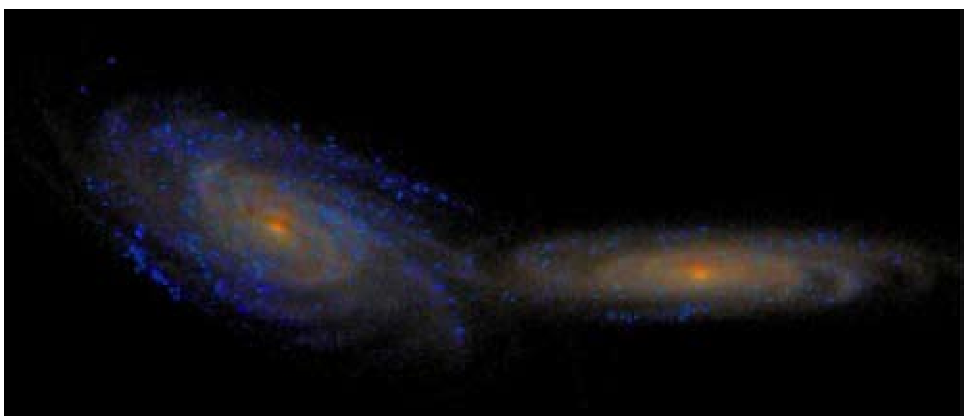

Figure 2: *An early stage of a simulated merger between two spiral galaxies run on the Columbia supercomputer. In this realistic color composite of u-, r-, and z-band images, places where new stars are forming appear blue, and dust lanes are yellow or brown.*

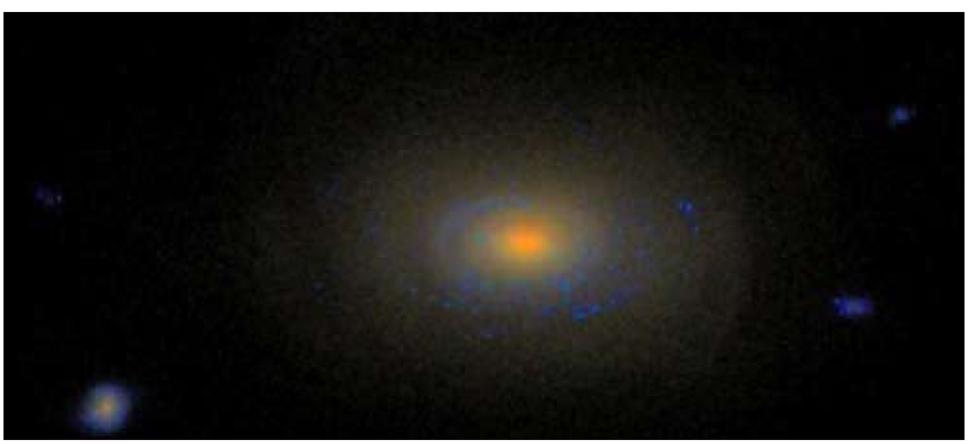

Figure 3: *This is a late stage of the same galaxy merger simulation, showing the formation of an elliptical galaxy.*

IMPACT OF EXTENDED IONOSPHERE ON MAGNETOSPHERIC DYNAMICS

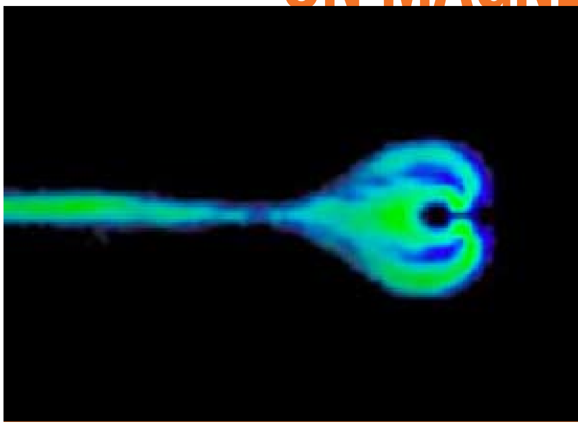

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Figure 1: *A 3 million-particle simulation generated this distribution of auroral wind oxygen ion pressure in the Y=0 orthogonal plane.*

Project Goals and Objectives: Recent observations have established that plasmas of terrestrial origin fill the magnetosphere and inflate it as they attempt to escape. This (Figure 1) is contrary to the classical picture of solar plasmas entering the magnetosphere and producing space storm effects including the ring current, which has the effect of inflating the magnetosphere. In current models, the ionosphere is assumed to be confined by gravity to a thin layer of the upper atmosphere. We use global simulations of the solar wind interaction to 1) produce ionospheric boundary conditions that are used to drive heating and expansion of the ionosphere against gravity, and 2) produce dynamic three-dimensional global electromagnetic fields, within which ionospheric particles' motions are computed to determine their circulation, importance, and impact on the system.

Project Description: The computation of individual ionospheric ion trajectories in three-dimensional electromagnetic (and gravitational) fields is relatively time-intensive, and very large numbers of trajectories are required to achieve adequate statistics for computation of bulk plasma properties (Figure 2). This is exacerbated by the fact that most solar wind particles simply flow past the magnetosphere without entering it. Only a small fraction of order 1% or less of the particles actually enter. For ions of terrestrial origin, the problem is rather that the particles escape and must be continually replenished.

In a computation of this kind, a very large number of particles have been used. To date, our runs have used several times 100 million particles, with many more runs remaining to be done. This particle number is almost an order of magnitude larger than in the largest computations carried out in this field to date, and significantly exceeds the long-term growth rate of magnetospheric simulations, which roughly follows Moore's Law.

Relevance of Work to NASA: This work, supported by the Geospace Science Theme, Heliophysics Division, is an important part of NASA's continuing quest to increase our understanding of the sun, heliosphere, and its interactions with the planets, including the ablation of planetary atmospheres, as well as the development of space weather around the planets, which often involves the battle between planetary sources of plasma and the solar wind plasma.

Computational Approach: We use a massively parallel test particle approach that is readily parallelizable using the cluster approach. We release particles with a Monte Carlo (random selection) approach in both configuration and velocity space, and in time. Our fields evolve dynamically so that particles must be spread in many dimensions, which is why so many are required to get at least 100 particles in every cell (for <10% statistical errors).

Results: We have been able to generate a simulation with a useful spatial (1 Earth radius) and temporal (4-minute) resolution, while still being able to look at the kinetic properties of the particles in each space and time cell, for the entire magnetosphere. A dynamic range of 10^2 per dimension allows sufficiently accurate statistical characterization of the plasmas for evaluation purposes. In some cases, features of interest motivate development of greater resolution (Figure 3), and additional particles can be added to provide this in the future.

Role of High-End Computing: Direct numerical simulations are an indispensable tool for the theoretical study of the solar wind interaction with planets, which forms space weather. Such computationally intense calculations, however, can only be carried out on moderately to massively parallel systems, such as the NASA Center for Computational Sciences' Halem supercomputer, which have the capacity to provide a large set of dedicated processors. At present, we do not have, but are developing, applications with a high-bandwidth requirement—for handling significant amounts of inter-processor communication.

The large number of particles needed to generate accurate, detailed magnetospheric simulations required the large aggregate memory available on Halem and consumed approximately 130,000 processor-hours. This work was a full investigation of less than 10 real-time hours of the magnetosphere.

Future: The amount of data and information content for the final model's extended ionosphere is substantial and will be organized into a "theoretical virtual observatory," allowing queries similar to those applied to the large observational databases. Special parallel algorithms will also be developed to analyze the large databases produced—to track the development history of solar storms and their magnetospheric responses for days and weeks at a time.

Co-Investigators

- Mei-Ching Fok, NASA Goddard Space Flight Center
- Dominique Delcourt, Centre d'Etudes des Environnements Terrestre et Planétaires
- Joel Fedder, LET Corp.
- Steven Slinker, Naval Research Laboratory

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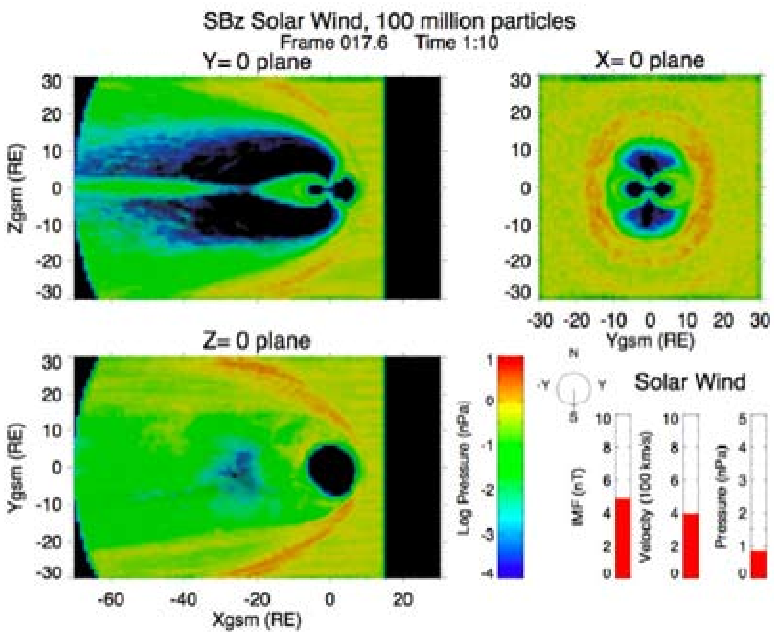

Figure 2: Distribution of solar proton pressure is depicted at specified time in three orthogonal planes at X=0 (upper right), Y=0 (upper left), and Z=0 (lower left). The pressure scale and solar wind properties are indicated at the lower right.

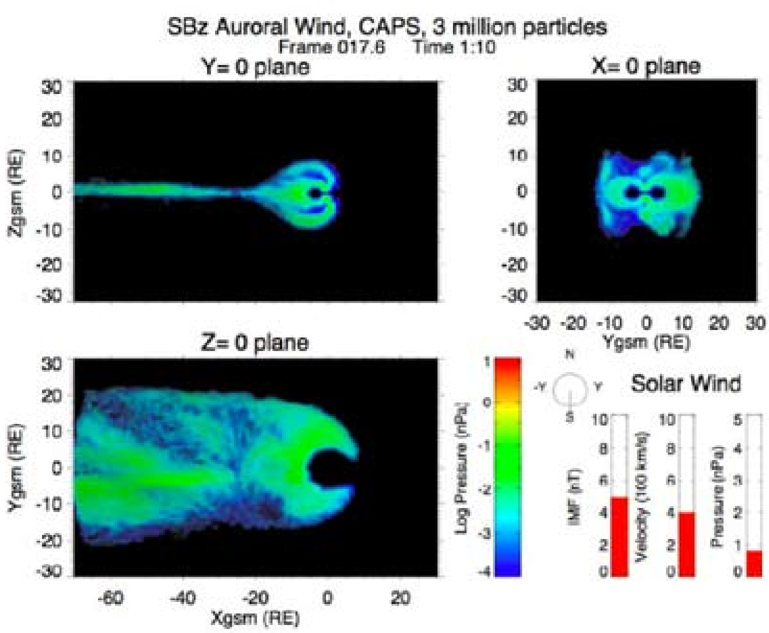

Figure 3: At the specified time during the simulation run, the distribution of auroral wind oxygen ion pressure is depicted in three orthogonal planes at X=0 (upper right), Y=0 (upper left), and Z=0 (lower left). The pressure scale and solar wind properties are indicated at the lower right.

MODELING THE EXPLOSION OF TYPE Ia SUPERNOVAE

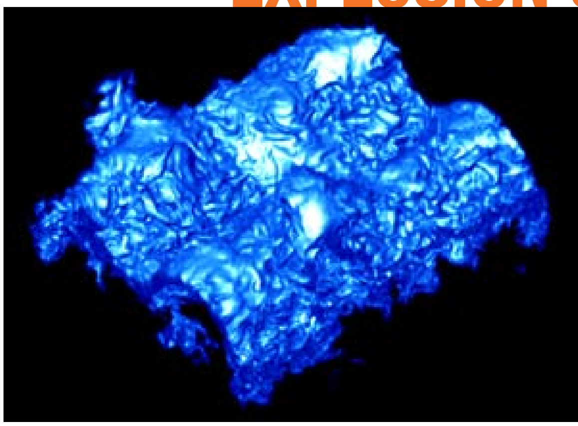

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Figure 1: *Burning (by nuclear fusion) bubble floating in carbon-oxygen fuel with a fuel density of 1.5 x 107 grams per cubic centimeters and a gravitational field about 109 cm/s^2. As the bubble rises, drag with the surrounding fuel causes it to roll up and become a torus. The torus does not split but is surprisingly persistent and stable.*

Project Goals and Objectives: The aim of this work (funded by the Astrophysics Theory Program) is to gain a better, first-principles understanding of how Type Ia supernovae work by studying the way in which burning propagates inside a carbon-oxygen white dwarf exploding as a Type Ia supernova. It is known that the observable properties, especially the light curves of interest to the cosmologists, are very sensitive to how much material burns, and at what temperatures and densities. Yet the flame is also known to be subject to numerous instabilities, as well as the turbulence generated by rising plumes of buoyant ashes. A critical open question is whether the subsonic burning front propagating outward from the center of the white dwarf can, at some point, transition to a detonation (a deflagration-detonation transition). Through resolved simulations of turbulent flames (Figure 2), we seek to answer this question.

Project Description: We employ a unique hydrodynamics algorithm (low Mach number hydrodynamics) to allow for efficient simulation of flames. This code was developed in collaboration with the Center for Computational Science and Engineering at Lawrence Berkeley National Laboratory. These burning fronts are initially very subsonic (Mach < 10^{-3}), placing long-time evolution simulations out of reach of traditional compressible hydrodynamic codes. In the low Mach number formulation, the pressure is decomposed into dynamic and thermodynamic components, the ratio of which is of order Mach number squared. Only the dynamic pressure appears in the momentum equations, filtering sound waves out of the system. Adaptive mesh refinement gives us a further efficiency boost by allowing us to focus resolution on the flame front. We apply this code to small-scale simulations of the thermonuclear flame front in the star, resolving the structure of the flame itself.

Relevance of Work to NASA: Type Ia supernovae—nature's biggest thermonuclear explosions—are both inherently interesting and poorly understood. These supernovae are responsible for many of the isotopes in nature, including two-thirds of the iron group. They are also important to cosmologists as standard candles, and an understanding of the physics underlying their diversity is essential to "precision cosmology." These topics spill over into observational programs by many of NASA's missions, predominately the Hubble Space Telescope, James Webb Space Telescope, and the Joint Dark Energy Mission.

Numerical Approach: The low Mach number equations take the form of partial differential equations describing conservation of mass, momentum, and enthalpy, together with an elliptic constraint on the velocity field. We solve the low Mach number hydrodynamics equations using a second-order accurate approximate projection method. A fractional step procedure is used, including advection, projection, and reaction steps. In the advection step, an unsplit Godunov method is used to advance the state to the new time level, yielding a provisional velocity field that does not yet satisfy the elliptic constraint. The projection step enforces the constraint by solving a Poisson equation via multigrid techniques. Finally, the reactions are coupled via Strang splitting.

Computational Approach: This code has scaled well to 504 processors on the Columbia supercomputer. In addition to the turbulent flame study, which is the focus of the current project, we have modeled the reactive Rayleigh-Taylor instability and flame bubbles in three dimensions.

Results: We produced the first resolved simulation of a reactive Rayleigh-Taylor instability inside a white dwarf and found that the buoyancy-driven turbulence has a Kolmogorov spectrum, which, while anisotropic on larger scales, becomes isotropic as the turbulent energy cascades down to smaller scales. This provides important input for the subgrid models used in large-scale simulations. We also found that the natural geometry taken on by a burning floating bubble in a gravitational field is a surprisingly stable torus (Figure 1).

Though discovered on scales of meters, we expect this result will carry over to full-star calculations on scales of thousands of kilometers.

Role of High-End Computing: This work was enabled through the extensive supercomputing cycles, data storage, and networking resources provided by NASA's High-End Computing Program, in addition to faster processing for reduced time-to-solution and accelerated science and engineering. The Program also provided valuable assistance with graphics, capturing the data generated. The wait time for computer cycles was shorter, and the computations more efficient than on other leadership supercomputers.

Future: A parameter study of turbulent flames is presently underway. By varying the density of the fuel, we sample different regimes where burning dominates over the turbulence and vice versa. This will allow us to build up a picture of the conditions that exist where a deflagration-detonation transition may take place. Full-star models in three dimensions are planned for the longer term—in about 2 years.

Collaborating Organizations

- Department of Energy's Scientific Discovery through Advanced Computing Program

Co-Investigators

- Ann Almgren, John Bell, Marc Day, Charles Rendleman, all of Lawrence Berkeley National Laboratory

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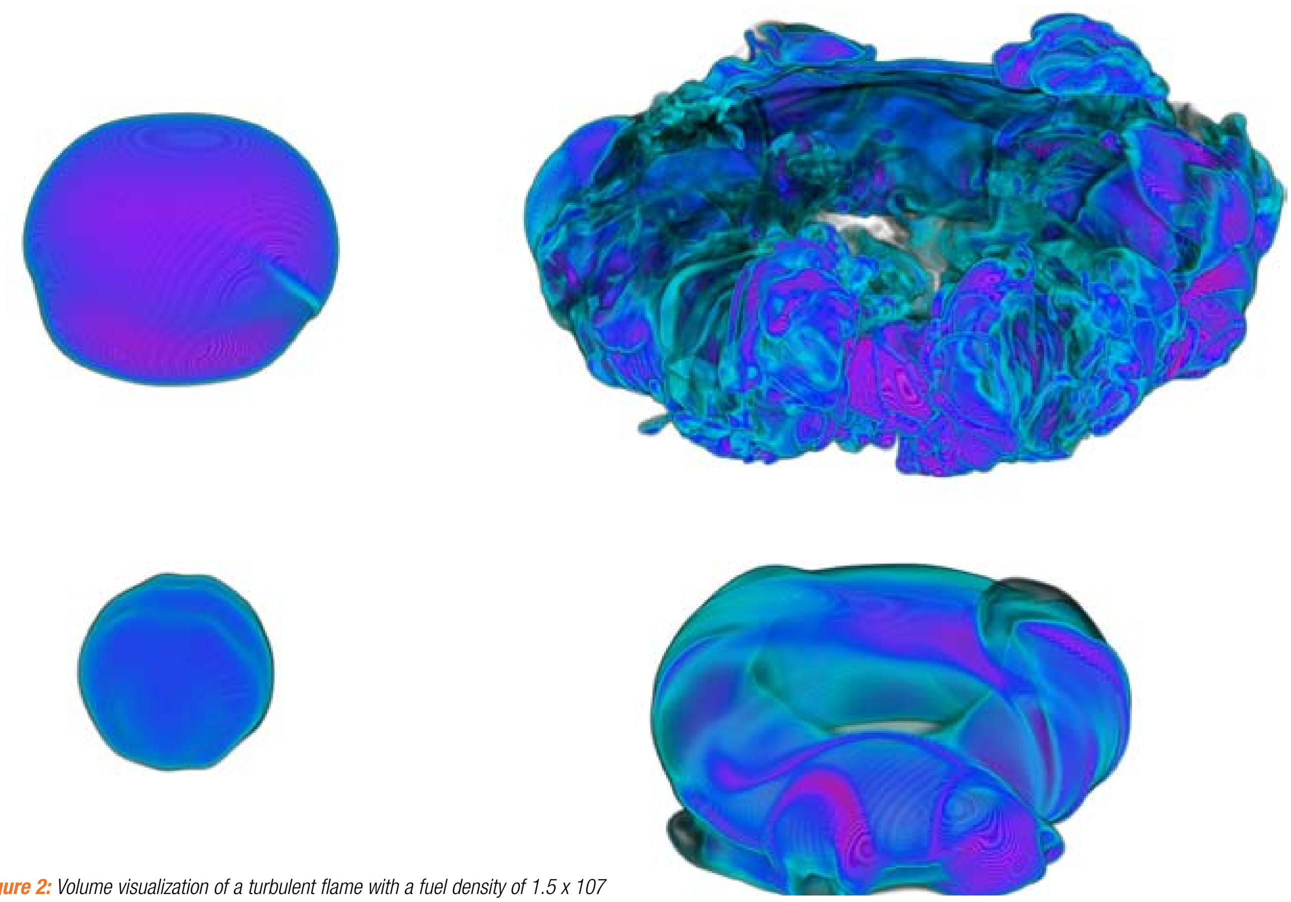

Figure 2: Volume visualization of a turbulent flame with a fuel density of 1.5 x 107 grams per cubic centimeters. The turbulent fuel wrinkles the flame dramatically, increasing its overall burning rate. At this low density, the turbulence dominates over the burning, marking the beginning of the transition to the distributed burning regime.

MODELING GAMMA-RAY BURSTS IN MASSIVE STARS

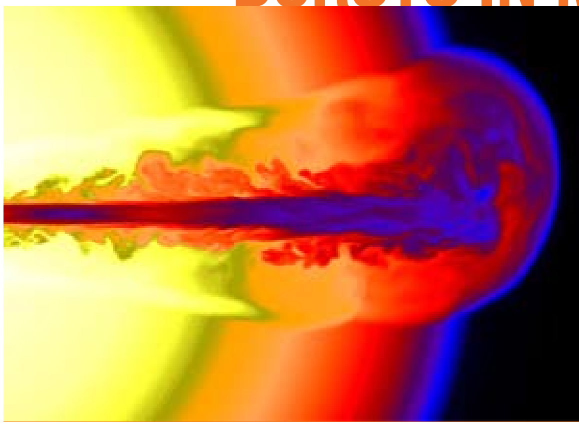

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Figure 1: *Magnetic interactions in and between the disk and the rapidly spinning black hole give rise to jets moving out along the rotational axes. These jets interact with the star and are focused by the interaction. Shocks in the star, plus a broader angle component of the jet, lead to the star's explosion as a supernova accompanied by a gamma-ray burst.*

Project Goals and Objectives: The aim of this work is to: understand how gamma-ray bursts (GRB) work; predict new high-energy transients that might be visible at different angles and at different redshifts; interpret discoveries by NASA missions dedicated to GRB studies—especially the High Energy Transient Explorer (HETE) 2 and Swift; and to develop the necessary relativistic codes and optimize them on massively parallel supercomputers.

Project Description: One-dimensional models of rotating massive stars are evolved including all known mechanisms for angular momentum transport. Collapse of the pre-supernova stars is mapped into two- and three-dimensional special relativistic, adaptive mesh codes. The more massive, more rapidly rotating stars collapse to a black hole and an accretion disk. Accretion is followed, and relativistic jets of various parameterized energies are introduced along the rotational axes. Jet propagation and breakout are followed until the jet enters a homologously coasting, relativistic phase.

Relevance of Work to NASA: This work, funded by the Astrophysics Theory Program, will help optimize the scientific return for HETE and Swift; predict and discover new phenomena; effectively utilize and capitalize on NASA's high-performance computers to gain scientific insight; and plan future high-energy mission strategies, for example, with Gamma-Ray Large Area Space Telescope and Swift follow-on missions.

Numerical Approach: Two codes were employed—each developed for, and optimized on massively parallel computers. One code, RAM, developed by MacFadyen (Princeton, IAS) and Zhang (Stanford, KIPAC), is a relativistic, adaptive mesh Eulerian code. This code implements a characteristic-wise, finite-difference, weighted essentially non-oscillatory (WENO) scheme using the full characteristic decomposition of the special relativistic hydrodynamical equations to achieve fifth-order accuracy in space. For time integration, the method of lines is employed with a third-order total variation diminishing (TVD) Runge-Kutta scheme. The implementation of adaptive mesh refinement and parallelization is based on the University of Chicago's FLASH code. RAM is modular and includes the capability to easily swap hydrodynamics solvers, reconstruction methods, and physics modules. In addition to WENO, a finite-volume module was implemented with the piecewise parabolic method for reconstruction and the modified Marquina approximate Riemann solver to work with TVD Runge-Kutta time integration. This code was used for studies of collapse and initial jet propagation. The second code, special relativistic hydrodynamics (SRHD), is also two- and three-dimensional Eulerian, but not adaptive mesh. In addition, SRHD features an explicit Eulerian Godunov-type shock-capturing method with high resolution, and was used to calculate jet propagation and breakout in massive stars.

Computational Approach: Two-dimensional studies of collapse using the RAM code typically took 10 hours on 86 of the Columbia supercomputer's processors. However, many calculations were necessary to debug the code and start to explore parameter space. Three-dimensional studies are more costly—for example, three-dimensional jet studies with SRHD took about a day each on 128 of Columbia's processors.

Results: We developed the necessary codes to study GRBs and supernovae in massive stars in two and three dimensions, and studied gravitational collapse with a range of angular momentum distributions and masses (Figure 2). We found oscillatory behavior that may affect the GRB light curves, and found complex behavior in jets breaking out from massive stars (Figure 1) that may translate into a variety of high-energy transients seen at various angles. We also found a minimum energy jet necessary to get out of the star before the central engine died. GRBs cannot occur at all energies however—one must have a threshold of power.

Role of High-End Computing: The extensive supercomputing cycles afforded by Columbia, in addition to smaller queues and more stable operation than experienced at other leadership supercomputing centers, were key to the success of this work. Assistance with graphics and a responsive help desk were also important.

Future: Future activities related to this work will include: writing up the work we have completed for the *Astrophysical Journal*; continuing to explore the collapse of model parameter space; calculating several models for the GRB and its accompanying supernova, including the light curve and spectrum of the supernova; exploring parameter space for jet breakout; estimating properties of transients seen at all angles; exploring models that produce a neutron star rather than a black hole; including better treatment of jet formation; and including magnetohydrodynamic processes (in collaboration with Arons at the University of California, Berkeley and Blandford at Stanford University).

Collaborating Organizations

- Department of Energy (Scientific Discovery through Advanced Computing Initiative)
- Scientific Discovery through Advanced Computing Initiative 2, through a collaborative agreement, "The Computational Astrophysics Consortium"
- Princeton Institute for Advanced Study
- New York University

Publications

1. Zhang, W., Woosley, S.E., and MacFadyen, A.I., "Gamma-Ray Bursts: Nature's Brightest Explosions," in SciDAC 2006 PI Meetings, *AIP Cong Proc*., 10 pages in press.
2. Woosley, S.E. and Heger, A., "The Supernova Gamma-Ray Burst Connection," 2006, in *Gamma-Ray Bursts in the Swift Era*, ed. Holt, S., Gehrels, N., and Nousek, J., AIP Conf Series, 838, 398–407.
3. Woosley, S.E., "The Supernova Gamma-Ray Burst Connection," 2006, BAAS, 207, 168.01, (Rossi Prize talk).
4. Woosley, S.E. and Bloom, J., Some images in: "The Supernova-Gamma-Ray Burst Connection," *Ann. Rev. Astron. Ap.,* 2006.
5. Zhang, W. and MacFadyen, A., "RAM: A Relativistic Adaptive Mesh Refinement Hydrodynamics Code," 2006, *Astrophysical Journal Supplement Series*, 164, 255–279.

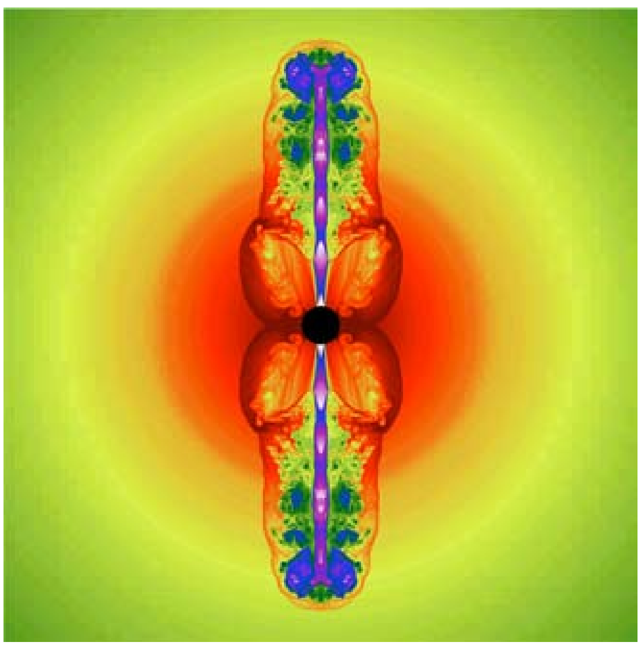

Figure 2: The collapse of a rotating massive star (14 solar masses) of helium and heavy elements creates a black hole surrounded by a swirling accretion disk. Several tenths of a solar mass enter the hole each second. Here, color represents log density at a time 20 seconds after the initial collapse, and the highest density in the equatorial plane near the black hole is 9 x 10^8 g/cm^3. The figure is 1,800 kilometers (km) across, and the inner boundary is at 13 km. A black hole of 4.4 solar masses has formed, and has been accreting for the last 15 seconds.

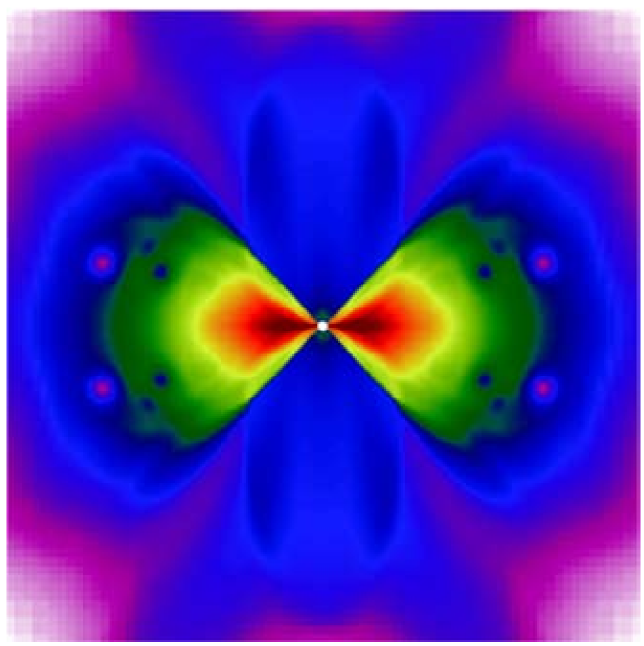

Figure 3: The jet erupts from the surface of the star about 9 seconds later. A classical gamma-ray burst results from a hyper-relativistic jet (Gamma about 200) blasted out of a massive star. Such a burst might be visible to an observer sitting inside about a 5-degree opening angle of the blue core of the jet here, but a variety of lower energy transients would be produced at larger angles by the ejecta running into circumstellar material.

SALINITY ANOMALY PATHWAYS IN THE PACIFIC OCEAN

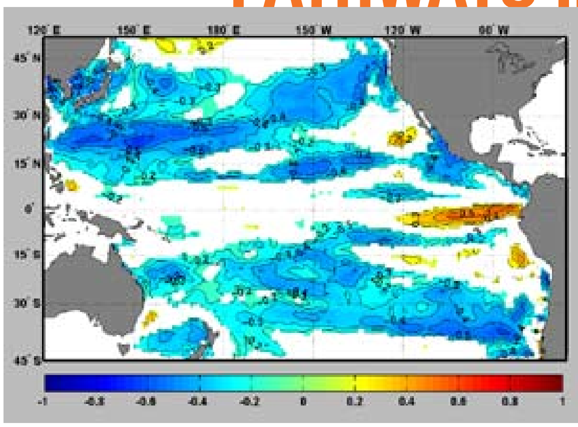

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Figure 1: *The correlation between the change in local salinity with the local rate of fresh water exchange with the atmosphere. Only correlations significantly above the 95% confidence limit are colored. Notice the high positive correlations in the eastern equatorial Pacific where El Niño effects are normally of largest magnitude. Along the rest of the equator, the correlations are deemed not significant. Away from this area, negative correlations dominate, indicating an inverse relationship, such as more rain produces saltier surface water. Clearly, other processes must be understood for salinity anomaly generation in these areas.*

Project Goals and Objectives: Oceanic salinity variations normally are either ignored or thought to be of secondary importance in the generation of short-term climate shifts such as El Niño. Part of the reluctance to investigate the salinity's role comes from a lack of any observational data. Coarser-scale ocean model runs have indicated that salinity may play an important role in the modulation in strength and frequency of events such as El Niño. The goal of this project is to run state-of-the-art, finer-resolution ocean models to determine more accurately the role of a variable salinity field on the dominant modes of variability in the Pacific Ocean.

Project Description: A potential mechanism effecting a modulation of the Pacific El Niño/La Niña cycle is a change in the central and western equatorial Pacific stratification due to high-salinity water that is propagated from the subtropics. High-salinity water is advected in shallow circulation cells both from north and south of the equator. Modeling and understanding the observed variability will not only help with the interpretation of salinity data to be obtained by NASA's Aquarius Mission (scheduled for launch in July 2009), but it will also contribute directly to helping meet the Aquarius Mission objective of inferring fresh water exchanges between the ocean and atmosphere from the salinity observations taken. Realistic modeling of relevant processes that includes the resolution of finer-scale instability waves on the Pacific Ocean equator requires a grid with at least eight times finer resolution than has been previously used for salinity variability studies of this kind.

Relevance of Work to NASA: The El Niño-Southern Oscillation (ENSO) cycle is the most important short-term climate change that can be observed during the expected life of a single satellite platform. This work builds on previous NASA efforts to create a modeling/assimilation/forecast system for ENSO events, and will help to understand how internal ocean variability affects the strength and frequency of these phenomena that have impacts on global weather and economic and social impacts.

Computational Approach: The Geophysical Fluid Dynamics Laboratory's Modular Ocean Model (MOM) was adapted to the local parallel computing architecture, as no version of the code existed for this architecture. In MOM, the Navier-Stokes equations of motion are discretized on a spherical grid for the Pacific Ocean basin using standard centered techniques, and upper layer boundary processes are computed based on the values of the local gradient Richardson number. The fast-moving external modes are split from the slower-moving internal modes for the computational efficiency of larger time-steps.

Results: One of the critical tasks of this project (supported by the Physical Oceanography Program, Earth Science Division) was to produce a model solution that is not only realistic compared to available observations, but also in balance with the surface forcing from exchanges of momentum and buoyancy with the atmosphere. The Pacific Basin spans 1/3 of the globe at the equator, and the spin-up time for such a large basin is many decades. Using the allotted resources, a spun-up, base integration for a 1/2-degree and a 1/4-degree horizontally resolved basin was obtained.

The scientific production runs are an additional 40 years of model time integration using forcing that is derived from the National Oceanic and Atmospheric Administration's National Centers for Environmental Prediction atmospheric analyses. This forcing produced an accurate representation of the observed modes of variability, including the very strong El Niños of 1982 and 1997, and the La Niña of 1988. Longer-time scale variability, such as the nearly 4-year warming in the equatorial Pacific during the early 1990s, is also apparent in the integrations. The results thus far have clearly indicated the dominant role of fresh water exchange (predominantly precipitation) in the eastern equatorial Pacific for salinity anomaly generation (Figure 1). The remainder of the equator yielded no significant correlation between salinity anomaly generation and fresh water exchange with the atmosphere. Away from the equator, advection plays a more significant role generating anomalies than local fresh water exchange with the atmosphere (Figure 2).

Role of High-End Computing: Because of the lack of direct salinity observations, numerical simulations provide the only plausible means for understanding the mechanisms responsible for salinity anomaly generation and propagation. The Aquarius Mission will provide global salinity observations at the surface once a month, but understanding the full three-dimensional structure of that variability, and how important surface mixing processes that occur on time scales much faster than a month affect that variability, will require models and assimilation of available data for analyses.

The wealth of higher-frequency and finer-scale phenomena apparent in a basin as large as the Pacific Ocean requires computational capabilities made available through the NASA Center for Computational Sciences and NASA Advanced Supercomputing Division. The spin-up run for the 1⁄4-degree integration alone required in excess of 150,000 processor-hours.

Future: The amount of output from the computer model from the spin-up and the production runs is substantial. Further production runs that will highlight the benefits of including satellite-derived surface forcing will also be performed. Data analysis packages to expose the relevant processes that are determining any changes in salinity anomaly production have been and continue to be developed. Resources permitting, we hope to perform several production runs highlighting the effects of various scales of temporal forcing on salinity anomaly generation.

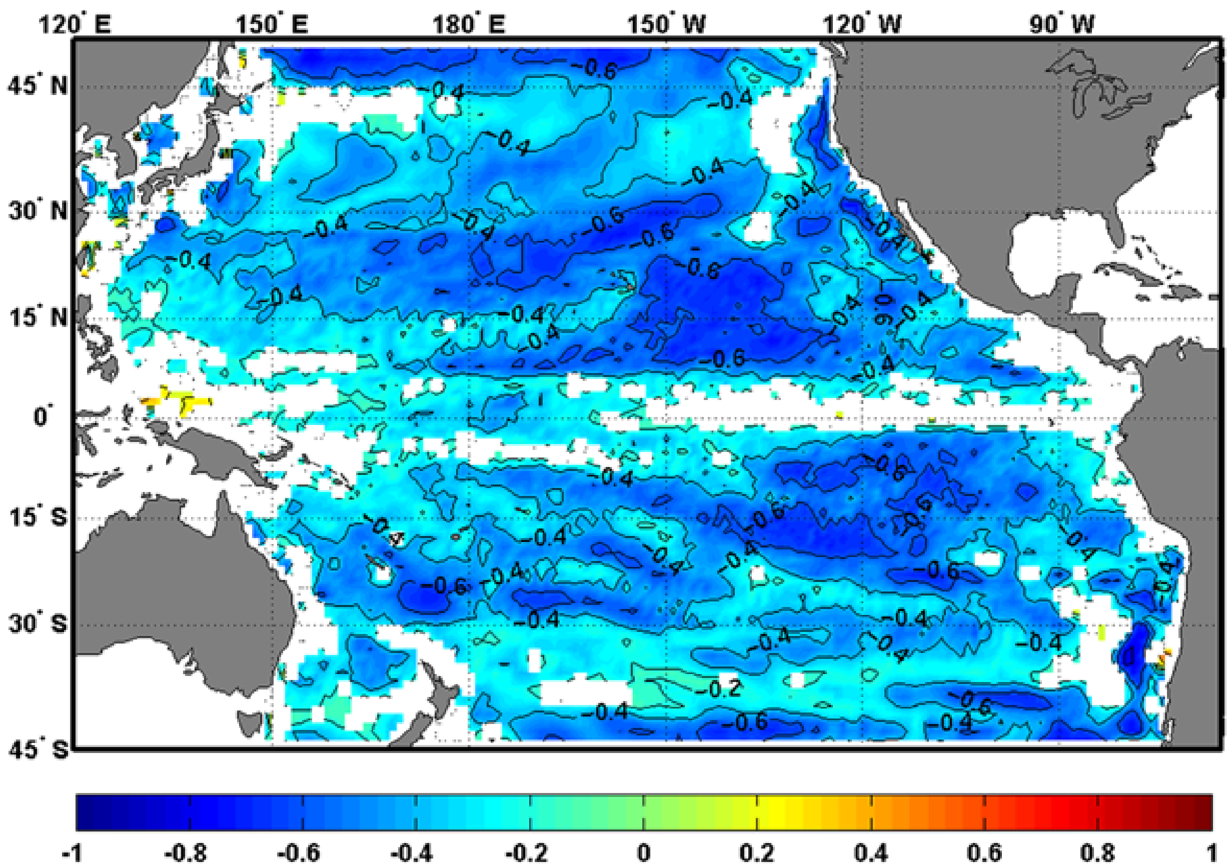

Figure 2: The correlation between the change in local salinity with salinity changes due to advective processes. Only correlations significantly above the 95% confidence limit are colored, and because of a sign convention, negative correlations indicate a direct relationship between salinity change and advection. The largest-magnitude correlations occur in the sub-tropics in the eastern and central Pacific. These areas lie along the path that the model indicates that salinity anomalies generated in the east take on their way to the subsurface equatorial waters in the western basin.

SEASONAL-TO-INTERANNUAL CLIMATE PREDICTION

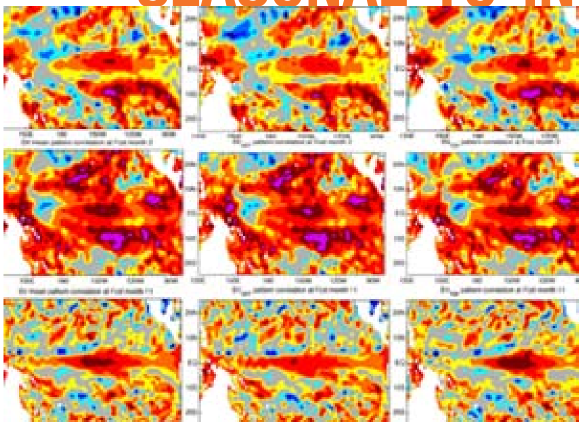

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Figure 1: *Close-up of sea-surface temperature anomaly correlation for monthly-mean July forecasts starting in different months and using different ensembles.*

Project Goals and Objectives: The goals of this project are to address many of the important problems of prediction, but with a focus on short-term climate variations: initialization (particularly the use of satellite data to initialize the ocean and land surface states), model forecast bias, characterization of uncertainty in predictions, and identification of the inherent predictability in the system.

Project Description: The longer time-scales in the ocean and land surface are the key sources of memory in the climate system, and provide the potential skill in predicting short-term climate variability. This project focuses on improving our coupled ocean-atmosphere-land-surface climate model and the assimilation methods used to estimate the state of the ocean as part of model initialization.

The current Global Modeling and Assimilation Office (GMAO) experimental forecast system—Coupled General Circulation Model, Version 1 (CGCMv1)—is exercised on a near-real-time basis as a continual check of system performance, and to investigate changes in predictability in the evolving background climate. The next planned coupled system—the Goddard Earth Observation System, Version 5 (GEOS-5) CGCM with updated components for the atmosphere, ocean, land surface, and sea-ice—is being integrated and tested.

Relevance of Work to NASA: Supported by NASA's Modeling, Analysis, and Prediction (MAP) Program, Earth Science Division, this work contributes to climate modeling for the MAP Program, and is one of NASA's contributions to the U.S. Climate Change Science Program. It helps enhance the utility of satellite observations for climate research and climate prediction applications, modeling and design, climate and weather prediction, and chemistry-climate interactions.

Computational Approach: The component models of the CGCM and the ocean analysis are finite-difference grid-point codes written in Fortran-90. For the GEOS-5 CGCM, the superstructure of the Earth System Modeling Framework (ESMF) is used to couple the components and integrate the ocean assimilation system. Parallelization is primarily Message Passing Interface.

Results: Using the NASA Center for Computational Science's Halem supercomputer, we have run ensembles of forecasts with the CGCMv1. These forecasts have been initialized with a univariate ocean assimilation system that assimilates temperature and salinity profile data. This system has comparable performance with other single-model operational systems. As an example, the model was one of the few to predict the cooling of the eastern Pacific sea-surface temperature (SST) in late 2005, and the subsequent warming in early 2006 (Figure 2). However, the model was not consistent in the forecasts initialized in late summer 2005.

To address issues with initialization of the coupled system and adequacy of the forecast ensemble spread, bred vectors (BV) have been implemented in CGCMv1. BV are designed to capture the dominant growing errors in the coupled system, and are applied as initial ensemble perturbations. From our investigations, BV in CGCMv1 are clearly related to forecast errors for both SST and equatorial subsurface temperature, particularly when the BV growth rate is large. Whereas the BV are not able to correct the false positive forecasts of SST anomaly that may be related to lack of predictability in the system, the overall statistics show an improvement in SST anomaly correlation at large forecast lags (Figures 1, 3).

To assimilate the surface data from satellite altimetry, we have developed an Ensemble Kalman Filter (EnKF) with online bias correction to compensate for differences between model and data means in sea-surface height. The EnKF also introduces a multivariate assimilation scheme that improves upon the univariate methods used in our production system. With the availability of the Columbia supercomputer, we were able to run the EnKF with an ensemble of up to 48 models totaling more than 1.4 billion state variables. We were able to run many simulations with 9, 17, and 33 ensemble members. These simulations allowed us to investigate the effect on assimilation performance of (1) the ensemble size, (2) the effect of using a time-dependent background error covariance model (as provided by the EnKF), and (3) the inclusion of remotely sensed sea-surface height observations, in addition to the traditionally used in situ temperature profile data.

Initial GEOS-5 CGCM tests have helped improve the updated ocean model, Poseidon V5. Short simulations have been conducted, and the ocean assimilation system has also undergone initial tests under the GEOS-5 infrastructure.

Role of High-End Computing: Climate prediction is a computationally intensive activity. The computational cost comes from a) the need to conduct ensembles of hindcasts over as long a period as feasible to assess statistical reliability of the forecasts and to remove climate drift, and b) the need for ensembles to assess uncertainty and predictability of the forecasts. We also use ensemble techniques to estimate the flow-dependent multivariate covariances for ocean data assimilation. Here too, the larger the ensemble size that can be simulated, the better the statistics are captured. As for any modeling and assimilation activity, tuning is required for the free parameters in the system to optimize the scientific performance. These sorts of experiments, both numerous and computationally intense, can only be carried out on massively parallel systems.

Future: The experimentation required to improve the models and initialization of the coupled system will continue. There are clear societal benefits to be gained by improved climate prediction. Improvements to GEOS-5 for seasonal-to-interannual climate prediction will focus on generating ocean state estimates.

Co-Investigators

- Siegfried Schubert, David Adamec, Christian Keppenne, Shu-Chih Yang, all of NASA Goddard Space Flight Center

Publications

1. Sun, C., Rienecker, M.M., Rosati, A., Harrison, M., Wittenberg, A., Keppenne, C.L., Jacob, J.P., and Kovach, R.M., "Comparison and Sensitivity of ODASI Ocean Analyses in the Tropical Pacific," *Mon. Wea. Rev.* (in press).
2. Yang, S.-C., Kalnay, E., Cai, M., and Rienecker, M., "Bred Vectors and Forecast Errors in the NASA Coupled General Circulation Model" (draft).

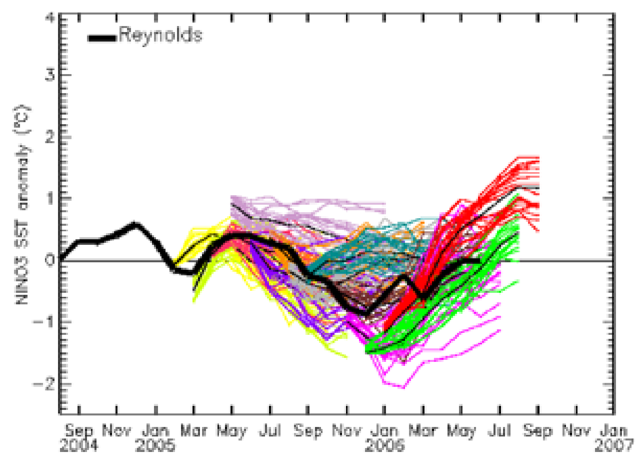

Figure 2: Forecast sea-surface temperature (SST) anomaly in the Niño-3 region (90-150°W, 5°S-5°N) from ensembles of the Global Modeling and Assimilation Office's Coupled General Circulation Model, Version 1. Different colors are used for different initialization months, with 19 ensemble members for each month. Forecasts are of 12-month duration. Anomalies are calculated relative to the appropriate forecast climatology from 1993–2005. The observed SST anomaly is superposed.

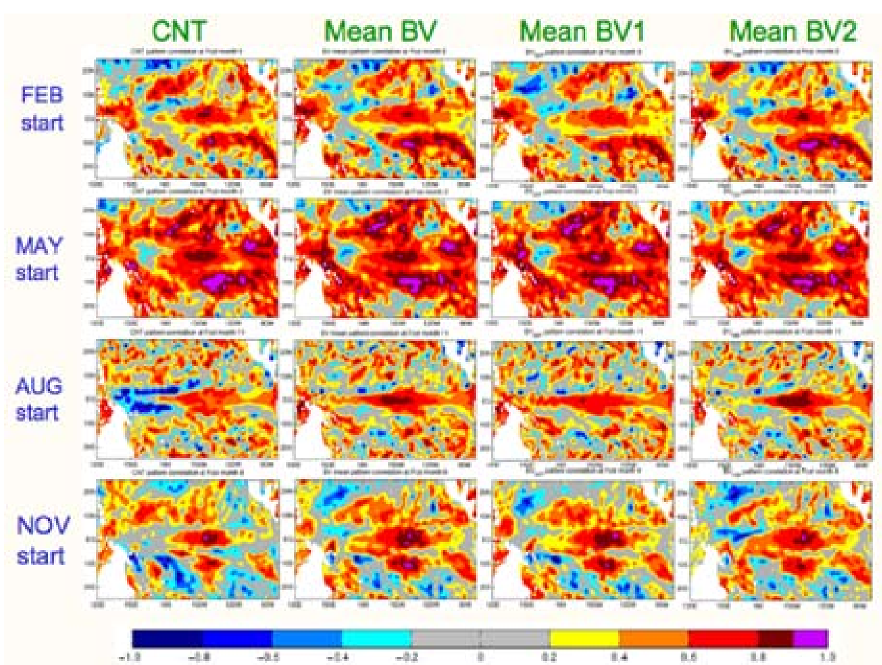

Figure 3: Sea-surface temperature (SST) anomaly correlation for monthly-mean July forecasts, with each row showing forecasts started from different initial months. The August start is the forecast with the longest lead for July forecasts. Each column shows the ensemble mean from different ensembles. The first column is the production forecast system. The second column shows a four-member ensemble mean, with ensemble perturbations from +/- the bred vectors using the SST rescaling norm (third column) and the D20 rescaling norm (fourth column).

SIMULATIONS OF THE SUN'S SURFACE

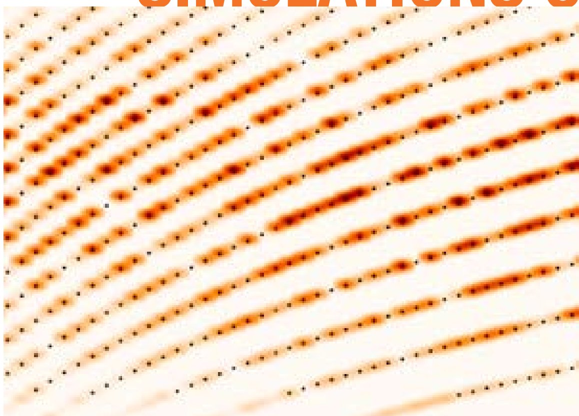

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Figure 1: *Close-up of solar acoustic waves seen in Figure 3.*

Project Goals and Objectives: The objective of this research, funded by the Living With a Star Program, is to improve our understanding of the interior structure and dynamics of the sun and other stars through improvement in numerical simulations of the complex multi-physics phenomena present. Specifically, we want to improve the quantitative soundness of helioseismic methods—our only direct observational probe into stellar interiors—by providing tests of the helioseismic inversion process using simulated data.

Project Description: Data is created as a collaboration of two distinct simulation efforts: (1) numerical solution of the acoustic propagation equations in the full solar body, and (2) calculation of the sound sources, which exist in the outer convective layers of the sun, and which drive the waves simulated in (1).

Relevance of Work to NASA: Having a clear understanding of the sun and other stars, including their evolution and dynamics, and their influence on the surrounding space and planets, is an important part of the Science Mission Directorate's charter to establish an understanding of Earth and other planets and their evolution.

Numerical Approach: The simulations of acoustic propagation, (1) above, require that the full solar sphere be simulated with methods that propagate linear waves with high accuracy and full coverage of the frequencies and wavelengths of interest. To accomplish these requirements, spherical harmonics are used in the angular directions, and B-splines are used in the radial direction.

Computational Approach: These two simulation efforts deal with different equations and require distinct numerical approaches; however, both demand Columbia supercomputer-class hardware capabilities, and achieve a high level of parallel scalability to 500 processors—the largest number on which they have been tested to date. We have every reason to believe the scalability will continue for larger numbers of processors. The convective simulation code in particular has been carefully engineered to minimize inter-processor communication as much as possible, given the requirements of physical dependence of the variables involved. The acoustics code uses the parallel structure of a legacy code, Anelastic Spherical Harmonic, which we ported to Columbia, resulting in excellent parallel performance.

Results: A hierarchical sequence of length scales is found—the scale increasing with depth. It is possible, though not yet proven, that these multi-scale structures cause the observed granule, meso-granule, super-granule hierarchy observed at the surface (see Figure 2). The solar acoustic excitation spectrum of spherical harmonic degree versus frequency is very accurately reproduced by the acoustic propagation code (see Figure 3).

Role of High-End Computing: The NASA Advanced Supercomputing facility at NASA Ames Research Center provided extensive supercomputing cycles on Columbia and the data storage needed to carry out this work.

Future: Much remains to be done—study of the effects of magnetic fields on the sound sources is just beginning. This is a crucially important phenomenon since it is in the active regions of the sun that magnetic effects are most important, and it is these regions that control space weather throughout the solar system. Local helioseismic imaging of sunspots is a new, critical component of the study of active regions, and simulations of the sources of sound in these regions, as well as their propagation through them, can significantly improve the accuracy and precision of the interpretation of the helioseismic observations. Further study of the size hierarchy in the outer 40 megameters should shed light on the long-standing question of the source of the surface structures. These structures are significantly modified in the vicinity of active regions, probably indicating that the subsurface structures are also different. The details of these differences will aid in our understanding of the production and evolution of active solar regions and the resulting space weather events.

Co-Investigators

- Thomas Hartlep, NASA Ames Research Center
- Alexander Kosovichev, Stanford University
- Thomas Duvall, NASA Goddard Space Flight Center
- Mark Miesch, University Corporation for Atmospheric Research

Collaborating Organizations

- Stanford University/Ames Center for Turbulence Research
- Stanford University/HEPL

Publications

1. Hartlep, T. and Mansour, N.N., "Acoustic Wave Propagation in the Sun," Center for Turbulence Research Annual Research Briefs, 2005.

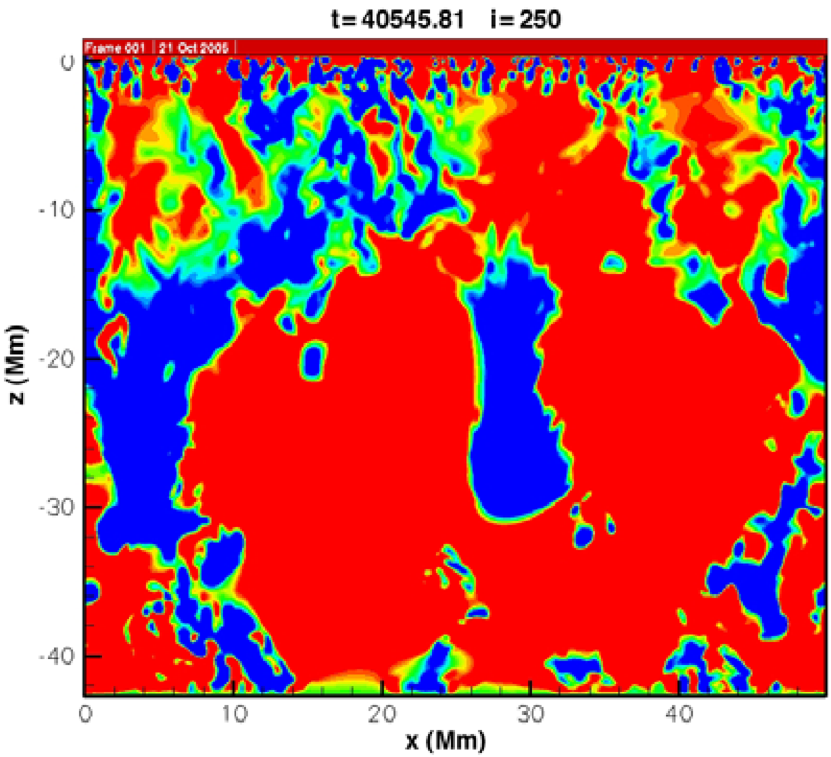

Figure 2: The vertical velocity in a slice of a three-dimensional simulation of the outer 42 megameters of the sun. The warm colors depict upward motion, while cool colors represent downward motion. To present more detail, all velocities higher than 50,000 cm/sec are shown blue, and those lower than -50,000 cm/sec are red.

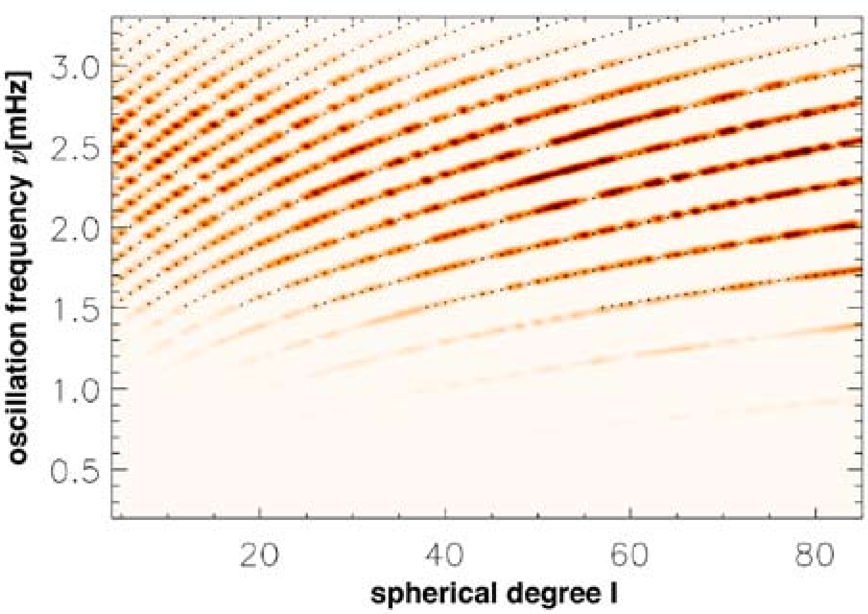

Figure 3: Power spectrum of solar acoustic waves as functions of spherical degree, l and frequency. The shades of color correspond to intensity: bright coloring represents low intensity, while the darker coloring denotes higher intensity. For comparison, black dots indicate oscillation frequencies obtained from solar observations.

SUBSEASONAL CLIMATE PREDICTION

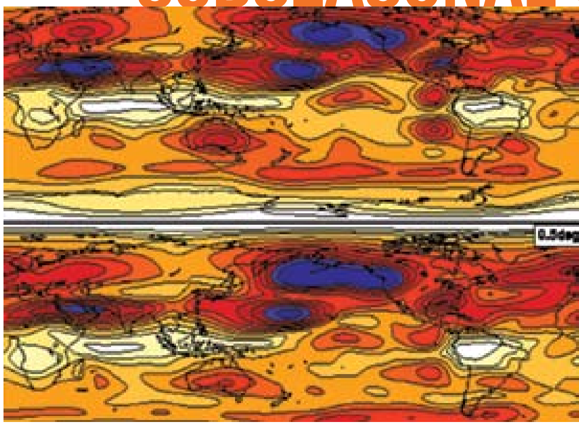

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***Figure 1:** Close-up of changes in variability associated with the 1999 La Niña event.*

Project Goals and Objectives: The proposed work seeks to take advantage of new global datasets (for example, precipitation, clouds, tropical heating estimates) and the next generation of comprehensive Earth system models and data assimilation capabilities developed in the Global Modeling and Assimilation Office (GMAO) to assess and advance subseasonal prediction capabilities. Our emphasis is on extracting the potential skill associated with tropical diabatic heating and land surface processes, and to assess the extent to which high-resolution versions of our climate model are able to simulate selected recent climate extremes.

Project Description: It is now well known that the climate prediction problem is probabilistic in nature. As such, the reliability of predictions must be understood and measured in probabilistic terms. Large ensembles of simulations and forecasts are thus necessary to provide estimates of uncertainty and information about how the tails of the probability density functions (the extreme events) change as a response to large-scale climate forcing. Our basic approach is to focus on the prediction of selected high-impact climate events (e.g., major storms, floods, droughts) since these provide an important test of our models and initial conditions (observations) and tend to have substantial economic and social consequences.

Relevance of Work to NASA: This work, primarily supported by the Modeling, Analysis, and Prediction Program, Earth Science Division, contributes to NASA's science mission to develop Earth system models and data assimilation capabilities aimed at improving climate and weather predictions. Subseasonal time scales (approximately 2 weeks to 2 months) are a critical component of the climate spectrum, linking weather and longer-term climate variability.

Computational Approach: The simulations were done with the GMAO atmospheric-land general circulation model (AGCM) run at various resolutions ranging from 2- to 1/2-degree horizontal resolution. The ensemble experiments were run in parallel to the extent possible given the machine load. On the Columbia supercomputer and at 1/2-degree resolution, the AGCM requires 6 hours to run 1/2 month of simulated time on 120 processors. The code uses distributed parallelism (MPI) and requires 256 megabytes of memory per processor.

Results: We show two results illustrating 1) the use of very large ensembles run at a relatively coarse model resolution and 2) high-resolution model runs with more modest ensemble size. Figure 1 shows a close-up of 1999 La Niña variability. The former looks at the impact of the El Niño-Southern Oscillation (ENSO) on weather, while the latter focuses on the simulation of the 2003 European heat wave.

Figure 2 compares the changes in variability associated with the 1997 (neutral), 1998 (El Niño), and 1999 (La Niña) winters at different AGCM resolutions (2-, 1-, and 1/2-degree). In each case, the AGCM is forced with observed sea-surface temperatures (SSTs). The last figure in each column is from observations (National Centers for Environmental Prediction reanalysis). The results show that all three resolutions produce similar changes in subseasonal and synoptic variability—changes that are consistent with the observations. This gives us confidence that we can use the coarse resolution runs as a basis for studying these changes, taking advantage of our ability to run very large ensembles at 2-degree resolution. As an example, we carried out an empirical orthogonal function (EOF) analysis of 324 January-February-March coarse resolution hindcasts. The results indicate a clear impact of ENSO on the variability associated with some of the EOFs. For example, EOF 8—a winter storm that impacts Southern California and northwestern Mexico—shows enhanced (reduced) variability during El Niño (La Niña), while EOF 9—a storm that affects the Pacific Northwest—shows enhanced (reduced) variability during La Niña (El Niño).

We also examined the impact of SSTs, soil moisture, and model resolution on simulations of the 2003 European heat wave. This extreme event is yet to be successfully simulated by any model. We analyzed the monthly mean surface air temperature over Europe from 1990 through 2003, comparing observations and the model at various resolutions. While the model runs show a general tendency for warmer values during 2003, and some are as large as the observed values, none of the larger simulated values are maintained throughout the summer as observed. Figure 3 shows the mean surface temperature from a 9-ensemble simulation compared to observations. Individual ensemble members (not shown) highlight the considerable variability in the results due to internal atmospheric variability. While some ensemble members also show very warm conditions, the model tends to put the warmest temperatures too far to the east.

Role of High-End Computing: The combined requirements of high model resolution and large ensembles make regional climate prediction a computationally challenging problem. In fact, we would argue that progress on this problem is fundamentally limited by the available computing resources at the world's major climate research institutions. Most climate predictions are necessarily carried out at relatively coarse resolution and with a very modest number of ensemble members—inadequate for making anything more than gross inferences about changes in the mean and variance of the largest scales. With the NASA Center for Computational Sciences and NASA Advanced Supercomputing facility computing environments, we are now beginning to be able to address the connections between weather and climate.

Future: We are continuing our work with large-ensemble, high-resolution AGCM simulations of selected recent climate extremes with the new GEOS-5 AGCM. Specifically, we will re-examine the linkages between extreme winter storms and global-scale climate variability during the 1997–99 ENSO and examine the impact (and predictability) of the Madden Julian Oscillation in producing enhanced U.S. west coast storminess during the winter of 2004–05.

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- Yehui Chang, Goddard Earth Sciences and Technology Center
- Philip Pegion, Science Applications International Corp.
- Randal Koster, NASA Goddard Space Flight Center

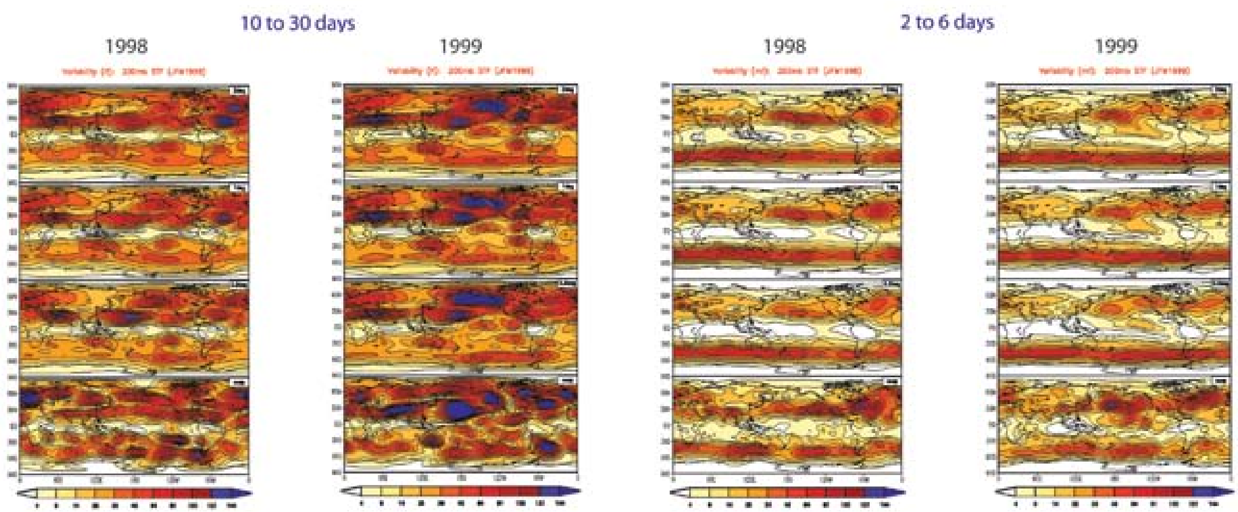

Figure 2: A comparison of the changes in variability associated with the 1998 (El Niño) and 1999 (La Niña) events at 2-, 1-, and 1/2-degree model resolutions. The last figure in each column is from observations (National Centers for Environmental Prediction [NCEP] reanalysis). All three resolutions show a marked increase in subseasonal (10- to 30-day) variability in the North Pacific during the La Niña year, similar to the observed change. The synoptic variability (2 to 6 days) shows the well-known southward (northward) shift in the Pacific storm track during El Niño (La Niña) years. The highest resolution shows, surprisingly, the weakest synoptic variability in the Northern Hemisphere.

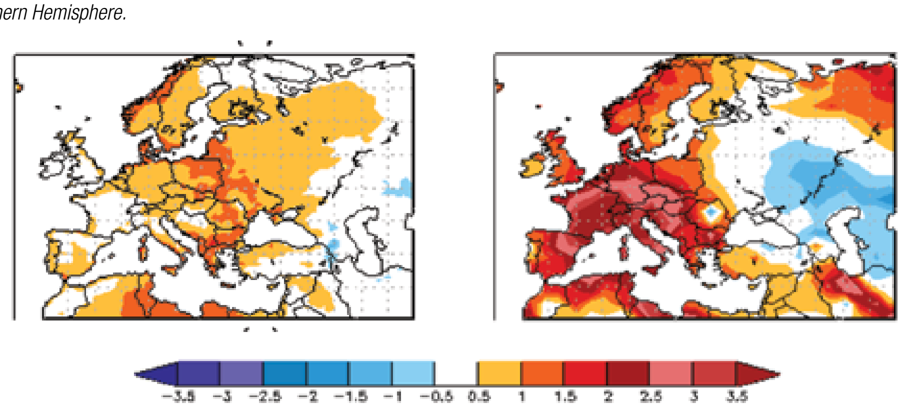

Figure 3: The 2003 June-July-August mean surface air temperature over Europe from the mean of 9 ensemble members run at 1/2-degree (left) and from observations collected by Climate Prediction Center Merged Analysis of Precipitation, at the National Centers for Environmental Prediction (right).

UNDERSTANDING SOLAR WIND-MAGNETOSPHERE-IONOSPHERE COUPLING

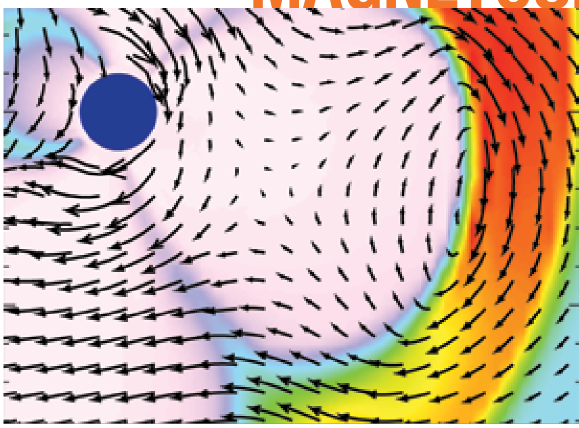

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Figure 1: *Close-up of the dayside magnetosphere for weakly driven conditions. Color-coded plasma density and vectors indicate magnetic field perturbations.*

Project Goals and Objectives: The polar cap potential (PCP) is a key quantity for understanding the nature of solar wind-magnetosphere-ionosphere (SMI) coupling. The accuracy of PCP predictions reflects to some degree our understanding of the SMI system. While there has been reasonable success at predicting the PCP for low to moderate solar activity levels, much less is known about SMI coupling during high activity intervals. Unresolved questions about the SMI system during strongly driven events provide critical challenges to our basic understanding of SMI coupling and space weather forecasting. This project addresses these questions through a combined data analysis and global magnetohydrodynamics (MHD) modeling investigation.

Project Description: Using a global MHD model, we simulated the coupled magnetosphere-ionosphere system for a large range of external driving conditions. From this set of simulations, the sequence and timing of key events in the evolution of the strongly driven magnetosphere were identified and characterized. Features identified in the simulations were compared to observations from NASA's currently operating space flight missions. The results of this combined simulation/data analysis are being used to discriminate between competing theories and models of magnetosphere-ionosphere coupling and predictions of the PCP.

Relevance of Work to NASA: The objective of this work, supported by the Geospace Science Program (GSP), specifically addresses GSP Goal II SEC 1.c to identify and understand the response of the magnetosphere and ionosphere to external and internal drivers. The PCP is a key parameter in specifying the nature of SMI coupling and is critical for space weather applications.

Computational Approach: We use a global MHD model based on standard MHD equations for ionospheric and magnetospheric plasma augmented with hydrodynamic equations for a collisionally coupled neutral thermosphere. The Integrated Space Weather Prediction Model (ISM) operates within a three-dimensional computational domain that extends continuously from the bottom of the ionosphere (taken to be ~80 km) extending upward through the magnetosphere and into the solar wind. The ISM code has been developed for operation on massively parallel computers. ISM is sponsored by the Defense Threat Reduction Agency.

Results: A large number of simulations of the coupled magnetosphere-ionosphere system have explored the range of responses of the system to changing external and internal drivers. A new picture of the magnetosphere during extreme conditions is emerging, which contrasts significantly with the more familiar and better understood magnetosphere during low to moderate activity levels. Key features in the configuration and dynamics of the strongly driven magnetosphere have been identified and favorably compared with in situ satellite observations, which improved understanding of the underlying physics and increased scientific returns from NASA's currently operating space flight missions. Figures 1 and 2 illustrate some of these differences observed in the perturbation fields and shape of the simulated dayside magnetosphere for weakly versus strongly driven conditions.

Role of High-End Computing: Numerical models of the magnetosphere-ionosphere system are a valuable tool for exploring the physics of this highly complex coupled system. Because of the large computational volume that has to be considered and the high-resolution grids that are necessary, such computationally intensive calculations can only be carried out efficiently on massively parallel systems. The computational speed afforded by parallel processing greatly expands the range of practical calculations that can be accomplished.

Future: As a result of this investigation, we will have a better overall understanding of SMI coupling and the physics of the magnetosphere during extreme conditions. This will lead to improved space weather forecasting and mission planning capabilities.

Co-Investigators

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- Nelson Maynard, University of New Hampshire
- William Burke, Air Force Research Laboratory/Hanscom Air Force Base
- Gordon Wilson, University of Alabama in Huntsville
- Daniel Weimer, Solana Scientific, Inc.

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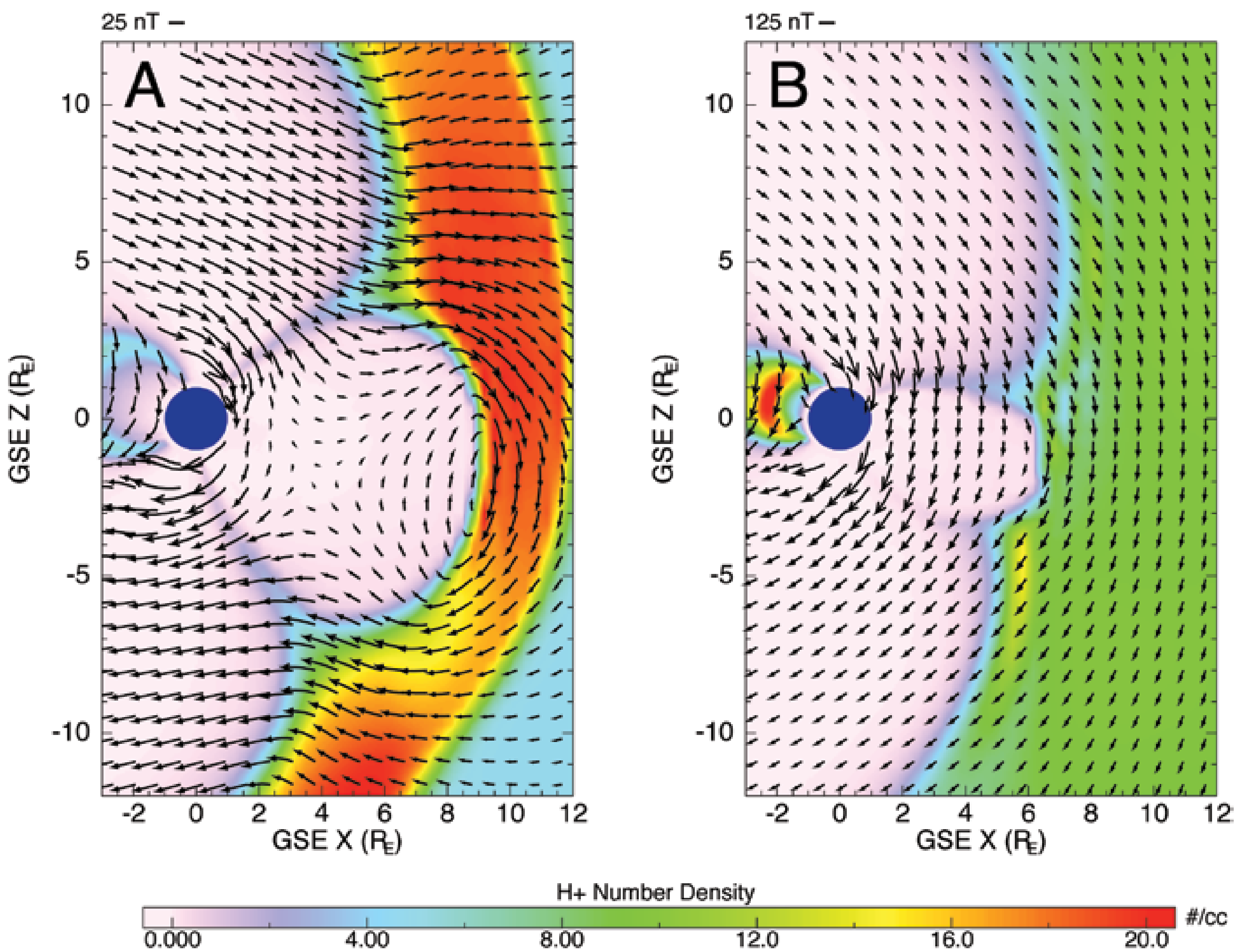

Figure 2: *Noon-to-midnight cross-section of the simulated magnetosphere with color-coded plasma density and vectors indicating magnetic field perturbations, contrasting the configuration of the dayside magnetosphere for (A) weakly driven versus (B) strongly driven conditions.*

MISSION DIRECTORATE

SPACE OPERATIONS

The Space Operations Mission Directorate provides agency leadership and management, including top-level requirements development, policy, and programmatic oversight of NASA space operations related to human exploration in and beyond low-Earth orbit. Current exploration activities in low-Earth orbit are the Space Shuttle and International Space Station programs which include NASA astronauts. The directorate is similarly responsible for Agency leadership and management of NASA space operations related to launch services, space transportation, and space communications in support of both human and robotic exploration programs.

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DELTA II HEAVY LAUNCH VEHICLE INVESTIGATION

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Figure 1: *Close-up of the top of the strap-on rocket motors used to increase the main engine thrust.*

Project Goals and Objectives: During the first three successful flights of The Boeing Company's Delta II Heavy launch vehicle (Figure 2), unexpected main engine control deflections were recorded. NASA Kennedy Space Center requested NASA Langley Research Center's assistance in explaining these deflections. With the cooperation of both NASA Kennedy and Boeing, NASA Langley initiated a research study, which included wind tunnel testing, computational studies, and an assessment of the vehicle's flight dynamics.

Project Description: Wind tunnel testing included three entries into the National Transonic Facility, a high-pressure wind tunnel located at NASA Langley. While the transonic forces and moments that could explain the main engine control deflections had not been previously characterized in the Boeing developmental testing, the telltale signs of transonic flow unsteadiness were recorded by the testing team (comprised of both NASA and Boeing engineers). NASA's previous experience with aircraft demonstrating similar unsteady transonic flows made the test planning and execution relatively straightforward for this space launch vehicle. Based on the wind tunnel test results, additional computational work was initiated, which focused on simulating the transonic and separated flow over the vehicle.

Relevance of Work to NASA: This work has contributed to the process of clearing the Delta II Heavy launch vehicle for continued flights of NASA payloads, including the upcoming Dawn mission to the Asteroid Belt slated for launch in June 2007. The aim of the Dawn Mission is to characterize the conditions and processes of the solar system's earliest epoch by investigating in detail two of the largest protoplanets remaining intact since their formations: Ceres and Vesta.

Computational Approach: Computational fluid dynamics modeling done by Boeing using NASA's OVERFLOW code was expanded to include the time-accurate simulation of unsteady flow about the full vehicle. Modeling of the vehicle accelerating through the transonic speed range was also performed.

Results: Both the wind tunnel and computational work complemented each other, constructing a complete picture of how the flow underneath the Delta II's solid rocket boosters was fluctuating in an unsteady fashion. This unsteady behavior was triggering significant flow squeezing out between some (not all) of the solid rocket boosters. The resulting asymmetries in the flowfield were determined to be the cause of the unanticipated and asymmetric moments on the vehicle, which were triggering the main engine control deflections. NASA's work in the area of flight dynamics has also resulted in improvements in mathematically modeling the behavior of the vehicle.

Role of High-End Computing: Computational simulation for this project would not have been possible without the availability of high-end computing resources such as the Columbia supercomputer. The high degree of geometric fidelity, coupled with the need for time-accurate simulation, required over 250,000 processor-hours. The availability of Columbia allowed these calculations to be performed in a timely fashion, in addition to enabling path-finding simulations of the accelerating launch vehicle. Furthermore, the High-End Computing Program application specialists assisted in debugging grid splitting issues along with the overall successful execution of OVERFLOW on Columbia.

Future: Several benefits have resulted from this investigation: first, the wind tunnel techniques associated with quantifying transonic unsteadiness have been transferred to The Boeing Company and will be considered in future testing; second, this study underscores the importance of running time-accurate computational simulations to look for unanticipated flow unsteadiness; third, The Boeing Company is currently identifying improvements to be made to the vehicle based on the results from this study, which will reduce the possibility of excessive main engine deflections in the future; and finally, lessons learned during this study are being applied to the testing and analysis associated with NASA's Crew and Cargo Launch Vehicles for Project Constellation.

Collaborating Organizations

- NASA Langley Research Center, Research and Technology Directorate
- NASA Langley Research Center, Center Operations Directorate
- NASA Kennedy Space Center, Launch Services Program
- The Boeing Company, Boeing Expendable Launch Systems

Figure 2: *Boeing Delta II Heavy launch of NASA's "Opportunity" Mars Exploration Rover.*

A FLUID-STRUCTURE INTERACTION STUDY OF INFLATABLE DECELERATORS AND VALIDATION OF METHODOLOGIES AGAINST WIND TUNNEL TEST DATA

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Figure 1: *Comparisons of wrinkle pattern and displacements: test article (left) and simulation (right).*

Project Goals and Objectives: The objectives of this work were to further develop and examine a novel, flight test-validated fluid-structure interaction methodology for reentry vehicles using gossamer-like structures (ballutes) for deceleration; and to show that the aerodynamic, aerothermal, and structural performances of the inflatable decelerator of a reentry vehicle can be predicted.

Use of inflatable decelerators has been suggested for several NASA flight projects in the past [1, 2], and balloons of various types have been proposed for missions to Mars on many occasions. However, the roadblock has always been the difficulties related to deployment and uncertainty associated with performance in Mars' harsh environment. Yet, analyses of space inflation concepts have all confirmed that use of inflatable decelerators is technically feasible, and have revealed the potential advantages over classical reentry strategies. Most notably, the ballistic coefficient of an inflatable decelerator is approximately two orders of magnitude lower than for conventional entry vehicles—the nearly fuel-free method of decelerating a space vehicle could reduce the typical mass of an interplanetary spacecraft by more than half [3].

Project Description: Coupled fluid-structure interaction studies of two configurations of inflatable decelerators (balloon-parachute: ballute) were carried out. A novel and test-validated method for mapping loads and displacements were employed to transfer data between the fluids and structural models such that the errors in the data transfer remains below 1.0% [4], see Figure 2. The first study was conducted on a gossamer-like trailing toroidal inflatable decelerator, and attempts were made to include the influence of the shocks emanating from an attached reentry vehicle (Figure 3). This study was followed by a detailed verification using a second set of computational fluid dynamics (CFD) and finite element software. This study examined several areas that could be viewed as potential contributors to the overall accuracy of the results.

The second study was conducted on a scaled wind tunnel test article (representing a clamped inflatable decelerator) at Mach 6 (Figure 3). The purpose of the second study was to validate the analysis methodology for the trailing toroidal inflatable decelerator. Requirements for the second study were relaxed not only to achieve quicker solution cycles, but also to examine the accuracy of analysis versus computational time. All studies used an accurately coupled fluid-structure interaction procedure, which was proven accurate enough to produce a maximum displacement within 6.7% of that observed from the wind tunnel test data.

Relevance of Work to NASA: Use of inflatable decelerators translates to smaller, less expensive vehicles that can be better equipped to conduct long-term NASA science experiments, or achieve faster trip times. When aerocapture devices are combined with solar electric technology, previously unreachable outer planet destinations become practical [5].

Computational Approach: Both TetrUSS and MSC.Nastran were employed as the workhorse applications to support this work, while FUN3D/HEFSS and MSC.Marc were used to spot-check results in the fluids and structural areas respectively. Methodology for the load and displacement mapping is per [4] and validated per [6]. A salient feature of the present study is the development of a consistent, coupled aero-structural analysis process capable of handling dissimilar aerodynamic and structural surface meshes. Figure 2 shows a graphical representation of the entire process which consists of six modules: aerodynamic analysis, load convergence, transfer aero loads to structural model, structural analysis, transfer displacements to aerodynamic model, and adjust aerodynamic field grid.

Results: The fluid-structure analysis of a trailing toroidal ballute revealed a superb match among the geometries and mesh of Computational Structural Model (CSM) and Computational Fluid Model (CFM). This near-perfect match is attributed to the method used for mapping the loads and displacements from/to CFM to/from CSM, while conserving virtual work. The method of loads and displacement mapping considered the minimization of errors during all interpolations. At the towline attachments, the stretched CFM and displaced CSM coincide flawlessly, see Figure 3. The mesh density around the towlines, however, appeared to be insufficient. An increase in mesh density around these areas in both the CFM and CSM will perhaps allow for a better load and displacement distribution, and thus the material wrinkling in these areas can be captured more accurately.

The test-validation study showed that fluid-structure interaction analysis results can be matched to wind tunnel test data. When examining test data and analysis results for the 4-inch diameter ballute, wrinkle patterns were similar, and the difference between predicted maximum displacement and that from the test data was 6.7% [7].

Role of High-End Computing: The fluid-structure interaction models created as the basis of this work were formed using CFD analyses conducted using the Columbia supercomputer. The entire project required approximately 20 solutions, each (at a condition of Mach 30) consumed 48 processors for three days. The runtimes were computationally expensive due to the number of species, which is a function of temperature and Mach number—the higher the temperature, the higher the number of species, and the more interactions required.

Future: While only basic research on materials for a ballute and the associated computational analyses are being conducted at present, NASA will inevitably incorporate a ballute in the design of future spacecraft for travel to Mars and other inter-planetary missions. Ballutes are a viable means for building space vehicles with the hefty fuel capacity required for further, faster journeys into space.

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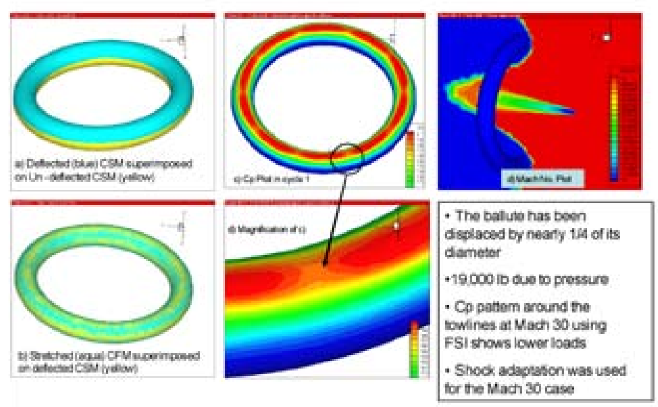

Figure 3: Coupled fluid-structure interaction toroidal ballute.

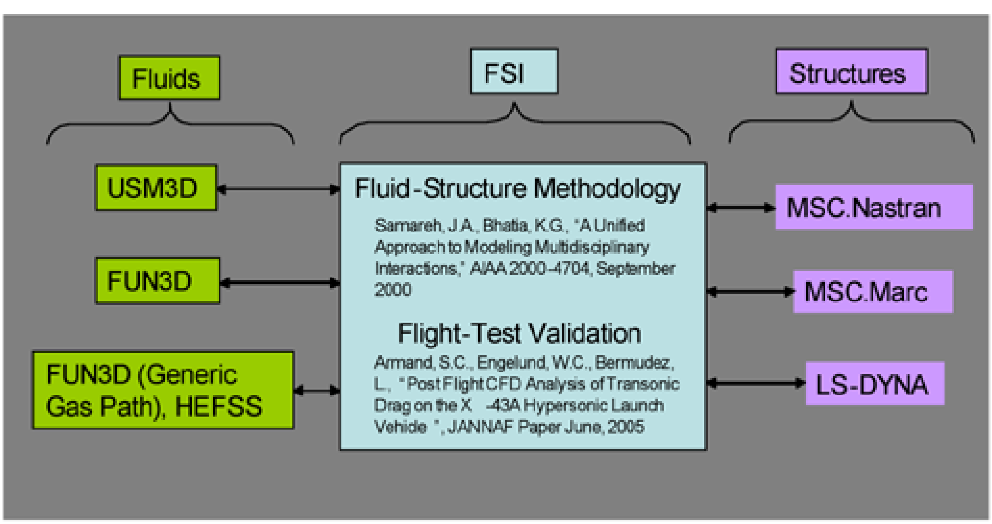

Figure 2: Coupled fluid-structure interaction methodology.

HIGH-FIDELITY SIMULATIONS OF UNSTEADY FLOW THROUGH TURBOPUMPS AND FLOWLINERS

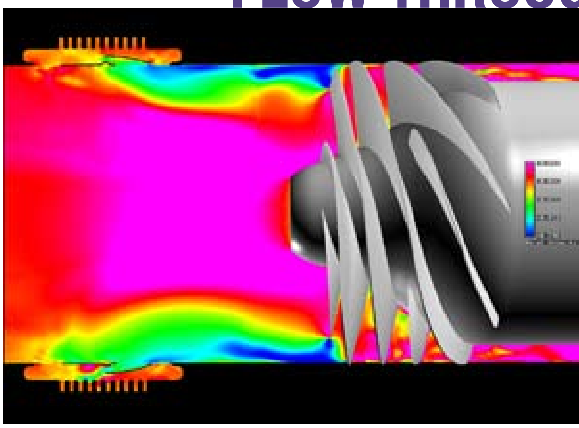

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Figure 1: *Instantaneous axial velocity contours on a vertical plane (12th rotation).*

Project Goals and Objectives: We are working to provide a high-fidelity computational framework for design and analysis of the entire fuel supply system of a liquid rocket engine, including high-fidelity unsteady turbopump flow analysis. This effort will decrease design costs, improve performance and reliability, and provide developers with information such as transient flow phenomena at startup, impact of non-uniform flows, and impact on the structure.

Project Description: A number of computational models have been developed, and time-accurate computations carried out to characterize various aspects of the flow field surrounding the flowliner. We have found that the Low-Pressure Fuel Turbopump (LPFTP) inducer creates backflow regions that extend upstream including the flowliner regions, and that the extent of the backflow varies with inducer design and operating conditions. This unsteady interaction between the backflow and flow in the bellows cavity poses high-frequency loading on the flowliners—considered one of the major contributors to the high-frequency cyclic loading. This can result in high cycle fatigue damage to the flowliners just upstream of the LPFTP. In this work, we investigate the effects of backflow in several different flowliner models including one with the inducer by itself (Model I) and another based on the first, but with the addition of the flowliner geometry (Model II).

Relevance of Work to NASA: This work is especially relevant to ensuring the safe and efficient operation of the Space Shuttle Main Engines (SSMEs). Applying our computational framework enables us to solve current problems with the SSME—for example, we have applied this framework to the investigation of the root cause of fuel-line cracks as a part of NASA's Engineering Safety Center Independent Technical Assessment.

Computational Approach: The incompressible Navier-Stokes flow solver based on the artificial compressibility method was used to compute the flow of liquid hydrogen in each test article. All computations included tip leakage effects with a radial tip clearance of 0.006 inches, a pump operating condition of 104.5% of rated power level, a mass flow rate of 154.7 pound-mass per second, and a rotational speed of 15,761 revolutions per minute.

The objective of studying Model I was to compare unsteady pressure values against existing data. To resolve the complex geometry in relative motion, an overset grid approach is employed. The geometrically complex body is decomposed into a number of simple grid components. Connectivity between neighboring grids is established by interpolation at each grid outer boundary. Addition of new components to the system and simulation of arbitrary relative motion between multiple bodies is achieved by establishing new connectivity without disturbing the existing grids. This computational grid has 57 overset zones with 26.1 million grid points.

The grid system for Model II includes 38 upstream slots, 38 downstream slots, the overhang area between liners, and the bellows cavity. This model is very similar to the ground test article (Model I). It consists of 264 overlapped grids with 65.9 million grid points. The flowliner component consists of an axisymmetric chamber around the external wall of the pipe, and two rows of slots in the streamwise direction.

To speed up and automate the grid generation procedure, script systems have been developed to automatically and rapidly perform the various steps of the grid generation process prior to the use of the flow solver. Special procedures were developed to automatically create grids for each component type. The present computations are performed utilizing the INS3D computer code, which solves the incompressible Navier-Stokes equations for both steady-state and unsteady flows.

Results: The findings include a significant backflow generated by the inducer reaching 15–20% of the tip velocity and a jet flow of 10–15% of the inducer tip speed, which penetrates into the bellows cavity, creating an unsteady recirculation region in the cavity (Figure 1). The reverse flow as shown in Figure 2 (represented by the red particles) and unsteady recirculation regions create an unsteady interaction between the duct and the bellows cavity, resulting in high-frequency cycle loading. The backflow also creates swirl in the bellows cavity on the order of 10% of the inducer tip velocity.

Role of High-End Computing: Many benchmark calculations of the SSME flowliner have been carried out to characterize the performance of the Columbia supercomputer. These benchmarks included the use of various parallel paradigms as well as communication protocols between nodes (where each node includes 512 processors). Global shared memory in each node allows efficient implicit solution procedures to be implemented in parallel for expensive high-fidelity, time-accurate calculations such as the SSME flowliner which contains 67 million grid points and 267 zones. Use of Columbia significantly decreased the overall turnaround time for these calculations, making the analysis of the flowliner crack problem more feasible. In addition, the Program's scientific visualization specialists provided extremely valuable interactive tools to handle large-scale particle tracing data to help quickly pinpoint flow features of interest anywhere in time or space.

Future: This work has direct applicability to assisting with design of the next-generation engines for a heavy-lift Crew Launch Vehicle being developed for Project Constellation. In particular, we will be carrying out stewardship-type calculations to help address the integration issues introduced with the design's multi-engine configuration.

Collaborating Organizations

- NASA Engineering Safety Center
- NASA Glenn Research Center
- NASA Johnson Space Center
- NASA Kennedy Space Center
- NASA Langley Research Center
- NASA Marshall Space Flight Center

Co-Investigators

- Dochan Kwak, NASA Ames Research Center
- William Chan, NASA Ames Research Center
- Jeff Housman, University of California, Davis

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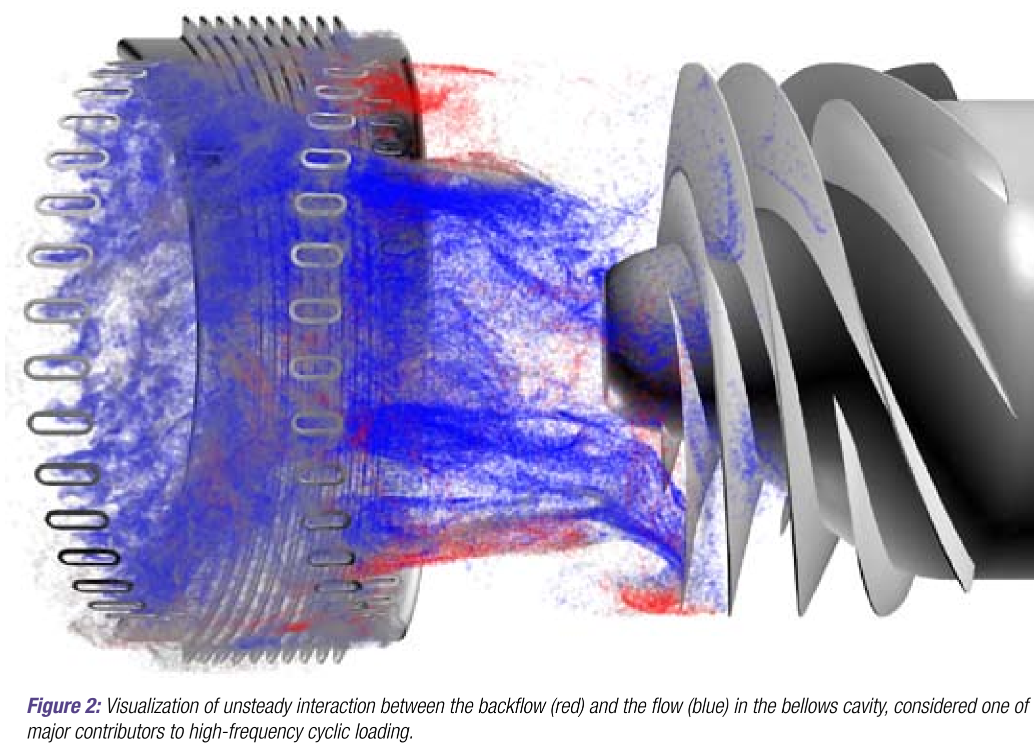

Figure 2: Visualization of unsteady interaction between the backflow (red) and the flow (blue) in the bellows cavity, considered one of the major contributors to high-frequency cyclic loading.

MPS FLOWLINER CRACK INVESTIGATION

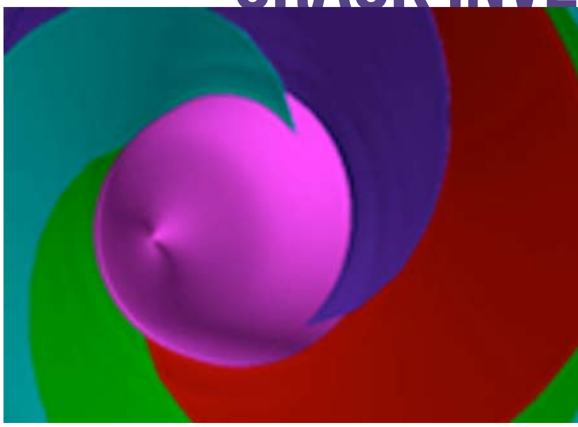

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Figure 1: *Close-up of vapor fraction in a flowliner simulation.*

Project Goals and Objectives: The goal of this work was to identify the driving mechanisms causing cracks found in a flowliner upstream from the low-pressure fuel pump in the Shuttle's Main Propulsion System (MPS).

Project Description: During a post-flight inspection of the liquid hydrogen feed lines leading to the Space Shuttle Main Engines (SSMEs), cracks were discovered in the slots of a gimbal joint flowliner just upstream from the low-pressure fuel pump inducer. An investigation was initiated following this discovery to determine the cause of the cracks and to formulate a strategy for either eliminating the driving mechanisms or increasing the durability of the liner. In support of the investigation, numerical simulations were performed for the feed line, the flowliner, and the inducer—in parallel with extensive experimental testing. The experiments were run in air, water, and liquid hydrogen to determine the acoustics, unsteadiness, and cavitation from the fuel pump. The simulations were run for the same fluids, and used to help guide the experiments and provide additional insight into the fluid dynamics phenomena in the pump.

Relevance of Work to NASA: While this work helps ensure the safety of the Space Shuttle, the analysis tools and techniques will have direct applicability to other engines employing the flowliner technology—the J-2X engine, for example. This particular engine, which is currently being designed to support the upcoming Project Constellation and its Crew Exploration Vehicle, will likely utilize flowliners.

Numerical Approach: A large matrix of three-dimensional unsteady simulations were performed for the feedline and inducer operating at engine conditions—in water to support water flow tests conducted at NASA's Marshall Space Flight Center, and in air to support air flow tests also conducted at NASA Marshall. These simulations were performed using NASA Marshall's PHANTOM code, a finite-difference flow solver capable of solving for liquids, gases, and two-phase turbomachinery flows. The code uses block structured O- and H-type grids, and was recently modified to use dynamic memory allocation. The computational simulations contained 3–5 million grid points, depending on whether the flow was assumed to be single- or two-phase, and the predicted results exhibited good agreement with the experimental data across the range of fluids and flow conditions tested. The simulations also helped identify the hydrodynamic mechanisms causing the cracks.

Results: Based on the calculations (assuming air, water, and liquid hydrogen) and experiments, the investigation team was able to determine what was accounting for the large unsteadiness, and at what frequencies they were occurring. It was concluded that a majority of the unsteadiness was being generated by the pump located downstream from the flowliner, which was causing pressure waves and backflow (Figure 1). In addition, it was determined that residual stresses from the flowliner manufacturing process were also contributing to the generation of the cracks. In an effort to remedy the situation, all holes in the flowliner were polished, and those with the cracks welded. No further issues have been detected since.

Role of High-End Computing: An average simulation was run on 12–48 processors of the Columbia supercomputer within a 24–48 hour timeframe. Typical simulations required 4–6 of these runs to obtain a time-periodic solution.

Future: This work is officially completed. The investigation team has gained a considerable amount of insight into the interaction between the pump and adjacent components, and this knowledge will be applied to the J-2X and future engine programs.

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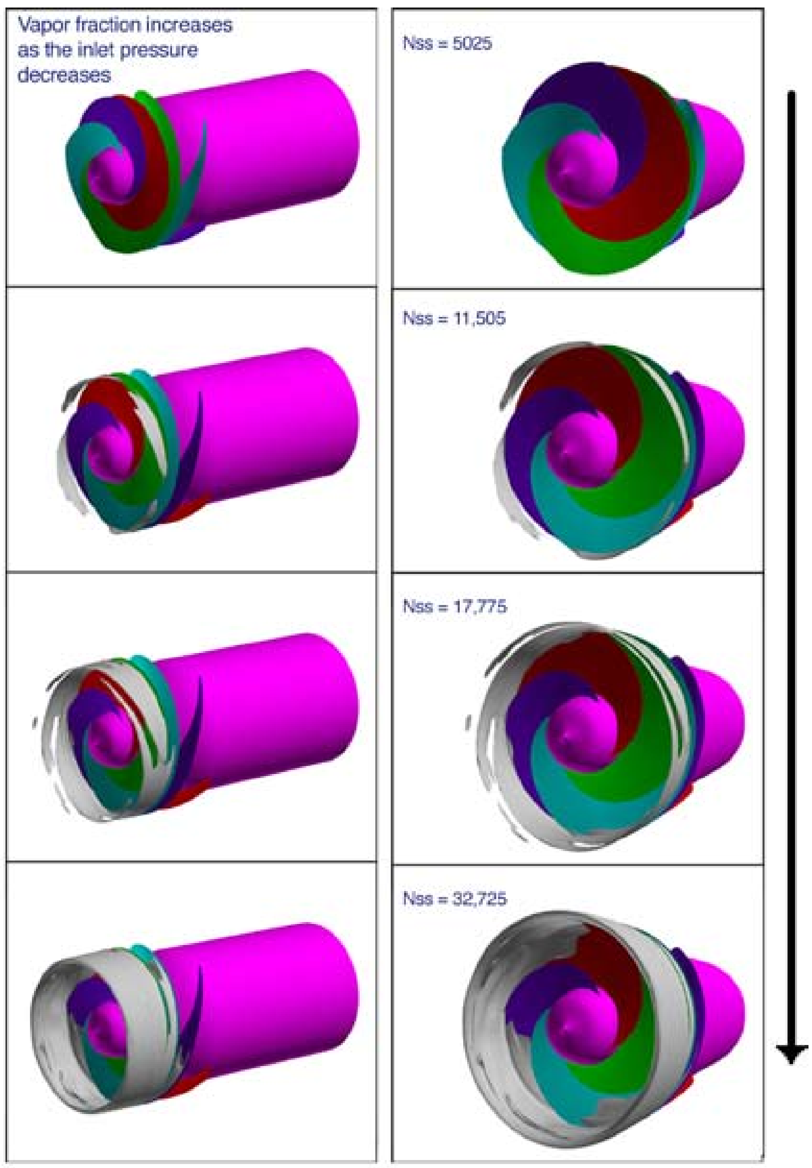

Figure 2: *Effects of cavitation near the flowliner—vapor fraction increases as the inlet pressure decreases (from left to right).*

PLUTO/NEW HORIZONS: RP-1 QUALIFICATION TANK FAILURE ANALYSIS

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Figure 1: *Close-up of the Atlas V 551 Series Launch Vehicle as shown in Figure 2.*

Project Goals and Objectives: On September 13, 2005, failure of an Atlas V Common Core Booster RP-1 Tank occurred during qualification testing. At this time, the Pluto/New Horizons Atlas V launch vehicle was slated to launch on January 17, 2006 (Figure 2). An anomaly investigation team of engineers and analysts was created to determine the root cause of the failure, and to determine the flight worthiness of the vehicle. The goal was to launch on time to avoid any costly delays in reaching Pluto.

Project Description: The qualification tank failure occurred during the last test case that was to be performed on the tank, which had previously survived an extensive series of pressure cycles and external load tests. Material properties and fatigue were investigated thoroughly to narrow down the cause of the failure. Once a cause was determined, a path to flight worthiness was established.

This path to Pluto/New Horizon's flight worthiness would involve the use of the finite element model (FEM) with existing test data. Numerous analyses were performed to correlate the model to the test cases. This activity not only corrected issues with the model, it increased the accuracy of future analyses.

Relevance of Work to NASA: Launching a satellite to Pluto not only requires excellent engineering, it takes precision timing. A one-month launch slip would cause the spacecraft a five-year delay in arrival to Pluto. Performing the finite element analysis in a timely manner was crucial for a successful and on-time launch.

New Horizons' core science goals reflect what the science community has wanted to learn about Pluto for the past two decades. The craft will map the surfaces of Pluto and Charon with an average resolution of one kilometer (versus the Hubble Space Telescope which can only capture a 500-kilometer resolution). It will map the surface composition across the various geological provinces of the two bodies, and will determine the composition, structure, and escape rate of Pluto's atmosphere. NASA has also outlined a list of lower priorities, including the measurement of surface temperatures and the search for additional satellites or rings around Pluto.

Computational Approach: Analysts and engineers were faced with three significant obstacles. First, the initial FEM results indicated stresses were above the material's yield allowable, indicating that the material is in the plastic strain region of the stress-strain curve. With the material in this region, it would either assume permanent deformation or exceed the ultimate stress. This finding indicated that a time-consuming, non-linear finite element analysis would need to be performed. Second, the material used is anisotropic, meaning the material capability is direction-dependent. Predicting the exact material behavior was difficult because the stresses are applied at an angle between these two directions. Third, the structure is complex to model and poses many variables such as the manufacturing technique used.

The FEM analysis has shown an adequate capability to explain the loading conditions that lead to yielding. The previous tank analysis failed to numerically explain the behavior of the structure under yielded conditions. Numerical tools can be effectively applied in a limited role to compare local loading conditions between flight and test load combinations, but it is extremely unlikely that the tools can be used to quote absolute analytical margin against a handbook allowable.

Results: Comparative stress analysis is being used to assess flight-load combinations and their resulting predicted stresses with respect to the stresses calculated by the same models for qualification test cases. In this regard, FEMs are being used to resolve and express effective stresses resulting from pressure and external loads. The fact that these stresses are not being used to quote margins against an allowable makes predictions that can be compared between flight limit and qualification test cases.

The findings of the qualification failure investigation, coupled with the physical understanding of the problem, the empirical evidence gathered within the existing flight tanks, and the extensive cases survived by the qualification article, support the development of a reasonable and conservative flightworthiness rationale.

Role of High-End Computing: Finite element analysis of a 1+ million-node model requires a powerful server to perform the computationally intensive calculations in a timely manner. Due to the lack of available computer resources and time to perform the calculations, NASA engineers and analysts required use of the Columbia supercomputer to perform analyses. Use of Columbia was essential to meeting the goals of the analysis—Columbia allowed NASA engineers to perform over 50,000 processor-hours of calculations in 2 months to successfully complete all analyses and launch Pluto/New Horizon's on time.

Future: In the future, the investigation team will complete an RP-1 tank redesign to gain margin over the previous design. Efforts to determine the optimal design are ongoing and continued access to Columbia will be required to process the large number of calculations needed to evaluate the effect of each redesign.

Figure 2: *Launch of the Atlas V 551 Series Launch Vehicle carrying Pluto/New Horizons on January 19, 2006 at 2 p.m. EST from Complex 41 on Cape Canaveral Air Force Station.*

SHUTTLE REENTRY HEATING AERODYNAMICS

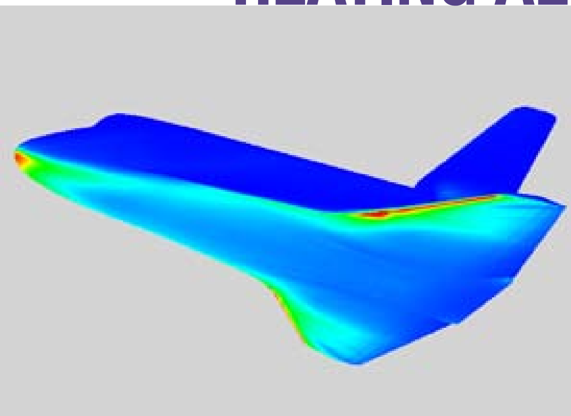

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Figure 1: *Heating rate distribution on the Shuttle at peak heating conditions during reentry.*

Project Goals and Objectives: The aim of this work is to ensure the safety of NASA's Space Shuttle fleet through the use of computational fluid dynamics (CFD) techniques. Specifically, assessing the health of the Shuttle's thermal protection system for reentry into Earth's atmosphere following any debris-related damage resulting from foam or ice shed during launch and ascent of the vehicle.

Project Description: During the course of a Shuttle mission (for example, STS-114, STS-121, STS-115, and future missions), NASA's Damage Assessment Team (DAT), comprised of CFD experts from NASA Ames and Langley Research Centers, analyzes any damage sites on the Shuttle resulting from foam or ice debris shed during launch and ascent. Several nodes of the Columbia supercomputer are dedicated to this effort throughout the duration of a Shuttle mission, enabling the assessment team to determine (within 24 hours or less) the health of the Shuttle's thermal protection system for reentry into Earth's atmosphere. Based on these analyses conducted using Columbia, DAT is able to make recommendations to the Space Shuttle Program chair regarding the damage sites—to either leave them "as-is" or repair them before reentry.

Despite an effort to develop a simplified engineering model for characterizing heating at damage sites (known as the Cavity Heating Tool), the assessment team is finding that the aerodynamic heating is very site-specific, thus making it necessary to maintain an on-orbit CFD capability to help resolve marginal damage sites that might be recommended for repair.

Relevance of Work to NASA: The safety of NASA's Shuttle fleet and crews is critical to the agency's successful space program. DAT's charter to provide on-the-fly assessment of damage sites to the orbiter—specifically regarding the health of the Shuttle's thermal protection system for reentry into Earth's atmosphere—is of paramount importance to ensuring successful missions.

Computational Approach: Detailed aero-thermal analyses by The Boeing Company, NASA Johnson Space Center, NASA Ames, and NASA Langley help determine the heating and structural stresses on the orbiter at each damage site. The High-Fidelity Rapid Aerothermal CFD analysis (developed at NASA Ames and NASA Langley) is then used on the more critical damage sites to augment information derived from engineering heating estimates.

The site-specific re-entry heating environment is fed into the Boeing Thermal Math Model and Finite Element analysis for determining the fitness of the tile(s) and the airframe for reentry. DAT then recommends that the damage site either be: "used-as-is" or repaired.

Results: In advance of Shuttle missions, solutions of the full orbiter are computed at several trajectory points, providing baseline re-entry heating for the Shuttle (Figure 1). The baseline solutions are used as the basis for local solutions on damage sites such as cavities, gap-fillers, and breeches. Damage on tiles such as that seen in Figure 2 can produce higher heating than would be present on undamaged tiles (Figure 3). Such computations typically require 2-million grid points, and 10 hours on hundreds of Columbia's processors.

Frequently, gap fillers protrude from between tiles creating a disturbance to the laminar flow on the underside of the vehicle. The disturbance (vortex) can lead to elevated heating due to the downwash of the vortex (Figure 3). In addition, the vortex can often trigger transition from laminar (low heating) to turbulent flow (high heating). These elevated heating levels are evaluated on a case-by-case basis to determine if downstream regions of the vehicle are vulnerable to the higher heating.

Role of High-End Computing: During each Shuttle mission, a few of Columbia's nodes are set aside and placed in stand-by mode for any necessary on-orbit CFD analysis work.

DAT typically consumes approximately 3,000 processor-hours on Columbia for each damage site analyzed, and results are captured within 24 hours. The team remains on stand-by to analyze multiple damage sites during the course of a mission (seven sites were analyzed during the STS-114 mission in July/August 2005).

Future: DAT will continue providing their CFD expertise both in preparation of upcoming Shuttle missions and during missions. Approximately 16 more Shuttle flights are anticipated between November 2006 and the conclusion of the Space Shuttle Program in 2010 when the International Space Station is slated to be complete. To help facilitate this work, High-End Computing Program application optimization specialists are working to enhance performance of the Data Parallel Line Relaxation and Langley Aerothermodynamic Upwind Relaxation Algorithm codes for use during future Shuttle missions.

Co-Investigators

- Dave Saunders, Chun Tang, Grant Palmer, Kerry Trumble, Tahir Gokcen, Peter Gnoffo, Steve Alter, Maria Pusonetti, all of NASA's Damage Assessment Team

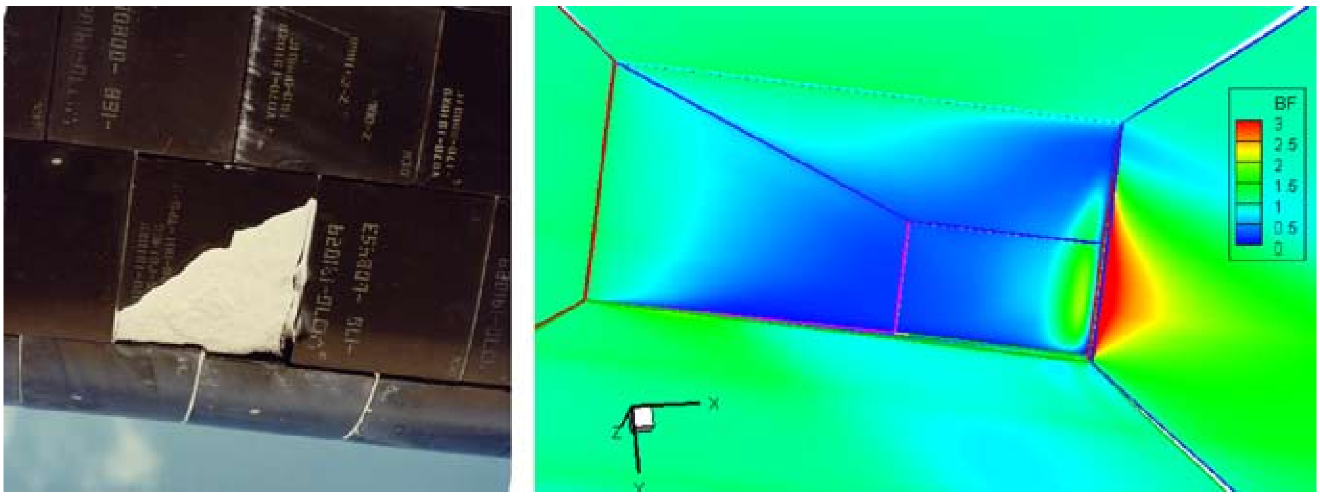

Figure 2: Tile damage on STS-2 (left); Chine simulated heating on the damaged tile (right).

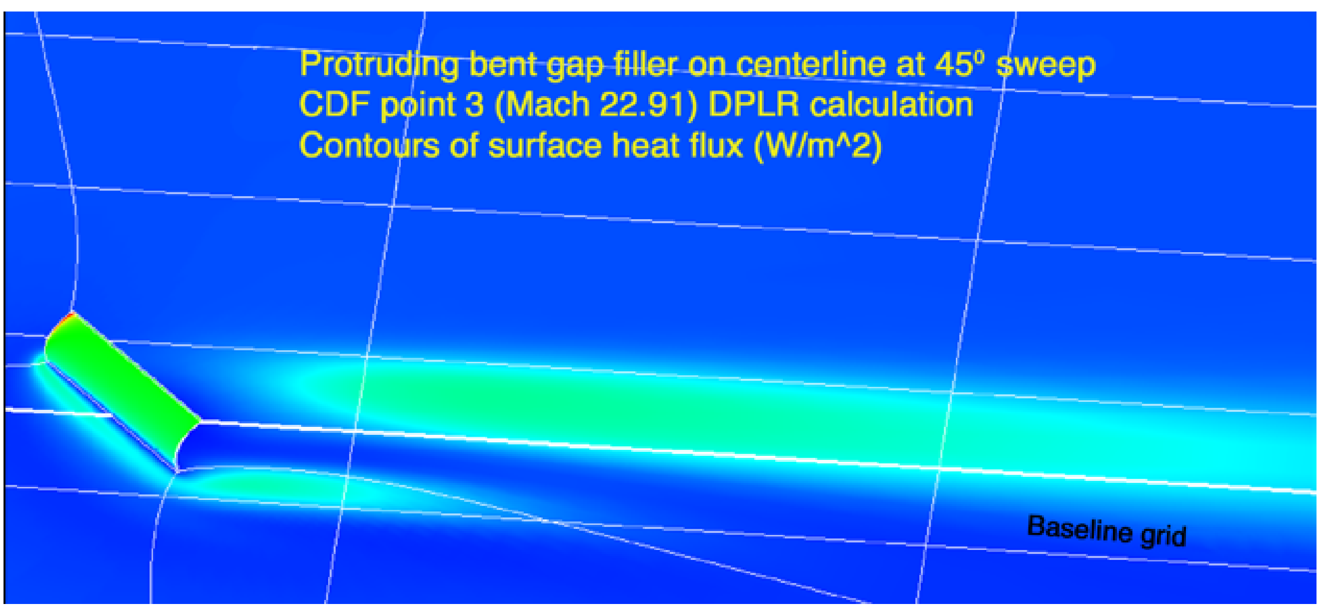

Figure 3: Simulated heating on a gap filler protruding from the underside of the Shuttle.

SPACE SHUTTLE RTF ASCENT AERODYNAMICS AND DEBRIS TRANSPORT ANALYSES

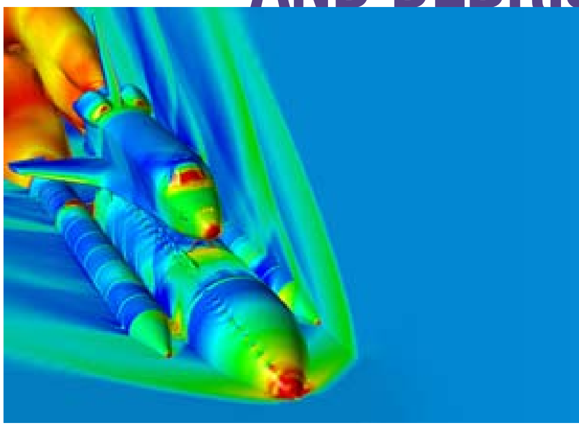

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Figure 1: *Pressure coefficient on the Space Shuttle Launch Vehicle and in the near-body flowfield.*

Project Goals and Objectives: This project supports Space Shuttle ascent environment assessments, and provides key inputs required to perform debris transport analyses of ascent and entry debris that threaten the orbiter.

Project Description: High-fidelity flowfield simulations are a critical part of NASA's Space Shuttle Return to Flight (RTF) efforts. Results from computational fluid dynamics (CFD) simulations of the Space Shuttle Launch Vehicle (SSLV) support a wide range of activities—from reassessment of databases created before the first Shuttle launch—through creation of redesigned External Tank (ET) aerodynamic environments. Additionally, unsteady six-degree-of-freedom (6-DOF) simulations are used to model debris aerodynamics for use in probabilistic risk assessments of various debris sources on the launch vehicle. These solutions provide insight and detailed information not available from wind tunnel or flight test data.

Relevance of Work to NASA: The safe return-to-flight of the Space Shuttle is NASA's top priority, as it paves the way for completion of the International Space Station, and is a precursor to the success of the Exploration Program.

After a large piece of foam debris shed from one of the Protuberance Air Loads (PAL) foam ramps on the Shuttle's ET during the STS-114 launch in summer 2005, an aggressive effort was launched to remove the PAL ramps. Removal of the ramps required extensive assessment of local and global aerodynamic environments. CFD simulations of the launch vehicle without the PAL ramps were used to design wind tunnel tests to measure local buffet environments and provide static airloads on the protuberances affected by the PAL ramp removal. Flight measurements captured during STS-121 in July 2006 showed no sign of aeroelastic excitation, confirming preflight predictions. The ability to rapidly produce high-fidelity simulations has been a critical element of the Shuttle Program's ET redesigns and debris analyses.

Computational Approach: Complex flowfield interactions between the Shuttle, ET, and Solid Rocket Boosters result in numerous shock boundary layer interactions, illustrated in Figure 1. Realistic simulation of these shock-boundary layer interactions requires solutions of the unsteady Reynolds-Averaged Navier-Stokes (RANS) equations. A complete unsteady simulation of the entire vehicle, over the full flight envelope, is beyond the scope of existing CFD capabilities—these assessments required a large, integrated effort involving computational simulations and experimental efforts. The numerical simulations included steady-state RANS analysis of both the entire SSLV and a number of isolated components. These computations utilized NASA's OVERFLOW code, and the complex geometries were discretized using the overset gridding technique, incorporated in a sophisticated script system built using the Chimera Grid Tools software package. Development of aerodynamic models of free-flying debris released in a supersonic flowfield was accomplished using unsteady 6-DOF calculations from the Cart3D code. Large numbers of these unsteady runs were used to quantify the seemingly random behavior of a particular type and shape of debris as it decelerates. The input variables for each of the individual runs were generated from a Monte-Carlo draw. The drag and cross-range data from the Monte-Carlo runs were then used to build distribution functions that serve as aerodynamic models in both deterministic and probabilistic debris analyses.

Results: The analyses performed to support the removal of the PAL ramps represent the most extensive use of CFD for evaluating Shuttle aerodynamic environments to date. Detailed simulations of the complex geometry shown in Figure 2, enabled extraction of detailed distributed loads that were difficult or impossible to measure with wind tunnel tests. Additionally, debris transport results were used to produce launch commit criteria for ice balls formed at foam defects during a Shuttle countdown. This tool is used to ensure that the vehicle does not launch with any hazardous ice formations.

Role of High-End Computing: The Columbia supercomputer's ability to rapidly reallocate resources and provide on-demand capability for high-priority work has been instrumental to the success of Space Shuttle redesign activities. The Shuttle Program has relied heavily on the system to dramatically increase safety of manned space flight. One of many tasks accomplished on Columbia was the delivery of 218 SSLV ascent CFD simulations covering the flight envelope at ten different Mach numbers: from 0.6 to 2.2. The overset grid system contained over 78 million grid points in 569 zones. The simulations required approximately 400,000 processor hours on four of Columbia's 512-processor nodes. All of these cases were completed in a span of 18 days, and produced more than 3 terabytes of data. This analysis was on the critical path for the launch of STS-121, and was used to generate the airloads database for the redesigned ET (required to certify the vehicle for flight).

Future: At least one more redesign of the ET ice/frost ramps is planned prior to the end of the Shuttle Program in 2010 to produce a minimal foam application design. A comparison of one proposed configuration and a wind tunnel test article are shown in Figure 3. Work continues on refining the ascent debris probabilistic risk assessments, and future activities will entail refining the debris aerodynamic models for lower-priority debris threats. Additional ice debris simulations will also be run to help refine the launch-commit criteria related to ice ball formation on the ET's surface.

Collaborating Organizations

- NASA Johnson Space Center
- NASA Ames Research Center
- The Boeing Company

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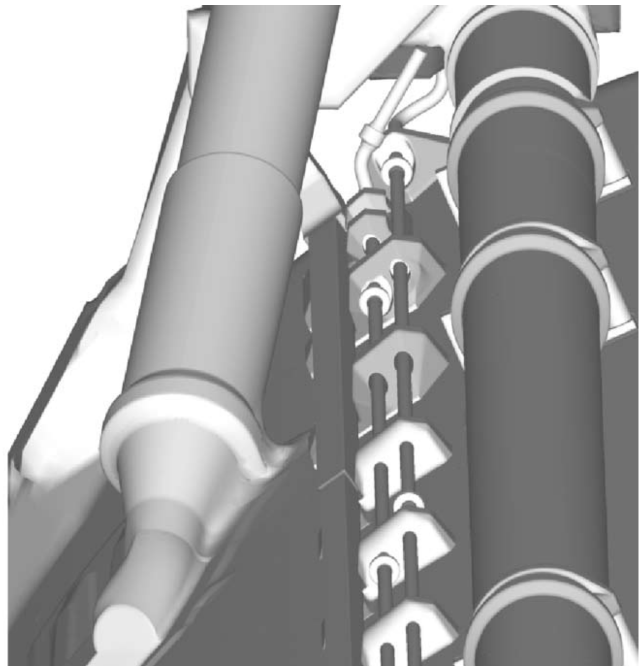
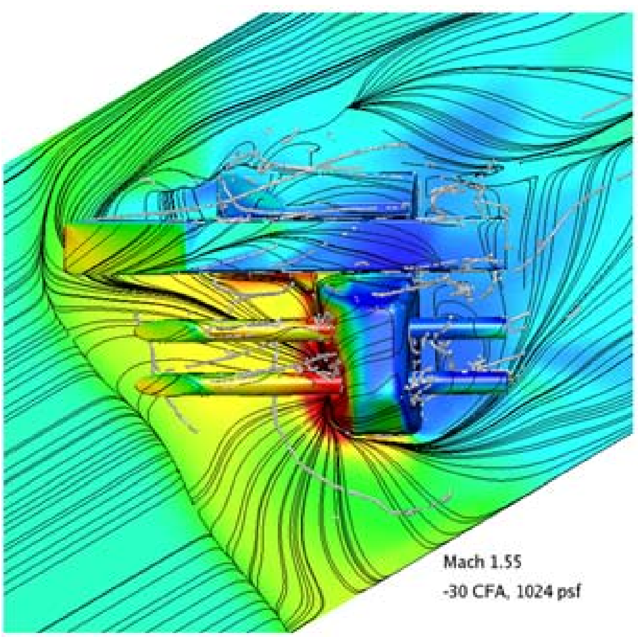


Figure 3: External Tank aft attach hardware computational fluid dynamics geometry details.



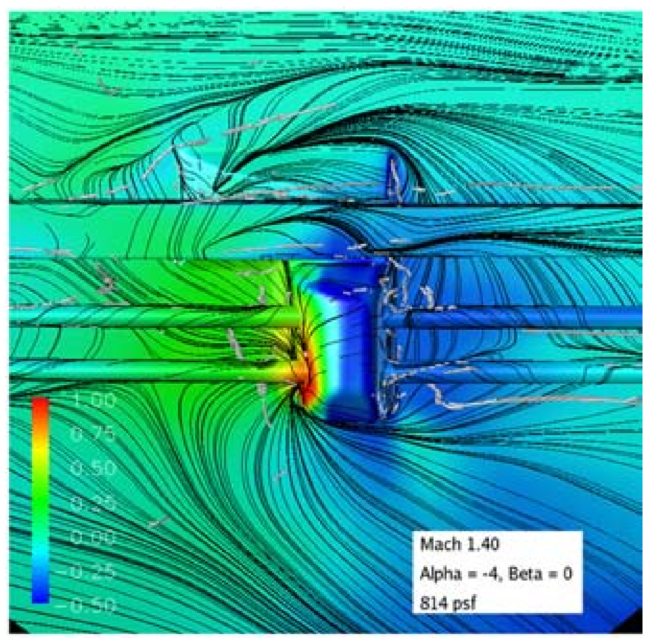


Figure 2: Reshaped ice/frost ramp comparison, showing surface pressure coefficient and flowlines, in addition to vortex cores. Full launch vehicle ramp is shown on the right, and a wind tunnel component test simulation is shown on the left.

SSME HIGH-PRESSURE OXIDIZER TURBOPUMP KNIFE-EDGE SEAL CRACK INVESTIGATION

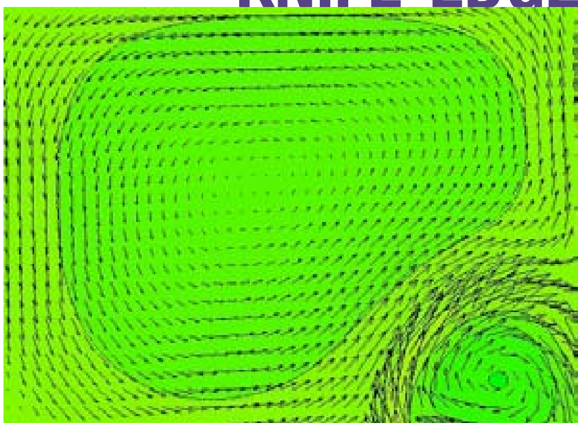


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Figure 1: *Close-up of flow patterns in a knife-edge seal, as seen in Figure 2.*

Project Goals and Objectives: During a routine inspection of the Space Shuttle Main Engine (SSME) following a Shuttle mission, cracks and missing material were discovered on two of the seals in the secondary flow path of the SSME high-pressure oxidizer turbine. NASA has put an analytical and experimental program in place with the goal of identifying the sources of these cracks, and determining ways to mitigate their potentially harmful effects.

Project Description: To help balance and control fluid flows in the SSME, knife-edge seals (seals with sharp "teeth" protruding from them) in the secondary flow path of the SSME high-pressure oxidizer turbine are designed to decrease pressure and limit the amount of flow. While no problems surfaced as a result of these recently discovered cracks in the seals and missing pieces of material, it was important to identify their root causes and devise a solution to prevent such occurrences in the future. NASA engineers, in collaboration with Pratt & Whitney and Rocketdyne (now merged and known as Pratt & Whitney Rocketdyne) formed the Knife-Edge Seal Investigation team to investigate the causes of these cracks and devise a solution. The team used a combination of experimental tests (including air rig and hot fire tests) and computational simulations to investigate the problem. The computational models were generated specifically to study the flow unsteadiness surrounding the knife-edge seals. Output from the computations included the frequency and amplitude of the flow fluctuations generated by the seals, as well as the pressure drops across the seals (Figure 2). The experiments and computations were designed to complement one another, and the experimental results were used to validate and anchor the computational models.

Relevance of Work to NASA: While the obvious benefits of this work are ensuring the safety of the Space Shuttle, the type of seals studied in this work are used in a variety of liquid fuel engines important to NASA. For example, the J-2X engine, which is being designed to support the upcoming Project Constellation and its Crew Exploration Vehicle, scheduled to replace the Space Shuttle in 2010; and the RS-68 engine, which will be used for the Ares V Cargo Launch Vehicle, also in support of Project Constellation.

Numerical Approach: A large matrix of two- and three-dimensional simulations was performed for the original and redesigned seals (redesigned by Pratt & Whitney) operating at both engine and airflow test rig conditions. The simulations were performed with the Loci-CHEM code from Mississippi State University, a finite-volume flow solver with combustion kinetics for generalized (including unstructured and hybrid) grids. The three-dimensional grids contain 9–15 million grid points, and represent one of the first attempts to quantify the flow unsteadiness in a series of knife-edge seals. Pre-test three-dimensional predictions showed good to excellent agreement with the results of airflow test data obtained during air rig testing at NASA's Marshall Space Flight Center.

Results: The numerical results obtained using the Loci-CHEM code have helped identify the aerodynamic sources responsible for the high stresses and cracking in the original seal geometry, and have confirmed that the redesigned seal geometry operates with much less flow unsteadiness. The redesigned seal is currently going through an extensive certification process at NASA's Stennis Space Center, which includes several ground runs during which the engines are run "full-out" to mimic real operating conditions.

Role of High-End Computing: The large processor count afforded by the Columbia supercomputer facilitated quick turnaround time—on average, each simulation was run within a 24-hour time period on 70–100 processors. Two such runs were typically needed to obtain a steady solution, while 10–15 runs were needed to obtain a time-periodic unsteady solution.

Future: Should future analyses be required on the knife-edge seals, NASA can now confidently apply the Loci-CHEM code and feel very comfortable with the results—this area of study was relatively untapped prior to this work.

Co-Investigators

- Lisa Griffin, Suzanne Dorney, both of NASA Marshall Space Flight Center

Publications

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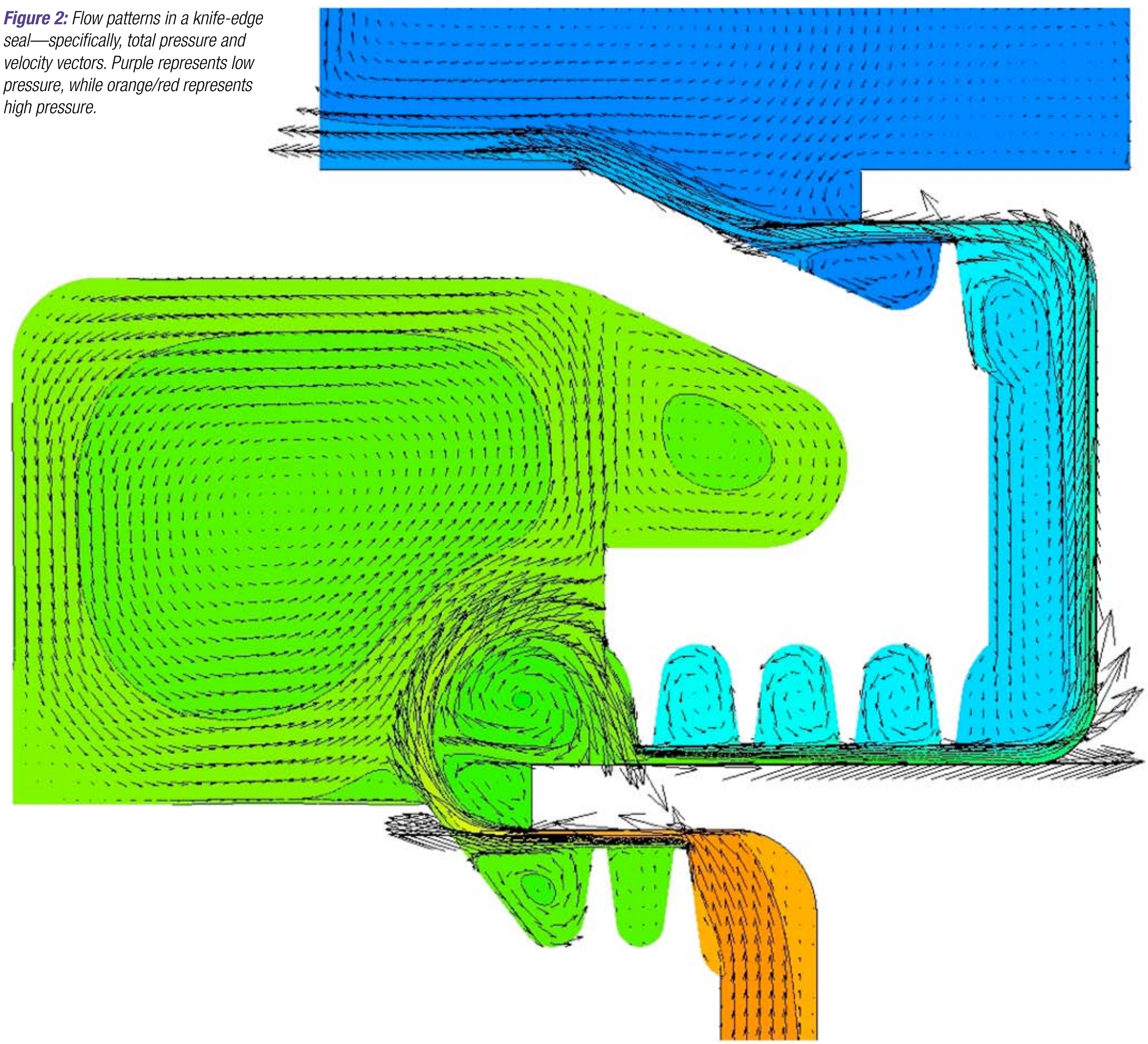
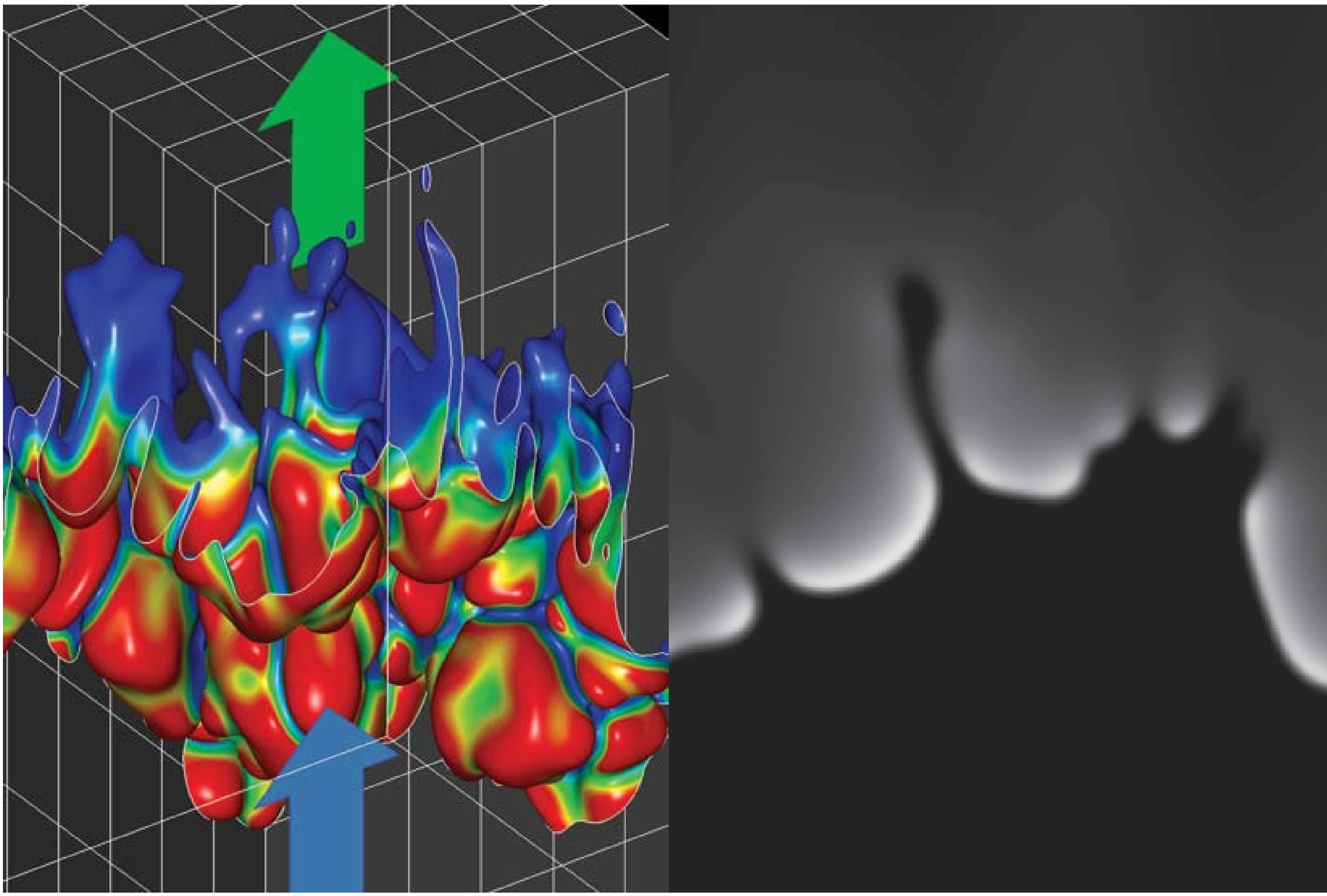
Figure 2: *Flow patterns in a knife-edge seal—specifically, total pressure and velocity vectors. Purple represents low pressure, while orange/red represents high pressure.*

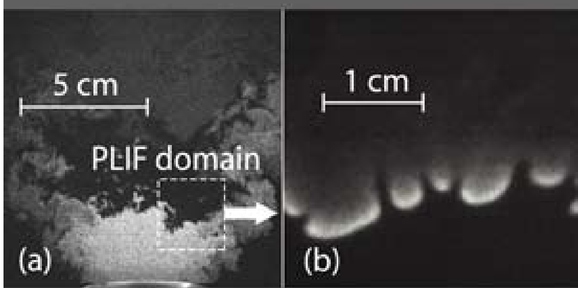




NATIONAL LEADERSHIP COMPUTING SYSTEM

NASA's National Leadership Computing System (NLCS) initiative provides access to NASA's largest supercomputers to selected non-NASA researchers doing cutting-edge, computationally intensive science and engineering of national interest. NLCS demonstrates the Agency's support for important national priorities, and its commitment to continued U.S. leadership in high-end scientific and technical computing and computational modeling. By inviting industry and academia participation, NASA can help advance U.S. technology and education, and assist U.S. competitiveness. In return for NLCS awards, much of the resulting knowledge will be made publicly available.

HIGH-FIDELITY SIMULATIONS ENABLING CLEAN COMBUSTION SYSTEMS



NATIONAL LEADERSHIP COMPUTING SYSTEM

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Figure 1: *Experimental diagnostics of a turbulent hydrogen flame in a low swirl burner. (a) Mie scattering image (laser-sheet-illuminated inert particles seeded in jet fuel; white region indicates premixed fuel, white/dark interface indicates temperature jump at flame surface), and (b) planar laser-induced fluorescence (PLIF) image of hydroxyl profile indicates region of combustion reactions. The pair of images shows that the flame surface is highly wrinkled, but also that the hydrogen flame burns in cellular structures separated by regions of local extinction.*

Project Goals and Objectives: The goal of this work is to perform detailed numerical simulations of lean turbulent premixed flames to enable a fundamental understanding and quantitative characterization of the coupling of turbulence and flame chemistry over a broad array of premixed gaseous fuels. The research focuses on fuels that exhibit unstable flame-front burning modes due to interactions with turbulence in the inlet stream. The work also involves the development of new diagnostic techniques for exploring large multi-scale, multi-dimensional, multi-component reacting flow simulations.

Project Description: Future energy needs must be met while minimizing environmental impacts and attaining high efficiencies. Thus, there is considerable technological interest in designing advanced fuel-flexible turbine combustion systems that can operate on lean hydrogen or syngas mixtures that can be burned in gas turbines. These new devices must operate in combustion regimes where turbulence/chemistry interactions have significant effects on flame dynamics and stability (see Figure 1), but where standard thin-flame theory for premixed flames cannot be directly applied. As a result, conventional engineering models based on this theory are not applicable, and current experimental diagnostic procedures cannot provide a characterization of the flame dynamics adequate to form the basis of predictive models. High-fidelity numerical simulation using models that incorporate detailed chemistry and species-transport provides essentially the only viable mechanism for obtaining a more detailed characterization of these flames. By integrating this simulation capability with new approaches to analysis of simulation data, it is possible to make direct and quantitative comparisons between simulations and experimental diagnostics, and directly link observed flame behavior to basic chemical reaction processes.

Relevance of Work to NASA: As a commitment to continued U.S. leadership in high-end scientific and technical computing and computational modeling, and in response to the recommendations of the Federal High-End Computing Revitalization Task Force, NASA extends access to the Columbia supercomputer to include research from outside of existing NASA projects. Lawrence Berkeley National Laboratory's work on efficient fuel combustion helps advance NASA's mission to develop technologies for safer aircraft and higher capacity airspace systems, while ensuring environmental compatibility. Moreover, hydrogen is among the fuels considered, so this study provides basic information about hydrogen flame instabilities relevant to a broad array of NASA missions.

Numerical Approach: The simulations are carried out with the low Mach number adaptive mesh refinement code, LMC [1]. The LMC code integrates the multi-species reacting Navier-Stokes in the low Mach number limit [2, 3], but without models for turbulence or turbulence/chemistry interactions. The low Mach number approximation exploits the natural separation of velocity scales in low-speed problems, removing acoustics and the need to evolve them from the analytic description of the system. Evolution of the system proceeds at a time step size constrained by the fluid velocity rather than the acoustic wave speed, considerably increasing the maximum numerical time step for typical low-speed combustion applications. The LMC code is implemented in the context of a block-structured approach to adaptive mesh refinement (AMR), originally developed by Berger and Colella [4] for hyperbolic conservation laws. With AMR, the regions to be refined are organized in rectangular patches, with several hundred to several thousand grid points per patch. Grid patches are distributed across parallel computing processors to balance the computational load dynamically during the simulation. The patches are created and destroyed as the simulation progresses to dynamically refine features of interest. In typical combustion applications, for example, the highest levels of grid refinement are focused around the flame-front and strong vortex structures in the turbulence. The AMR low Mach number algorithm results in computational savings of approximately three orders of magnitude (compared to a comparable uniform-grid compressible simulation). Computational savings enables this study on present-day high-end computing architectures.

Results: Following an initial set of two-dimensional scoping studies to identify appropriate operating regimes [5], we have carried out several time-dependent three-dimensional turbulent flame simulations geared at reproducing flame surface instabilities observed in experimental burner configurations. The study considers turbulence parameters (integral scale, intensity) and flame mixtures typical of a laboratory-scale "low swirl" nozzle burning a lean hydrogen-air fuel mixture. The simulations are performed in an idealized configuration consisting of a doubly periodic three-dimensional box with inflow-outflow boundaries representing the inner core region of the burner. A feedback control algorithm confines the flame to the finite rectangular computational domain. Figure 2 shows a representative snapshot of a lean hydrogen flame from this study. The comparison of the computed hydroxyl profiles with experimental measurements indicates that the simulation is able to accurately capture the observed cellular structure of this lean hydrogen flame. Preliminary analysis of the simulation data [6] confirms that the structure of the flame cannot be explained in terms of a wrinkled flame—thus underscoring the difficulties in studies of these types of fuels in the context of the standard flame theories.

Role of High-End Computing: This work on carrying out detailed numerical simulations of turbulent lean premixed flames takes full advantage of the power, configuration, and shared-memory capabilities afforded by the 2,048-processor Columbia system. The ability of the LMC code to take advantage of the 2,048 system's shared-memory architecture was due in part to assistance provided by the High-End Computing (HEC) Program's application performance scaling specialists. Additionally, HEC networking support for this work required transfer of up to 0.9 terabytes of data per day across the wide area networks between Columbia and the Department of Energy's Lawrence Berkeley National Laboratory.

Future: Additional simulations are under way for different fuels, including lean methane and propane mixtures, because these will exhibit substantially different burning modes than the hydrogen cases shown in Figure 2. We are currently developing deterministic path-line and stochastic data sampling and analysis procedures to shed light on the complex flow/chemistry interactions leading to local extinction in the hydrogen flames, and to identify the physical processes responsible for the differences between the fuels. A critical aspect of the analysis includes developing a process by which we can relate the observed flame behavior to those described in the classical combustion literature. This will aid in the extension of these new insights into engineering models used more universally for combustion system design and optimization.

Co-Investigators

- Robert Cheng, Ian Shepherd, John Bell, Mike Lijewski, all of Lawrence Berkeley National Laboratory's Combustion Laboratory

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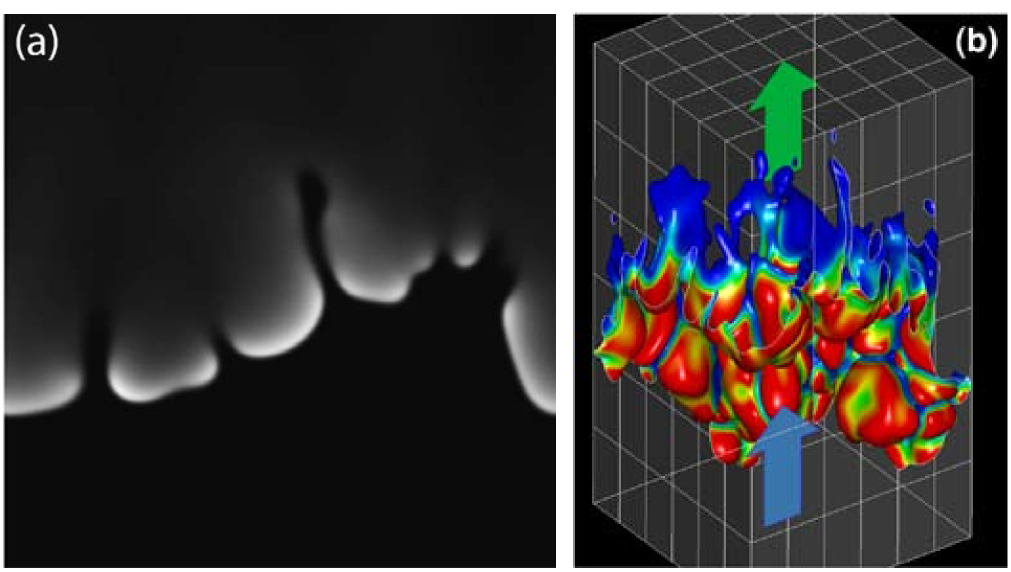
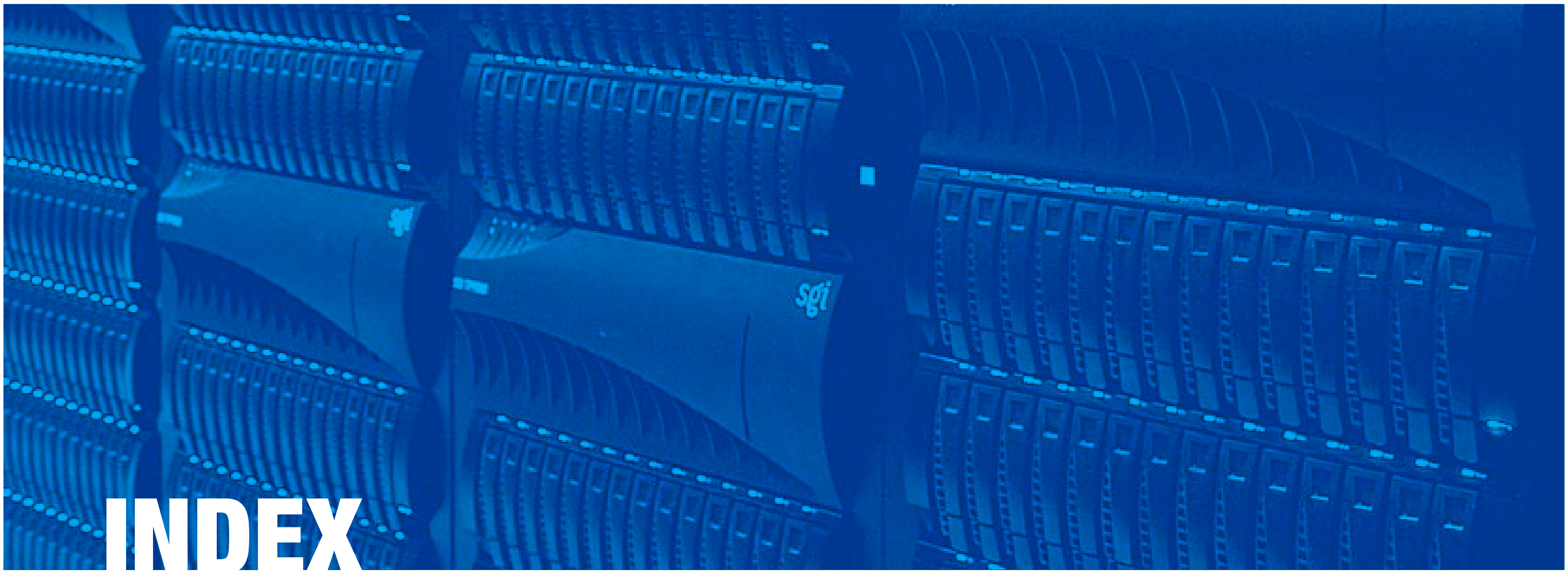


Figure 2: *(a) Typical computed hydroxyl profile from a three-dimensional numerically controlled flame simulation (compare with Figure 1b), and (b) a representative isotherm (temperature = 1,200 Kelvin) from the time-dependent simulation, colored by the local fuel consumption rate. Red color indicates stable burning; blue indicates extinction.*



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Images shown on back cover (from left to right):

- Explore, a 1,152-processor SGI Altix 3700 BX2 supercomputer housed at the NASA Center for Computational Sciences.
- Part of the Columbia supercomputer's one-petabyte data storage system housed at the NASA Advanced Supercomputing facility.
- Long view down the backside of two of the 20 nodes that comprise Columbia, a 10,240-processor SGI Altix system housed at the NASA Advanced Supercomputing facility.
- A portion of Halem, a 1,392-processor HP AlphaServer SC45 supercomputer housed at the NASA Center for Computational Sciences.

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