NASA Supercomputing Support Services (NS3) Acquisition

Pre-Solicitation Conference
NASA Ames Research Center
July 28, 2006

Agenda

Time	Topic	Presenter
9:00 - 9:30	Procurement Overview	Jill Willard, Contracting Officer
9:30 - 10:30	Technical Overview	Bryan Biegel, Deputy Chief (acting), NAS Division
10:30 - 10:40	Break	
10:40 - 11:30	Open Q&A	Jill Willard; Bryan Biegel
11:30 - 12:30	Tour of main computer room and VisLab	Bill Thigpen, Deputy Project Manager for Columbia; Chris Henze, Visualization Group Lead; Bryan Biegel
12:30	Exit NAS Building	

NASA Supercomputing Support Services (NS3)

PROCUREMENT OVERVIEW

Solicitation Information

- Solicitation Number: NNA06125494R
- Websites
  - Federal Business Opportunities: http://www.fedbizopps.gov/
  - NAIS (NASA Acquisition Internet Service): http://procurement.nasa.gov/
  - NASA/ARC Business Opportunities Page: http://procurement.nasa.gov/cgi-bin/EPS/bizops.cgi?gr=C&pin=21
  - NS3: http://procurement.nasa.gov/cgi-bin/EPS/bizops.cgi?acqid=118311
- Register at NAIS to receive the following e-mail announcements
  - Pre-solicitation and post-award notices and amendments
  - Notices of solicitation and solicitation amendment releases
  - General procurement announcements

Communications Guidance

- Copies of these viewgraphs and the Presolicitation Conference attendance list will be posted to website
- All revisions to the RFP will be in writing; nothing said here today should be construed as a revision unless subsequently confirmed in the final RFP
- All questions on the draft RFP or this conference should be submitted to Jill Willard, Contracting Officer
- “Open Door” communications policy will be in effect until the final RFP is posted
- Communications blackout will be invoked at RFP issuance - all communications will then be with Jill Willard, Contracting Officer

Freedom of Information Act (FOIA) Requests

- Requests for information on incumbents or other offerors: Will require FOIA request
- No proprietary information can be disclosed
- Terence Pagaduan, FOIA Officer
  - NASA Ames Research Center, Code EX, M/S 943-4
  - Moffett Field, CA 94035-1000
  - Telephone: (650) 604-1181
- URL: http://amesnews.arc.nasa.gov/foia/index.html
- Information that can be disclosed without FOIA request:
  - Incumbent: Advanced Management Technology, Inc.
  - Contract Number: NNA05AC20T
  - Type: Cost Plus Award Fee
  - Period of Performance: 4/1/2005 through 3/31/2007
  - Value: est. $49 million

Procurement Summary (1)

- NS3 is a follow-on to primary support contract for NASA Advanced Supercomputing (NAS) Division at ARC
- Procurement Vehicle: Full and open competition
- Type of Contract: Cost Plus Award Fee
  - Award Term was considered in addition, but was not selected
- Period of Performance: 3/1/2007 - 2/28/2017 (10 year limit)
  - Includes 30 day phase-in
- Periods
  - Two-year base and eight one-year options
- Subcontracting goals: 25%
  - Small Business 14%
  - Small Disadvantaged Business 5%
  - Women-Owned Business 5%
  - HUBZone 1%

Procurement Summary (2)

- Teaming Arrangements
  - Companies are responsible for own teaming arrangements
  - An Interested Parties list is posted and updated The list of attendees at this Presolicitation Conference will also be posted on website
- Award without Discussions
  - NASA's preferred and intended method of competition is to award without discussions
  - Offeror's intent to take exceptions to terms and conditions should be communicated to the Contracting Officer BEFORE offers are due

RFP Highlights - Section M

- Explains how the proposal will be evaluated
- Mission Suitability – Volume I
  - Numerically scored and assigned adjectival rating
  - Mission Suitability Subfactors are weighted
    - Technical Approach – Oral Proposal Presentation
    - Management Approach – Oral Proposal Presentation
    - Small Business Participation/Subcontracting Plan - Written
- Past Performance – Volume II
  - Adjectival Rating
- Cost/Price Proposal – Volume III
  - Government will compute Probable Cost (PC) for each Offeror
    - Based on Government's estimate of anticipated performance costs plus any fee proposed
  - Probable costs given confidence rating of "High," "Medium," or "Low"
    - Based on Government evaluators' assessment of Offeror's ability to meet requirements in the Statement of Work, approach and total cost and fee contained in its proposal

Procurement Schedule

Milestone	Tentative Date
Draft Solicitation Issued	August 2006
Comments on Draft Solicitation Due	September 2006
Final Solicitation Issued	October 2006
Proposals Due	November 2006
Contract Award	March 2007

NASA SUPERCOMPUTING SUPPORT SERVICES (NS3)

TECHNICAL OVERVIEW

Topics

- Purpose
- Take-Away Messages
- NAS in Context
- NAS Elevator Speeches
- Scope of Work
- Issues of Interest
- Backup: Recent NAS Highlights

Purpose of Technical Overview

- Not to repeat or expand on statement of work (SOW) or other RFP content
- To provide *context* for SOW and RFP
  - High Performance Computing (HPC) environment
  - NAS' HPC users and stakeholders
  - NAS culture

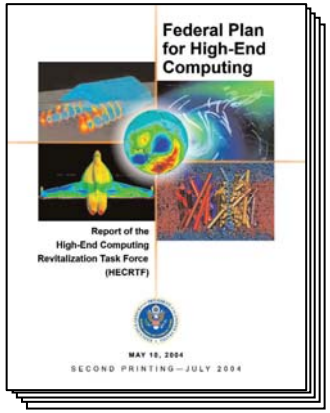
Take-Away Messages

Base Requirement: Support HPC resources and services of NAS Division

- NAS Mission: *Deliver **world-class** high performance computing (HPC) capability to **all NASA missions**, facilitating the rapid development and application of advanced knowledge and technology to enable mission success*
- Success requires highly skilled expertise in each technical area
- Contractor and NASA perform as highly integrated team
- Contractor expected to bring experience and best practices in operating world-class HPC facility
- Outcomes for NASA's computation-intensive and data-intensive challenges
  - Dramatic reductions in time-to-solution
  - Breakthroughs in accuracy and scale of solution
  - Rapid advances in scientific and engineering insight
- Goal: Enhanced mission impact for hundreds of simultaneous HPC users and projects across NASA Centers, Mission Directorates, and partner organizations
- **NASA has an inspiring mission; NAS is an exciting place to work!**

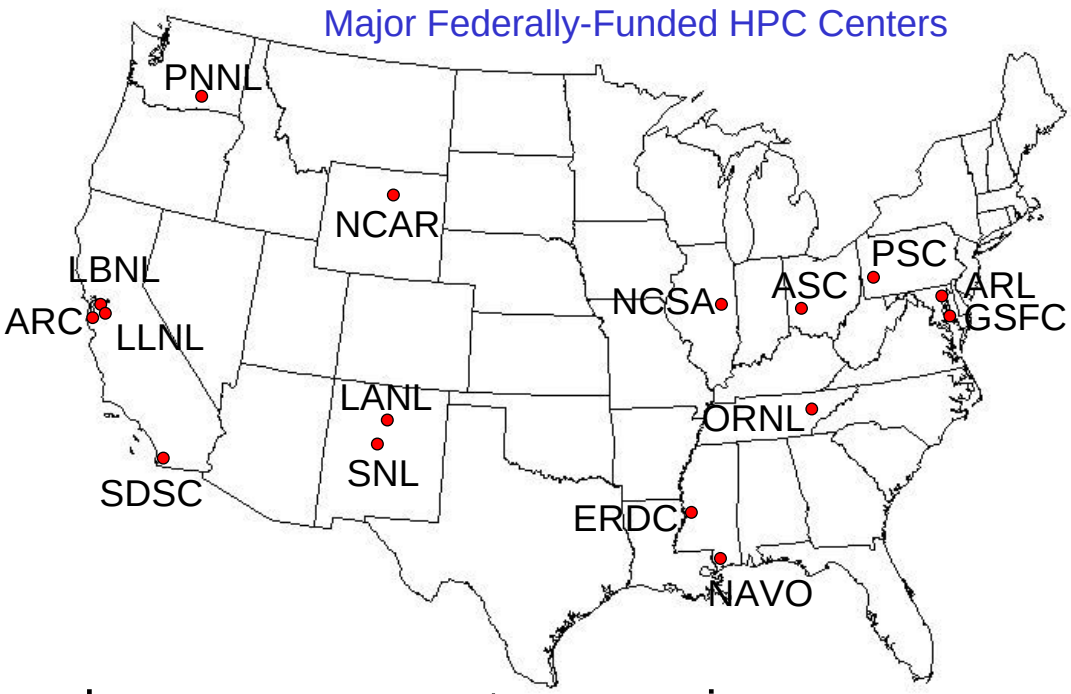
NAS in Context - Federal HPC Environment

- Leveraging HPC is key strategy of American Competitiveness Initiative
- Advanced Networking and HPC are OMB/OSTP R&D priorities
- Major HPC revitalization on-going in U.S.
  - Implementing 2004 plan of High-End Computing Revitalization Task Force (HECRTF)
  - First petascale systems expected FY08-09
  - Multi-agency, multi-vendor HPCS (High Productivity Computing Systems) Program is advancing HPC architectures, performance, usability
  - Coordination in all areas of HPC-related R&D through inter-agency NITRD (Networking and IT R&D) Program
  - Major procurements, petascale data I/O and storage, advanced networking, etc.



NAS in Context - HPC Community

- All major HPC user agencies and orgs participating in revitalization
- NAS communicates and collaborates through various means
  - NITRD and associated activities
  - HPCS reviews
  - HPC system reviews
  - Panels, conferences, workshops
  - Technical interchanges (publications, seminars)

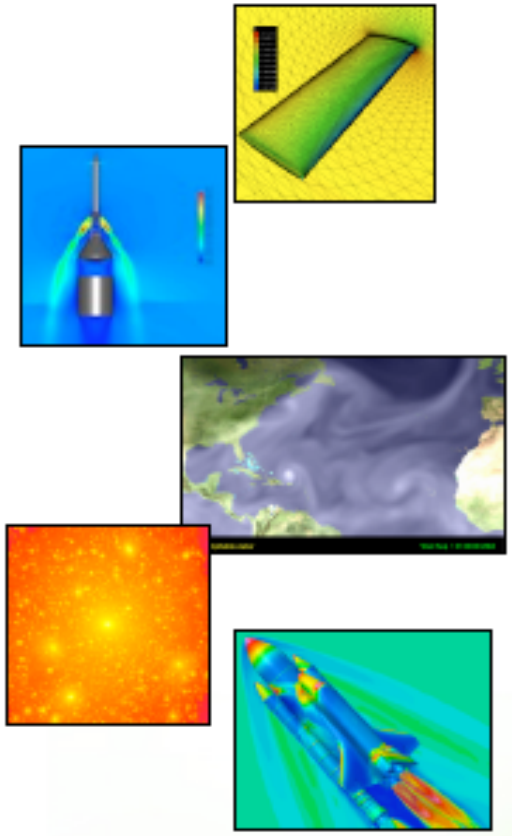


- HPC vendors, integrators, and program support companies are partnering to help realize the potential of HPC to enable/enhance mission success

NAS in Context - NASA Mission Directorates

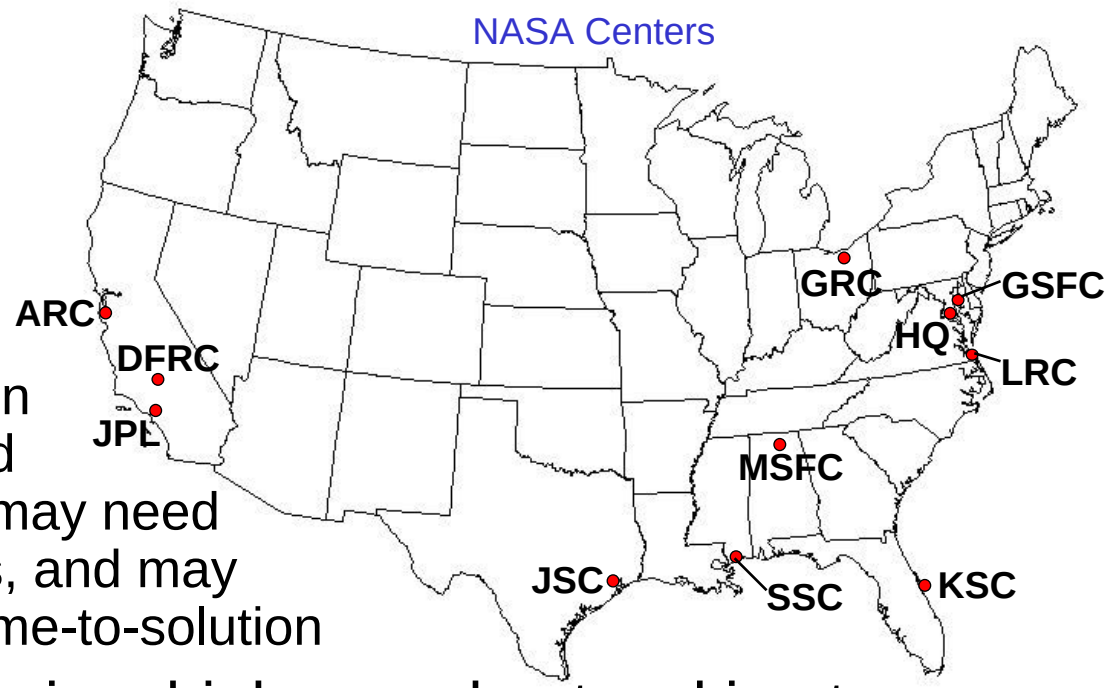
Support all Mission Directorates (MDs)

- Aeronautics Research (ARMD)
  - Develop and validate advanced aerospace vehicle models and concepts
- Exploration Systems (ESMD)
  - Design, development, and analysis of exploration systems and technologies
- Science (SMD)
  - Understand the Earth-Sun system, our own solar system, and the universe beyond
- Space Operations (SOMD)
  - Operate the Shuttle and International Space Station safely



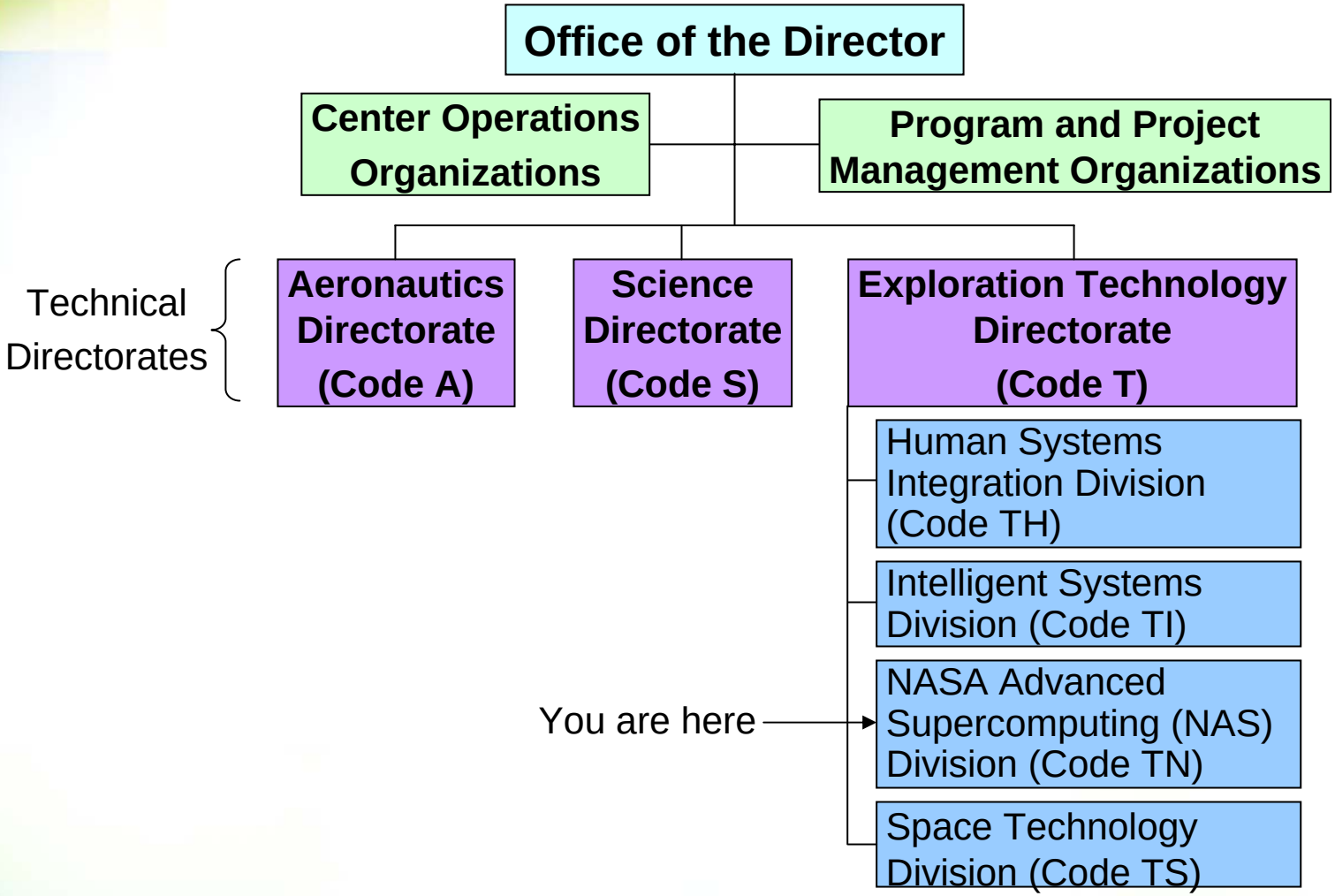
NAS in Context - NAS HPC Users

- NAS HPC users across all NASA Centers
- Many users at external sites (e.g., SMD PIs in academia)
- Two user classes:
  - Science: Applications often scale to very high resolution; users don't require quick turn-around
  - Engineering: Apps often difficult to scale beyond 100-200 CPUs; users may need to run large ensembles, and may need very short total time-to-solution



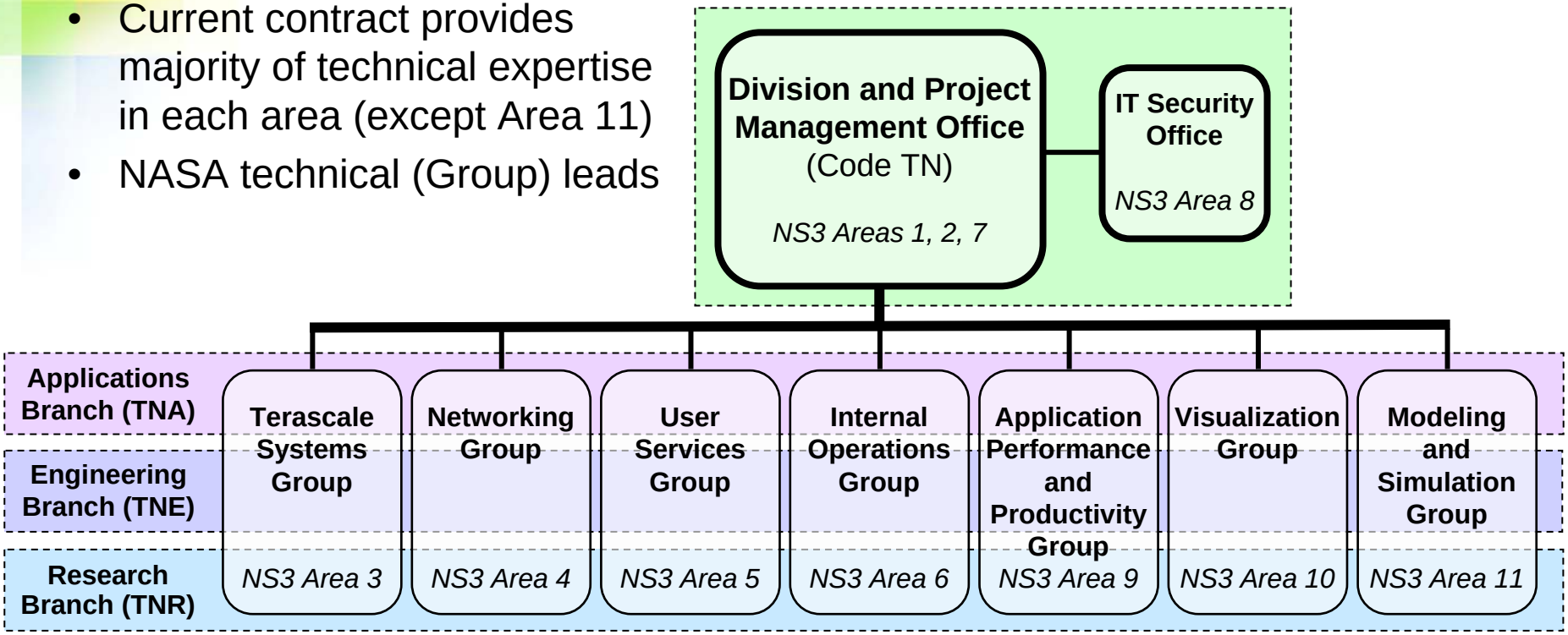
- Users productivity requires high-speed networking to user sites, and peering with external networks

NAS in Context - Ames Org (Simplified)



NAS Division Organization (July 2006)

- Current contract provides majority of technical expertise in each area (except Area 11)
- NASA technical (Group) leads



NS3 Technical Areas:

1. Program Management
2. Technical Integration
3. Supercomputing and Storage Systems
4. Networking and Communications
5. User Services
6. Facility Operation
7. HPC Enterprise Architecture
8. Information Technology Security
9. Application Services and Tools
10. Visualization and Data Analysis
11. Modeling and Simulation Projects

NAS in Context - NASA Funding

- Base Requirements funded by NASA Shared Capability Asset Program (SCAP)
  - Agency-level (above MD) funding, managed by SMD
  - Supports all Mission Directorates
  - Stability expected in funding for at least 5 years
- No dramatic changes expected in funding levels for contractor support during NS3 contract
- Tech Area 11 projects are more dynamic
  - Funded by program sponsoring modeling/simulation application
  - Depend on dynamic needs of MDs and programs
  - Recent funding very strong and growing to support ESMD
  - Currently mostly civil servants

NAS: Full Life-Cycle Support for Advanced Computational Modeling and Simulation

NASA Scientists and Engineers

Scientists and engineers set up computational problems, choosing effective codes and resources to solve NASA's complex mission problems.

Outcome: Dramatically enhanced understanding and insight, accelerated science and engineering, improved accuracy, and increased mission safety.

Performance Optimization

Data Analysis and Visualization

NAS experts apply advanced data analysis and visualization techniques to help scientists explore and understand large, complex data sets.

NAS software experts utilize tools to parallelize and optimize codes, dramatically increasing simulation performance while decreasing turnaround time.

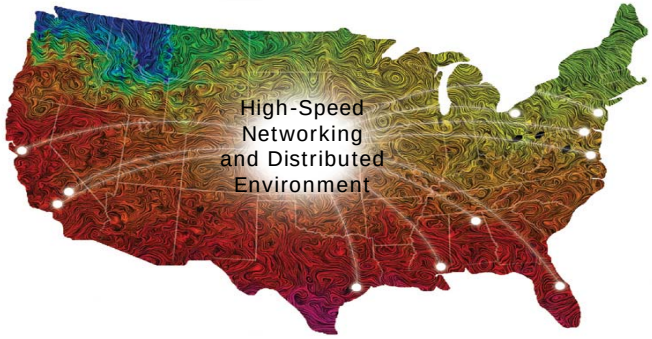
Supercomputers, Storage and Networks

NAS HPC environment (hardware, software, network, storage) executes optimized codes to solve NASA's large computational problems

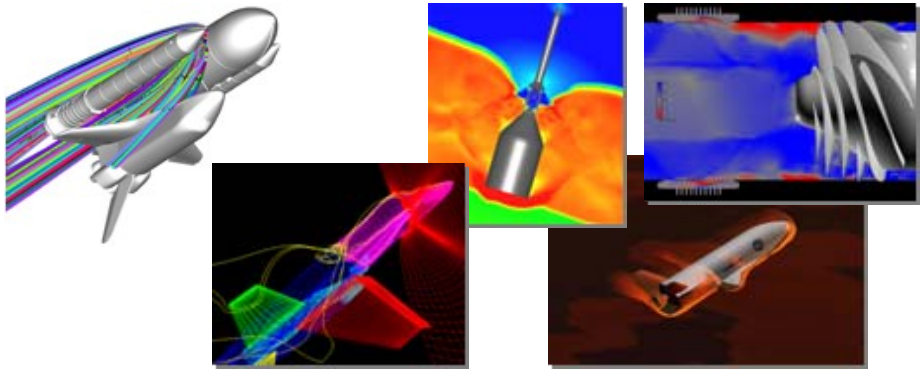
NASA Advanced Supercomputing: Comprehensive Application Support

Supercomputing Operations

Supercomputing User Services



NASA-Wide Supercomputing Environment



High-Fidelity Modeling and Simulation

NASA Advanced Supercomputing Division provides supercomputing, large-scale data storage, high-speed wide area networking, application performance optimization, data analysis and visualization environments, and high-fidelity modeling expertise in support of Agency Missions

Columbia: World-Class Supercomputing

- Goal: Enable NASA to use supercomputing for **broad** mission success
- Fast build: Order to full ops in 120 days; ~10X faster than similar systems; dedicated Oct. 2004
  - Unique partnership w/ industry (SGI, Intel)
  - Built from trusted components (Altix)
- Immediate impact: Full production and increasing capacity during build
- Leadership capability: currently 4th fastest supercomputer in world: 62 Tflops peak
  - Linpack runs at 51.9 Tflops
- Effective architecture: Easier application scaling for high-fidelity, shorter time-to-solution, higher throughput
  - 20 x 512p/1TB shared memory nodes
  - Some apps scaling to 2048p and beyond
- Supporting all Mission Directorates
  - >200 projects; >1000 accounts
  - Typically 100-200 simultaneous logins
  - Users from across and outside NASA
  - 24x7 support; high Quality of Service
- Result: Deep and Broad Mission Impact!

Systems: SGI Altix 3700 and 3700-BX2
Processors: 10,240 Intel Itanium 2
Global Shared Memory: 20 Terabytes

Front-End: SGI Altix 3700 (64 proc.)
Online Storage: > 1 Petabytes RAID
Offline Storage: >10 Petabyte Archive

Internal Network: NUMALink3/4
Internode Comm: Infiniband
Data Transfer: Gigabit Ethernet
Hi-Speed: 10 Gigabit Ethernet

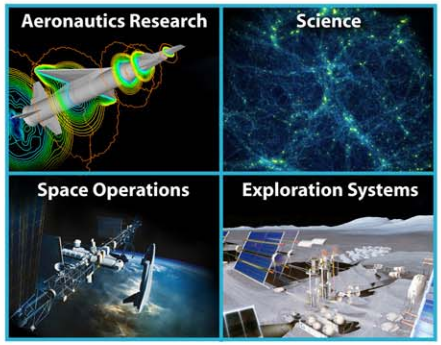
NASA Ames Research Center (ARC)

Success Through Partnerships

Partnerships with other agencies, mission customers, supercomputing technology vendors, and integrating expertise internally - enables NAS to support and enhance mission success across NASA

"LEADERSHIP" SYSTEMS

MISSION CRITICAL APPLICATIONS



NASA's Mission Directorates

NATIONAL

HECRTF

NSTC Report May 10, 2004

- Each agency should assess and make arrangements to provide for its own resources based on mission priorities.
- Agencies should examine the value of reallocating resource to respond to this opportunity.
- Provide access to shared leadership systems for the largest, most computationally intensive scientific endeavors.

NASA

One NASA

"Earth, Moon, Mars and Beyond"

NAS PROGRAM

Revitalized 3-Year Program

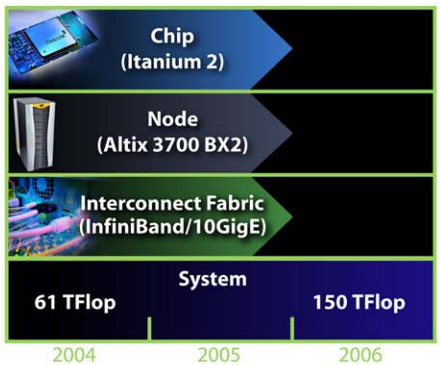
- Integrated balanced system
- Focused research and development
- Increased/sustained capital refresh

VENDOR TECHNOLOGY

INTEGRATED ENVIRONMENTS

Next Generation Codes & Algorithms	Rapid Deployment
OVERFLOW - *STS 107* Honorable Mention, 1998	- Systems
INS3D - *Pump Analysis* NASA Software of the Year, 1994	- Networks
CART3D - *STS 107* NASA Software of the Year, 2002	- Archives
Data Analysis & Visualization	**Computer Science Tools & Expertise**
- Hyperwall visualization systems	- Program development tools
- Process large data sets	- Automatic multilevel parallelization
- Interactive real-time visualization	- Scaling, porting, and optimization

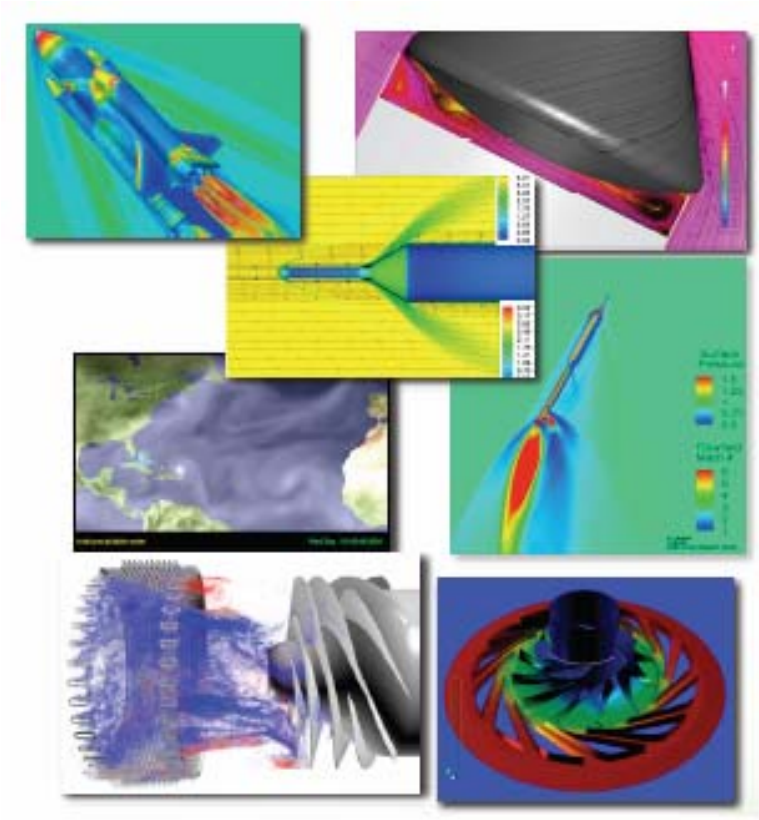
SUPERCOMPUTING



Columbia System

High-End Computing Columbia: Recent Mission Applications

- ARMD
  - Detached Eddy Simulation
  - Alternative Propulsion Systems
  - High-Speed Slotted Wing
- ESMD
  - CEV/CLV Launch Abort Risk Analysis
  - Aerothermal Analysis for TPS
  - Structural Analysis for Pluto Mission Launch
- SMD
  - High-Resolution weather prediction
  - Ocean modeling
  - Cosmological and galaxy evolution
  - Explosion of Type I-A Supernovae
  - Gravitational waves for LISA
- SOMD
  - STS-107 Investigation support
  - RTF: Aero ascent and debris analysis
  - Internal aerothermal CFD
  - RTF: External aerothermal CFD



Scope of Work (1 of 5)

- Baseline Technical Areas: Broad mission impact with HPC requires balanced environment, comprehensive user support, and programmatic excellence
  1. Program Management
  2. Technical Integration
  3. Supercomputing and Storage Systems
  4. Networking and Communications
  5. User Services
  6. Facility Operations
  7. NASA-Wide Architecture
  8. Computer Security
  9. Application Services and Tools
  10. Visualization and Data Analysis
  11. Modeling and Simulation Projects

Scope of Work (2 of 5)

1. Program Management
   - Create environment where contractor-Government teaming approach will succeed
   - Manage contractor support for all Technical Areas
   - Ensure accomplishment of deliverables on time and within budget
2. Technical Integration
   - Conduct or integrate high-level and cross-cutting technical activities
   - Develop and help to implement HPC best practices
   - Manage integrated product teams (IPTs), to resolve interrelated bottlenecks in application workflows
3. Supercomputing and Storage Systems
   - Support lifecycle (6-7 years) of HPC and storage systems, from concept to disposal
   - System Development: Engineering, procurement, deployment, integration, testing, and enhancement
   - Software Development: application scheduling, system monitoring and reporting
   - Operations: System monitoring and maintenance, software upgrades
4. Networking and Communications
   - Wide area networking (WAN): High-bandwidth connectivity between Centers and to outside
   - Local area networks (LAN): Wired, wireless, HPC system interconnect
   - LAN/WAN Development: Engineering, procurement, deployment, integration, testing, and enhancement
   - Operations: Network monitoring, security, and maintenance; problem resolution

Scope of Work (3 of 5)

5. User Services
   - Provide primary user support, including 24x7 helpdesk
   - Manage account and resource allocation approval, user reporting
   - Develop documentation and conduct user training in facility and system use
6. Facility Operations
   - Perform physical plant operations and maintenance and property control
   - Maintain and update website; develop multimedia and communications
   - Perform IT support for facility desktop and server computers
7. NASA-Wide Architecture
   - Support implementation of Enterprise Architecture for NASA HPC
   - Support creation of multi-Center HPC environment
8. Computer Security
   - Plan, implement, document, and monitor security of HPC and facility computers
   - Support compliance with Federal Information Security Management Act (FISMA) and other applicable Federal regulations and NASA policies for IT security

Technical Areas 1 through 8 are foundational HPC facility activities
- Highly integrated and interdependent

Scope of Work (4 of 5)

9. Application Services and Tools
   - Port application codes to HPC systems; solve execution problems
   - Scale and optimize application codes for fast execution
   - Benchmarking to understand performance of HPC systems for NASA applications
10. Visualization and Data Analysis
   - Develop advanced data analysis, visualization, and interactive environments for increased insight into data and computations
   - Develop advanced visualization systems for massive, complex data
11. Modeling and Simulation Projects
   - Conduct complex, mission-critical computational analyses

Technical Areas 9, 10, 11 are service-centric

- Application-focused: interface between facility and users
  - Primarily respond to specific or long-term needs of users
  - Critical members of IPTs; enable major application breakthroughs
- Often more independent work than areas 1-8

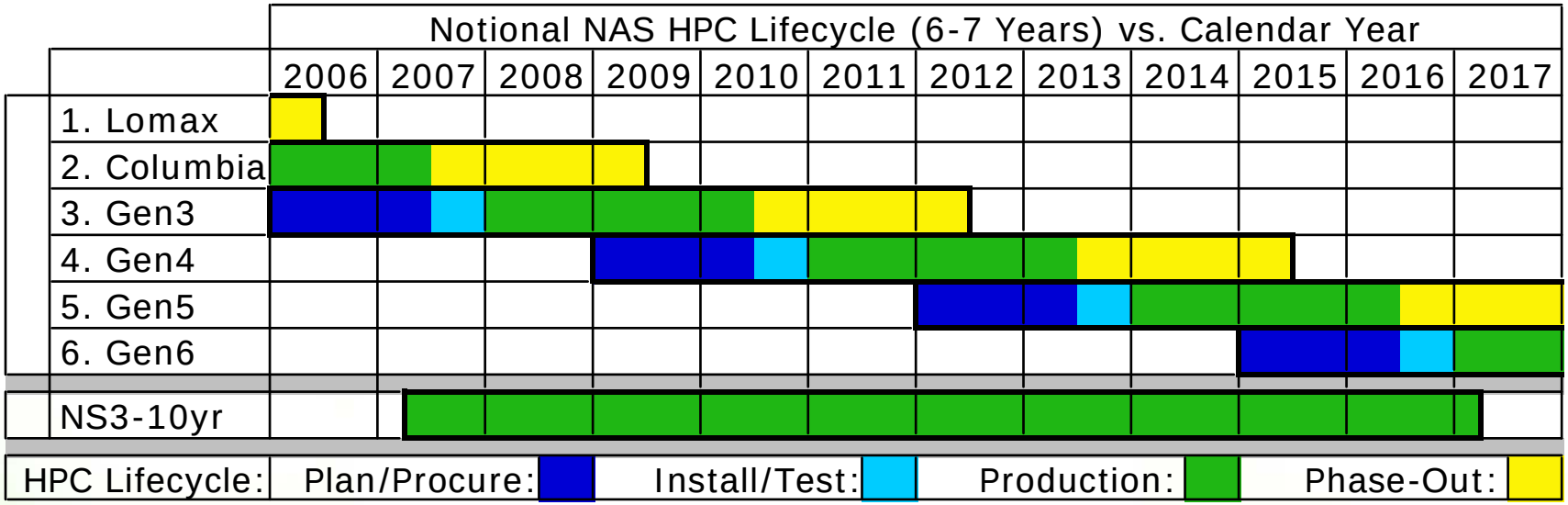
Scope of Work (5 of 5)

Additional Technical Areas: May be exercised during NS3

1. Other HPC Facility Support
   - NASA Center for Computational Sciences (NCCS) at Goddard Space Flight Center (GSFC), NASA's second major HPC facility, might request support under NS3
   - Other NASA Centers might also request NS3 support
   - Promote unified NASA HPC environment
2. Major HPC Procurements
   - Might be made through NS3 contract
   - Selection of procurement vehicle made by NASA based on expected best value before each major procurement
3. HPC-Related Research
   - Pursue significant hardware, software, and systems advances for NASA mission needs

Issues of Interest - Extended NS3 Term

- Provides continuity of services across HPC system lifecylces - average 6-7 years
- Enables experience and best practices to be carried forward across lifecycles for improved performance



Issues of Interest - Columbia Follow-On

- Goals
  - Meet NASA's growing demand for high-fidelity simulations
  - Leadership-Scale: Transition from Columbia 2048p to > 4x more capability
  - Capacity/Throughput: Maintain minimum ~60TF; seek > 4x more capacity
  - Mission-Critical: Maintain readiness for NASA's time-critical computations
- Columbia Attrition Schedule
  - Lease expiration: Oct 2006: 512-CPU Altix; Oct 2007: **11 512-CPU Altix systems**
  - NASA owns remaining 8 512-CPU Altix systems
- Acquisition Approach
  - Phased replacement of Columbia over 3 years (FY07-FY09) based on facility constraints, vendor benchmarking and proposals/quotes, and testbed evaluations for each phase
- "Best Value" Evaluation Factors (partial list)
  - Performance portability; Usability/user productivity
  - System Reliability, Availability, and Serviceability
  - Implementation (installation, operation) effort; Risk (system failure, instability)
  - Timing (technology availability); Opportunistic vendor partnerships
  - Robust technology roadmap over multiple generations

Issues of Interest - Leadership NAS Capabilities

- Setting the benchmark in rapidly and successfully procuring and installing HPC systems
- Integration and operation of large single-system-image computing
- Extending the capability of the CXFS global file system
- Global queuing to enhance system flexibility, usability, and utilization
- Advanced HPC usage monitoring and analysis
- Secure unattended file transfer
- Hyperwall-based visualization and exploration environments
- Concurrent visualization (i.e., during the computation)

Take-Away Messages

Base Requirement: Support HPC resources and services of NAS Division

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- Success requires highly skilled expertise in each technical area
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NASA SUPERCOMPUTING SUPPORT SERVICES (NS3)

BACKUP SLIDES:

RECENT NAS HIGHLIGHTS

June 2006 Highlight - Area 3 (HPC Systems)

- Two NAS staff members spoke about Columbia at the Gelato Itanium Conference & Expo (San Jose, April 23-26)—a third staff member sits on the board of directors for the Gelato organization
- One talk given, “Columbia Application Performance Tuning Case Studies,” was very well received and provoked many questions regarding specific tuning techniques covered in the presentation
- Attending and participating in the conference is an opportunity for technical interchange for NAS because it provides a forum for communicating directly with the platform designers about upcoming releases

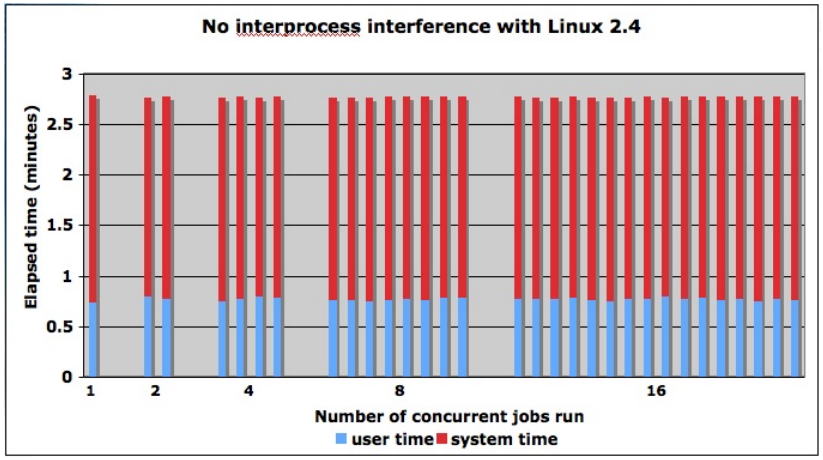


Figure from presentation by NAS staff member depicting running of multiple copies of a program with unaligned memory access, which do not cause interference between jobs on Linux 2.4 kernel.

June 2006 Highlight - Area 3 (HPC Systems)

- NAS HPC Systems Group evaluated and installed a file transfer program, “bbftp”—it improves transfer rates of large files into and out of Columbia environment 30- to 70-fold
- New mechanism recently provided scientists at NASA Langley (involved with Return to Flight work) with the ability to conduct frequent transfers of large files—accomplished significantly more computations and post-processing under time-critical conditions than they would have without the file transfer tool
- Improvement in file transfer speeds applies to both transfers local to Columbia system and between Ames and other NASA centers
- Due to the bbftp’s unwieldy command-line interface and file-transfer feature set, the NAS Systems Group developed more user-friendly wrapper program, “bbscp”
- bbftp will be used to perform analyses related to the upcoming STS-121 Shuttle mission

SCP vs BBFTP

bbftp improves transfer rates of large files in most cases by 30- to 70-fold—it is more streamlined than scp for the single purpose of transferring large files.

June 2006 Highlight - Area 3 (HPC Systems)

- In preparation for upcoming Return to Flight missions it is critical for NAS to ensure reliability of the Columbia supercomputer
- To keep Columbia running at maximum efficiency, preventive maintenance (PM) is performed on a regular basis—Columbia systems are rotated through a PM schedule every 6-7 weeks
- Goal: prevent problems before they occur—with due diligence on a round-robin PM schedule, unnecessary downtime has been dramatically decreased, resulting in increased productivity for NAS users

SGI Service Engineer performs regular preventative maintenance on a Columbia node.

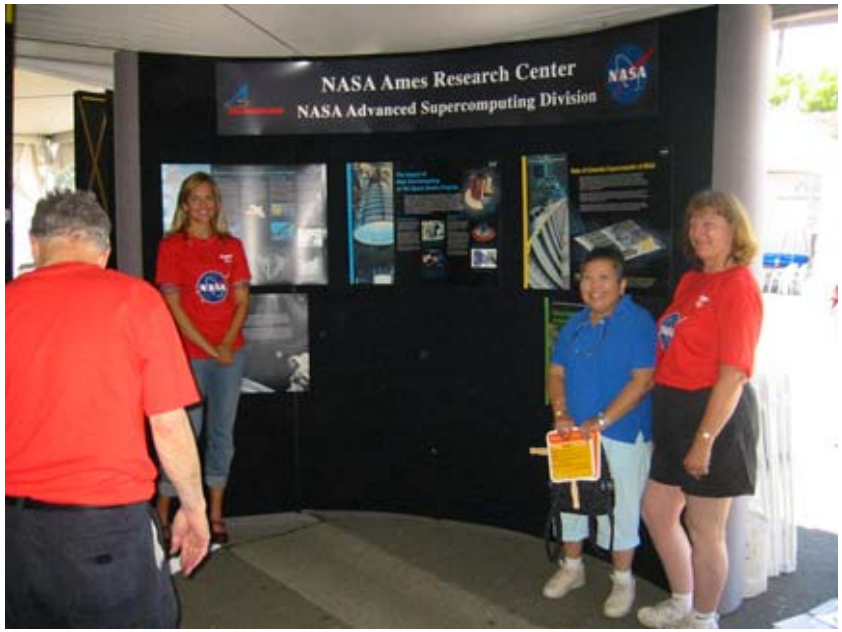
June 2006 Highlight - Area 4 (Networking)

- NAS Networking team completed the NASA Research and Engineering Network (NREN) system FISMA-compliant IT security plan which was accredited by the Ames Chief Information Officer
- 145-page document covers threats, vulnerabilities, and risk mitigations related to NREN's WAN system (including network connections into and out of the Columbia supercomputing environment)
- The document incorporates a contingency plan and detailed risk assessment for network outages and security break-ins, for example
- NAS Networking team has a coordinated process in place to ensure safety and integrity of data generated and stored within Columbia supercomputing environment

The NASA Research and Engineering Network system IT security plan was recently completed and accredited by the Ames Chief Information Office.

June 2006 Highlight - Area 6 (Internal Ops)

- Several Columbia-supported applications were displayed at a community event in Sunnyvale, Calif. June 3-4, 2006, drawing a crowd of more than 5,000
- This community event provided NAS with an excellent opportunity to educate the general public about some of the work being computed on the Columbia supercomputer, including Shuttle analysis and redesign work, and climate and ocean modeling
- This display will be used at three additional community events during the summer of 2006 to inform visitors about the important role NAS plays in supporting NASA missions



NASA civil servants and contractors on stand-by in front of Columbia display to share information about NAS' role in supporting NASA missions.

June 2006 Highlight - Area 8 (IT Security)

- NAS IT Security team recently deployed a Secure Unattended Proxy system that enables Columbia supercomputer users from an external host to carry out unattended operations within Columbia's secured computing environment
- The SUP addresses security challenges surrounding remote, unattended operations such as file transfers into the Columbia enclave under program control by allowing the user to acquire a limited lifetime, limited capability ticket using a SecurID fob for authentication
- In support of unified approaches to security and file handling, and to further enhance the collaborative computing environment between NASA Ames and NASA Goddard, NASA Goddard's Center for Computational Sciences is in the process of deploying a SUP at their site

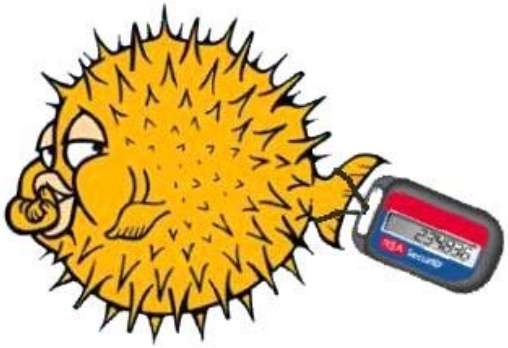
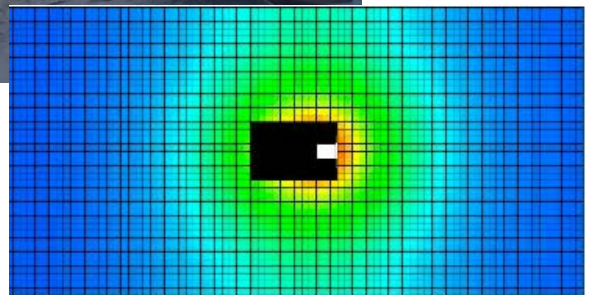


Image of the "OpenSSH fish" (Open Secure Shell) carrying a SecurID® token—two major components of the SUP software.

June 2006 Highlight - Area 9 (Applications)

- NAS Application Performance and Productivity (APP) group assisted NESC and JSC researchers with successfully porting SINDA code to Columbia, enabling them to conduct numerical analyses of damaged Shuttle Orbiter thermal tiles
- APP group ported SINDA by identifying and correcting several issues including an incompatibility JSC researchers were experiencing—some older syntax used in the code not recognized by Columbia's updated Linux OS
- Also assisted JSC in utilizing Columbia to run parallel copies of SINDA on independent datasets
- Given the large number of cases required for JSC's damaged tile study and the tight deadline, porting the software to the fast Columbia platform was key to speeding up analysis
- Background: SINDA code is an analytical tool used for solving heat transfer problems



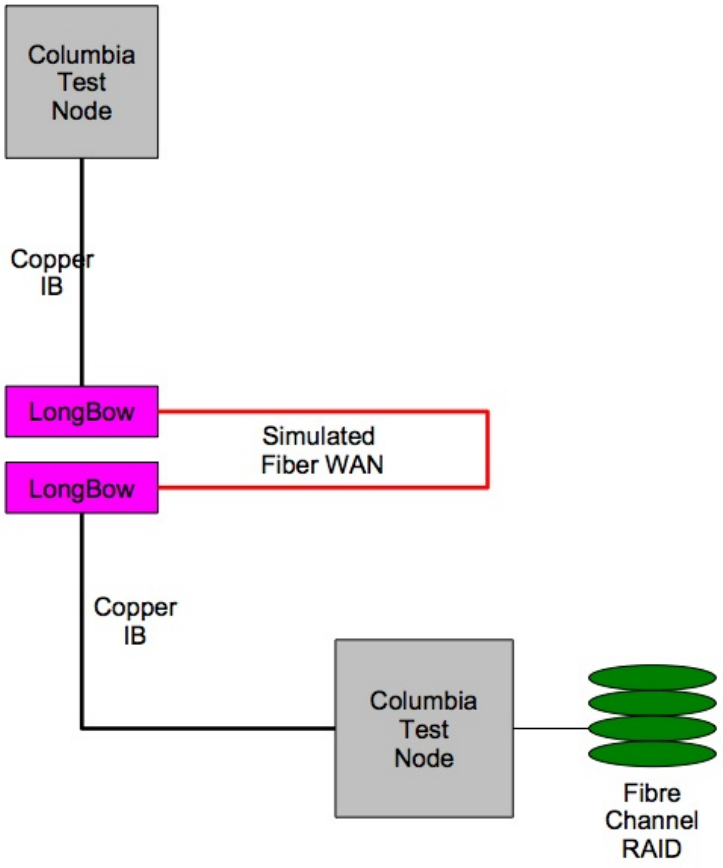
JSC researchers ran SINDA code to conduct numerical analyses of damaged Shuttle Orbiter thermal tiles. Lower image (courtesy of Boeing) depicts structure temperature contour plot generated using SINDA.

June 2006 Highlight - Publications and News

- Publications:
  - "Performance Characteristics of an Adaptive Mesh Refinement Calculation on Sclar and Vector Platforms"; CR 2006 Conference, May 3-5 in Ischia, Italy .
  - "Petascale Computing: Impact on Future NASA Missions"; Distributed European Infrastructure for Supercomputing Application Symposium, May 4-5 in Bologna, Italy.
  - "High-Fidelty CFD – Mature Technology"; Hydro Colloquim at the Naval Surface Warfare Center, Carderock Division, May 22.
  - "Performance Analysis of Cray X1 and Cray Opteron Cluster"; Cray User Group Conference 2006, May 8 – 11, Lugano, Switzerland.
  - "Performance Comparison of Cray X1 and Cray Opteron Cluster with Other Leading Platforms Using HPCC and IMB Benchmarks"; Cray User Group Conference 2006, May 8 – 11, Lugano, Switzerland.
  - "Hurricane Forecasts with a Global Mesoscale-Resolving Model: Preliminary Results with Hurricane Katrina (2005)"; for publication in Geophysical Research Letters
  - "Fleshing-out Pharmacophores with Volume Rendering of the Laplacian of the Charge Density and Hyperwall Visualization Technology"; for publication as a book chapter in "QTAIM: Quantum Theory of Atoms in Molecules"
- News:
  - "Black Holes Collide, and Gravity Quivers"; New York Times; May, 2, 2006; by Kenneth Chang

July 2006 Highlight - Area 4 (Networking)

- NAS Network engineers are currently evaluating the practicality of extending Infiniband over a WAN (e.g., between ARC and GSFC), which would facilitate more latency-sensitive applications such as Earth science modeling
- Initial steps involve local connections using Obsidian Longbow switches, then adding a metro-area “dark fiber” loop between the switches to increase inter-switch latency
- NAS engineers expect to wrap up their work with the LAN test environment in the next several months after which they hope to deploy the WAN version
- The outcome could provide an effective way to better support remote data access and/or system backup capabilities between centers



Infiniband Over WAN Test Environment Diagram.

July 2006 Highlight - Area 4 (Networking)

- NAS network engineers assisted with the June 7 emergency communications drill at ARC to evaluate center readiness for handling situations with limited or incapacitated telecommunications infrastructure
- The test was deemed successful, but uncovered several areas for improvement including the need for better documentation of emergency communications areas throughout ARC, and availability of backup power and on-hand technical support

The portable satellite communications equipment (TAZ), which acted as a backup communications link for the exercise.

July 2006 Highlight - Area 4 (Networking)

- A team of eight NAS staff members participated in the SGI User Group 2006 Technical Conference and Tutorials in Las Vegas, June 5-9, including delivering paper presentations and moderating/facilitating forums
- NASA's attendance at the annual SGI User Group meeting is important to the agency's HPC effort—it is a chance to exchange experiences and new ideas with HPC experts from across the nation and around the world
- As appropriate, new techniques gleaned from the meeting can be applied to the NASA computing environment to improve system performance, which enhances problem solving capabilities for NASA's mission-critical applications

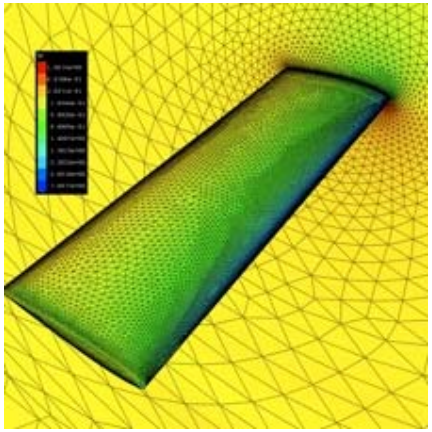
July 2006 Highlight - Area 6 (Internal Ops)

- Quick actions on the part of NAS support staff prevented arcing in a power distribution unit (PDU 2) from escalating into a facility fire that could have severely impacted the Columbia supercomputer
- These actions also minimized the impact on the two Columbia nodes powered by PDU 2
- This event demonstrates the importance of having 24x7 on-site staffing of the computer rooms
- After the power was shut off, the breakers were replaced, and the nodes rebooted—everything was running fine with the exception of one node coming up with just 508 of its 512 processors available

10,240 processor Columbia Supercomputer (top); Power Distribution Unit 2 that supports Columbia nodes C3 and C4 (above).

July 2006 Highlight - Area 9 (Applications)

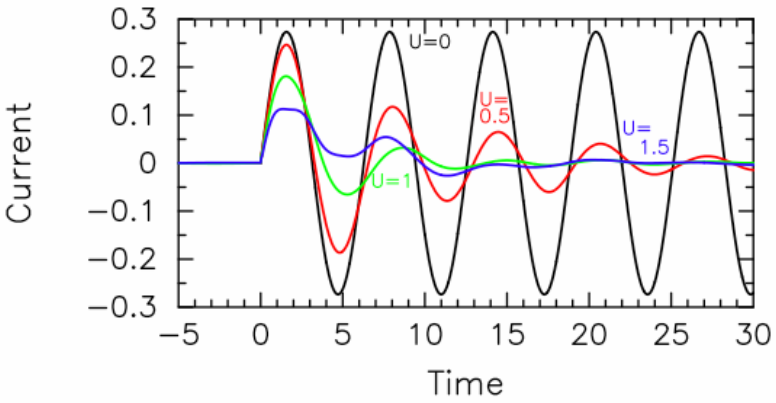
- NAS computer scientist recently optimized the USM3D flow solver (used for memory- and processor-intensive calculations of dynamic stability for aircraft), achieving a nearly four-fold speed-up
- The improved flow solver will significantly enhance productivity and creation of an aerodynamic database on the CEV and Launch Abort System, which will require 40-plus solutions per month for the next year
- USM3D, is a component of the aero analysis and design system, TetrUSS, which is used heavily on NASA's Columbia supercomputer and Department of Defense high-performance computing machines



USM3D flow solver applied to the HI-ARMS wing at a 12-degree angle of attack.

July 2006 Highlight - Area 9 (Applications)

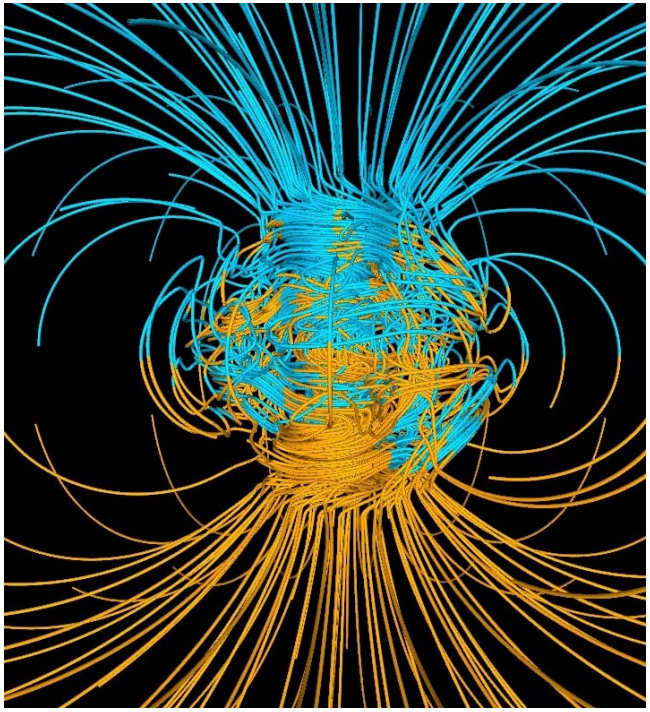
- NAS APP Group recently assisted Georgetown University Physics professor, Jim Freericks in successfully optimizing his code (a nonequilibrium dynamical mean-field theory solver) on the Columbia supercomputer
- The 6X+ speedup achieved will accelerate Freericks' progress on studying properties of Mott insulators (materials ideally suited for "smart electronics")
- The optimized code achieved 4 GFLOPS/process (> 60% of peak performance) and completed a medium test case on 64 of Columbia's processors in less than 40 minutes--compared to 4 hours with the original code



Bloch oscillations (alternating current driven by a large static electric field) are seen to decrease in amplitude as scattering is increased in the material (increasing U). When the material undergoes the Mott metal-insulator transition, the oscillations lose all of their regularity.

July 2006 Highlight - Area 9 (Applications)

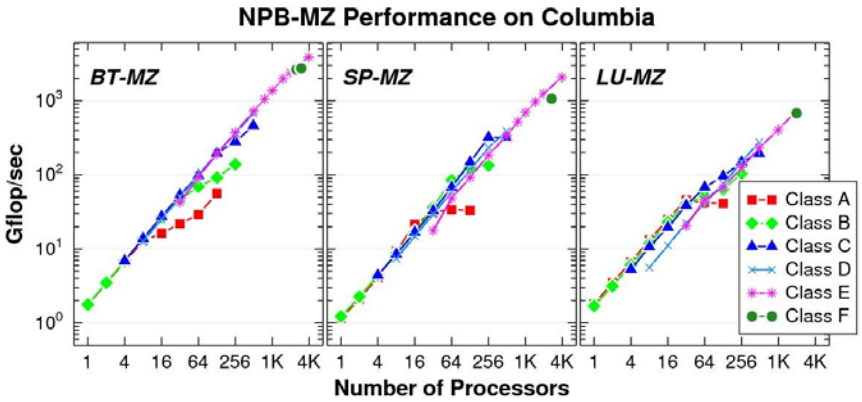
- NAS APP group recently assisted a UC Santa Cruz researcher with porting and parallelizing the GEO51 code to Columbia
- The APP group modified GEO51 to scale on shared-memory computer architectures such as Columbia
- This work yielded higher fidelity simulations of Earth's geomagnetic field (of geodynamo, the mechanism in the Earth's fluid core that maintains the geomagnetic field)
- Computer simulations using this code will significantly advance the understanding of the origin and evolution of zonal winds on large planets and global magnetic fields observed on some terrestrial planets



Snapshot of a magnetic field (illustrated as field lines) from one of the geodynamo simulations (yellow lines represent outward flow, while blue represents inward flow).

July 2006 Highlight - Area 9 (Applications)

- NAS computer scientists recently released two new versions of the NAS Parallel Benchmarks (NPB) to the high-performance computing community: NPB3.2.1 and NPB3.2-MZ
- NPBs are derived from important NASA applications and designed to mimic the workload of realistic applications— tuning Columbia to run NPBs well translates to performance gains in key applications on Columbia



Performance of new NAS Parallel Benchmark (NPB) NPB-MZ on NASA's Columbia supercomputer.

July 2006 Highlight - Publications

- "Unsteady Aerodynamic Computations of Parachute-Capsule Configuration by Using the Euler/Navier-Strokes Equations"; at AIAA Applied Aerodynamic Conference, June 5-8, 2006 in San Francisco, CA (also for publication in the Spacecraft Journal)
- "Aerodynamic Shape Optimization Using a Cartesian Adjoint Method and CAD Geometry"; 24th AIAA Applies Aerodynamics Conference, June 5-8, 2006 in San Francisco, CA
- "Propack 4 Experiences on Columbia"; the SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- "Unscheduled Interruptions on the Columbia Supercomputer"; SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- "Experience with PBSPro on a 4 x 512p Altix SuperCluster"; SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- "A Scalability Study of SGI Clustered XFS Using HDF Based AMR Application"; SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- "CXFS on the Columbia System"; SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- "A Scalability Study of Columbia using the NAS Parallel Benchmarks"; SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- "Addressing the Tension Between Strong Perimeter Control and Usability"; 11th ACM Symposium on Access Control Models and Technologies, June 7-9, 2006 in Lake Tahoe, CA
- "The NASA Space Communications Data Networking Architecture"; AIAA SpaceOps 2006, June 19-23, 2006, Rome, Italy

July 2006 Highlight - Presentations

- “Reentry-Vehicle Shape Optimization Using a Cartesian Adjoint Method and CAD Geometry”; 24th AIAA Applies Aerodynamics Conference, June 5-8, 2006 in San Francisco, CA
- “Capsule Abort Recontact Simulation”; 24th AIAA Applies Aerodynamics Conference, June 5-8, 2006 in San Francisco, CA
- “Columbia Application Performance Tuning Case Studies”; SGI Users Group Conference, June 5-9, 2006 in Las Vegas, NV
- “An improved AB Initio Potential Energy Surface for CH4”; International Symposium on Molecular Spectroscopy, June 19-23, 2006 in Ohio State University

July 2006 Highlight - News Events

- “Spaceship Work Saves NASA Ames Computing Jobs”; FCW; June 6, 2006; Aliya Sternstein
- “NASA and NSF Computers Simulate Sun’s Corona”; BBC News; June 27, 2006; Kandy Ringer
- “A New Sun Born in Computer Wears the Right Look for Eclipse”; Space Ref; June 27, 2006; Goddard Press Release
- “Computer Model Can Predict Solar Weather”; Space Daily; June 27, 2006; Staff Writers
- “IBM's BlueGene/L Tops Supercomputing List”; Enterprise IT Planet; June 28, 2006; Pedro Hernandez
- “Top 500 Supers: Brace Yourself for Petaflops Systems”; IT Jungle; June 28, 2006; Timothy Prickett Morgan
- “State Still Reigns in Supercomputing”; Inside Bay Area; June 29, 2006; Ian Hoffman
- “Voltaire Solutions Continue to Drive InfiniBand Growth on Top500 List; InfiniBand-based Supercomputers Grow 33 Percent Since November 2005; Year over Year Growth of 150 Percent”; Business Wire; June 29, 2006; Volitaire Press Release
- “Top500 Supercomputers: IBM Continues to Forge Ahead”; Heise Online; June 29, 2006; Robert W. Smith

Take-Away Messages

Base Requirement: Support HPC resources and services of NAS Division

- NAS Mission: *Deliver **world-class** high performance computing (HPC) capability to **all NASA missions**, facilitating the rapid development and application of advanced knowledge and technology to enable mission success*
- Success requires highly skilled expertise in each technical area
- Contractor and NASA perform as highly integrated team
- Contractor expected to bring experience and best practices in operating world-class HPC facility
- Outcomes for NASA's computation-intensive and data-intensive challenges
  - Dramatic reductions in time-to-solution
  - Breakthroughs in accuracy and scale of solution
  - Rapid advances in scientific and engineering insight
- Goal: Enhanced mission impact for hundreds of simultaneous HPC users and projects across NASA Centers, Mission Directorates, and partner organizations
- **NASA has an inspiring mission; NAS is an exciting place to work!**