NCCS/SIVO Open House

14 February 2008

Agenda

Welcome & Introduction
Phil Webster/NCCS, Mike Seablom/SIVO

About the NCCS

Cluster Upgrade	*Dan Duffy*
Data Sharing Services	*Harper Pryor*

About SIVO

Advanced Software Technology Group	*Tom Clune*
Scientific Visualization Studio	*Horace Mitchell*
ESD Education & Public Outreach	*David Herring*

Questions / Comments	*Phil Webster & Mike Seablom*
Tour of NCCS Facility	*NCCS Staff*

Software Integration and Visualization Office

SIVO-Who We Are

Advanced Software Technology Group
Tom Clune

- Develops & maintains application software
- Provides performance tuning of science codes
- Advocates professional software engineering practices
- Coordinates software integration efforts across Goddard and across NASA

Scientific Visualization Studio
Horace Mitchell

- Provides visualization services for a wide range of Earth and Space science customers
- Provides scientific visualizations targeted at NASA managers, policy makers, and the general public
- Develops visualization applications for use as analysis tools by scientists

MAP Integration Group
Gail McConaughy

- Serves the MAP program by selecting and implementing appropriate technologies that will benefit the development of Earth System models
- Develop software in support of Observing System Simulation Experiments (OSSEs)

Education & Public Outreach
David Herring

- Provides freely-available Earth Science visualizations through web-based publications
- Develops products for educators
- Coordinates Goddard Education & Public Outreach activities

NCCS & SIVO Partnership

NCCS

- High performance computing
- Data archival & stewardship
- Code development environments and modules support
- Scientific software code repository for SMD
- Data analysis environment and collaborative tools
- HEC networks
- Data sharing and publication
- User services

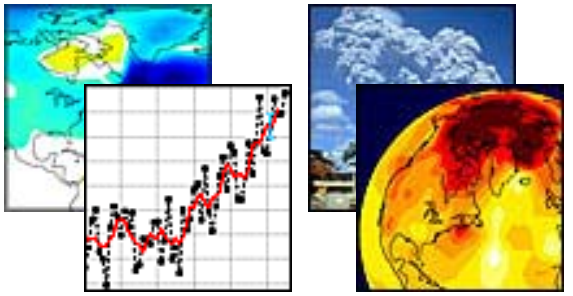
SIVO

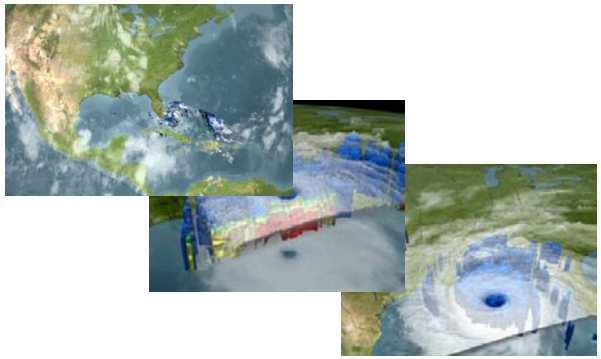
- Application support and benchmarking
- Software design, development, and implementation
- Code porting and optimization/parallelization
- Visualization services
- Consulting & Training

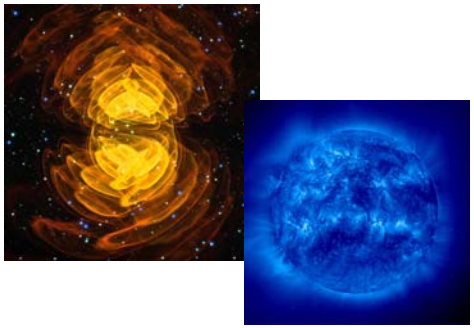
SIVO and the NCCS deliver a full range of HPC compute and data services to support the SMD science community.

NCCS User Community

- Support SMD modeling and analysis activities in Earth, space, and solar research:
  - Atmospheric modeling
  - Ocean modeling
  - Land surface modeling
  - Space and solar modeling
  - Coupled models and systems of models
  - Observing systems studies
- Extend HPC support to other SED science and engineering activities







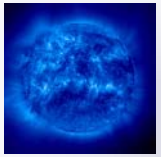
System Acquisition Philosophy

- Commodity-based approach to capacity computing:
  - Most flexible approach to support broad range of scientific & engineering applications
  - Builds a consistent HPC architecture
  - Reduces administrative cost and complexity
  - Architecture attends to data-centric needs of our users and applications
  - Supports flexible job execution opportunities – jobs not tied to specific resources
  - Ease of migration for users & Continuity of user experience
- Annual augmentation
  - Minimizes user impact while extended resources
  - Maintains balanced HPC environment
- ~3-year technology refresh
  - Provide sufficient opportunity to migrate users and applications to newer technologies
- Acquisition strategy based on:
  - Performance successes realized in Discover environment
  - Other lessons-learned
  - Characterized by standard HPC benchmarks
  - Maximize additional capacity with available funds
  - Competitive acquisition strategies to provide the best price performance

Data-Centric Conceptual Architecture

Data Portal & Data Stage

- Developing requirements for follow on system
- Significant increase in storage and compute capability



Collaborative Environments

- Web based tools
- Modeling Guru

Analysis

- Conceptual framework for analysis environment
- Matlab on Discover

DATA

- Single NCCS home, scratch, and application file system
- Data management initiative

Visualization

- Collaboration with Scientific Visualization Studio to provide tools
- Visualization nodes on Discover

High Speed Networks

Compute

- Significant upgrade to Discover
- Decommission Explore

Archive

- Increased disk cache for longer file retention
- Increase tape capacity to meet growth requirements
- Upgrade file server (newmintz) and data analysis host (dirac)

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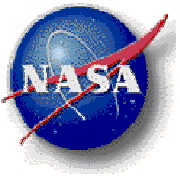
Tour of NCCS Facility	*NCCS Staff*

What are we going to do with Explore? Explore System Decommission

- Lease is due to expire at the end of September
- NCCS will not renew this lease
  - More cost effective to upgrade than it is to purchase the residual value and maintenance
- No significant changes to Explore are planned
  - Maintain the O/S with security patches and bug fixes as needed



Minimize User Disruption

- The primary goal in planning the cluster upgrade is to minimize the impact on the user community
- How will we do that?
  - Support in migrating applications and data from Explore to the Discover cluster
  - Consistent user environment
  - Consistent architecture
  - Scalable approach to both compute and storage needs; end result is a balanced system
  - Provide about a two month overlap between first stage of upgrade and decommission of Explore
  - First stage will be roughly twice the peak capacity of Explore

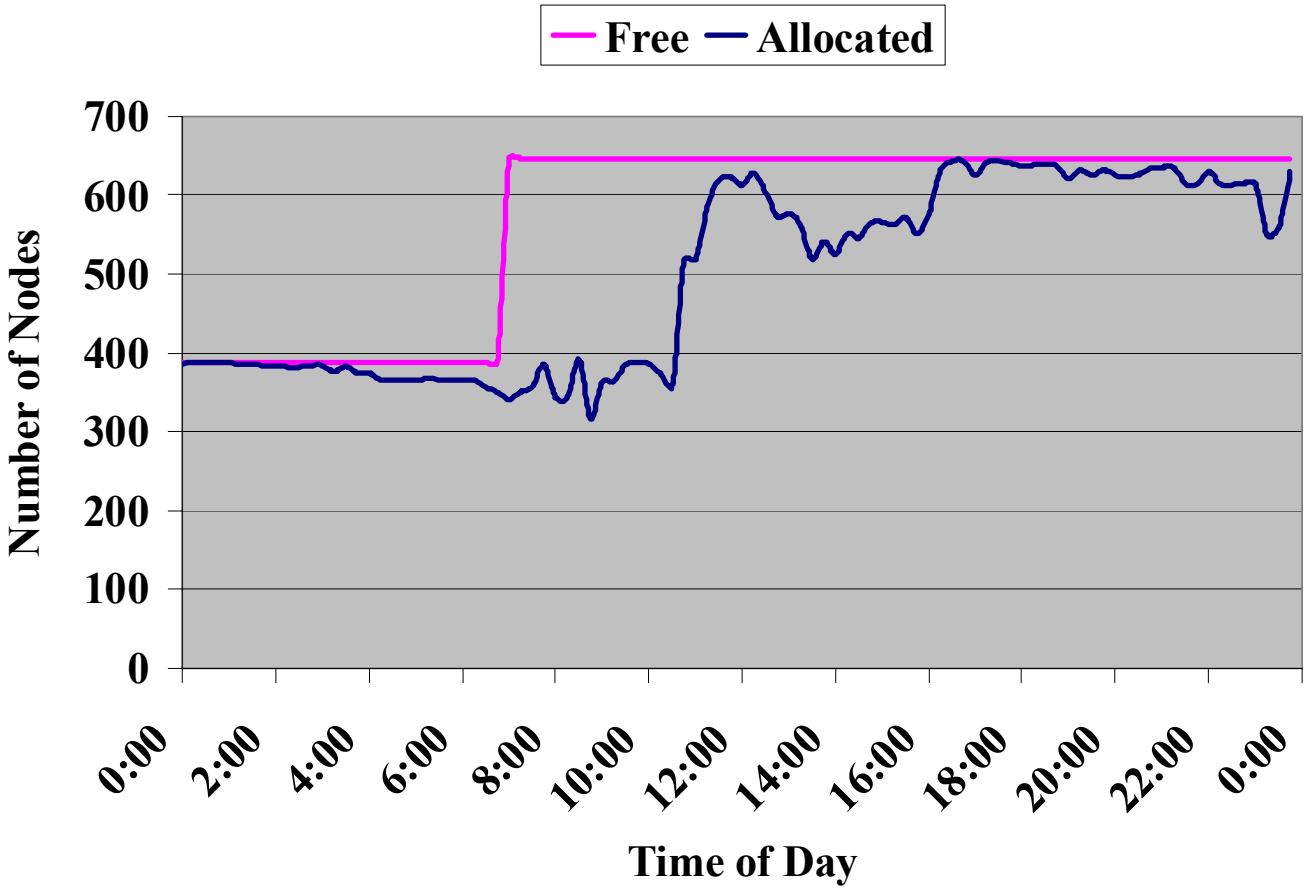
How are we going to provide a consistent architecture and user environment?

- Hardware
  - Intel Xeon processors
    - Binary compatible
    - Approximately the same speed (between 2.67 GHz and 3.0 GHz)
    - Quad-core rather than dual-core
  - Infiniband
  - 2 GB/core – which is an increase over existing environment
- Software
  - SLES
  - MPI
- User Environment
  - Modules
    - All the same modules will be available
  - PBS
    - Though you may need to make some changes to your scripts
    - Still exploring a more generic way to submit jobs so users do not have to specify or worry about landing on dual-core versus quad-core nodes

We have done this before

Addition of SCU2
11 September 2007

- Users went home on Monday night with only 388 nodes available for compute
- An additional 258 nodes were added to the PBS queues around 7:00 a.m. Tuesday morning
- By 11:00 a.m. Tuesday morning, the full 646 nodes were almost complete allocated

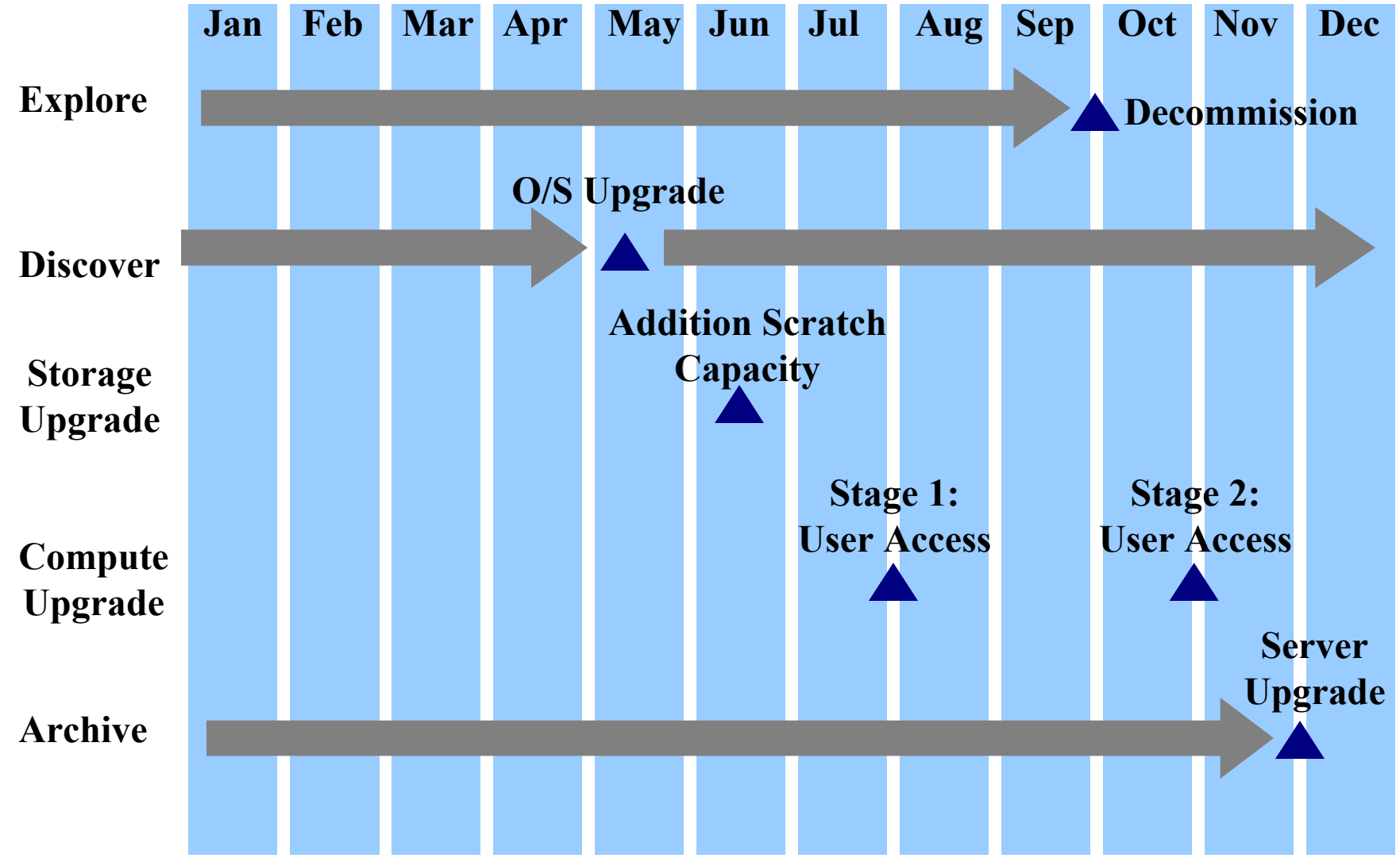


This is the kind of success we are targeting for the next upgrade!

There will need to be some changes

- Discover will need to be upgraded
  - Maintain compatibility with vendor supported software matrix
  - Provide compatibility with cluster upgrade
- Software Upgrade (2Q08)
  - O/S upgrade to SLES 10 SP1
  - Infiniband OFED 1.2
  - MPI Scali 5.6
  - Addition of Intel MPI
  - PBS 9.0
- Changes will be made on the test and development system and representative applications will be verified

Target Timeline & Milestones



What do you need to do to prepare?

- Support is immediately available to start
  - Getting an account on Discover
  - Porting your applications and scripts to Discover
  - Staging your data from Explore to the appropriate resource
- What about my data on Explore?
  - It is not going anywhere.
  - As always, you should save all critical files into the archive as soon as possible.
  - We will want to eventually clean off all the disks to reuse those disks elsewhere in the NCCS.
  - We will be asking you to stage your data from Explore into the archive or Discover as needed. The NCCS can help with this!
- How will we track this?
  - User services will track the migration of all groups from Explore to the new system.
  - As always, users can request support or ask general questions to support@nccs.nsaa.gov

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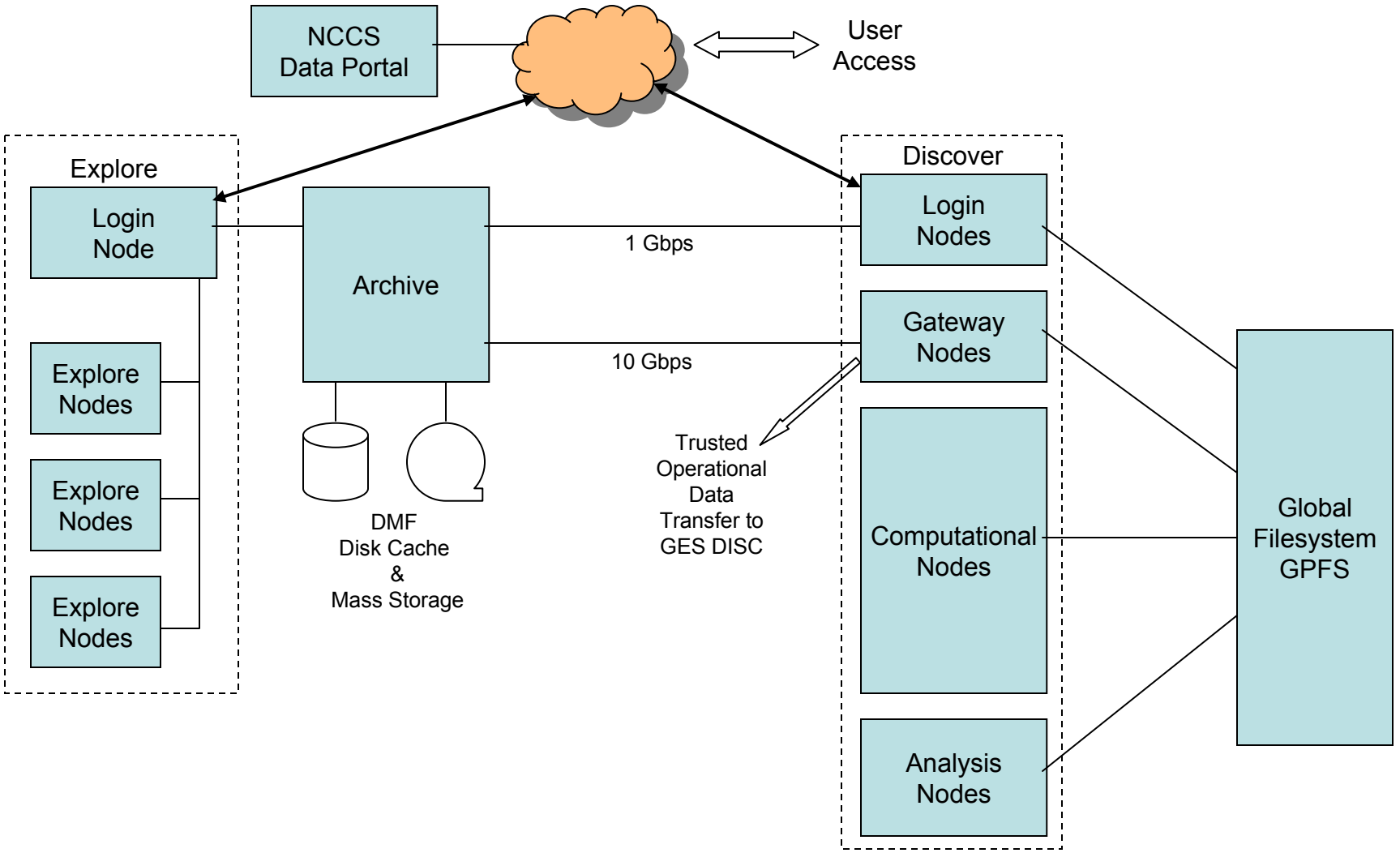
Tour of NCCS Facility	*NCCS Staff*

Data Sharing Services

NCCS supports a collection of service capabilities to better support scientific code development, job execution, data analysis, and collaboration with the scientific community.

- Shared on-line data repositories within the NCCS HPC environment for development team use
- Large, temporary input data holding areas to expedite production
- Access to production data output from the HPC analysis environment to support monitoring and assessment
- Data portal for sharing results with collaborators without requiring NCCS users accounts

NCCS Conceptual Environment



NCCS File System Attributes

- Shared on-line data repositories within the NCCS HPC environment for development team use
  - /nobackup areas established for finite timeframes to support group use
  - Examples: group access to shared codes, input or simulated data sets, etc.
  - Simply ask for assistance via support@nccs.nasa.gov
- Large, temporary input data holding areas to expedite production
  - /nobackup areas established for finite timeframes to support production use
  - Supports large input data sets to lesson mass storage impact on production
  - Simply ask for assistance via support@nccs.nasa.gov
- Access to production data output from the HPC analysis environment to support monitoring and assessment
  - /nobackup areas established for finite timeframes to support multiple access needs to large output data sets
  - GPFS file system is accessible from computation & analytic nodes
  - Simply ask for assistance via support@nccs.nasa.gov

NCCS Data Portal

- Sharing information and preliminary results with scientific collaborators without requiring NCCS user accounts

  - Approach:
    - Develop capabilities for specific projects and generalize for public use
    - Resources managed by the NCCS
    - Software development by SIVO and SMD users

  - Capabilities:
    - Web/Portal registration
    - Usage monitoring & reporting
    - Directory listings
    - Data download
    - Limited data viewing/display (GrADS, IDL, OpenDAP)

NCCS Portal Support

NCCS maintains Data Portal environment with:

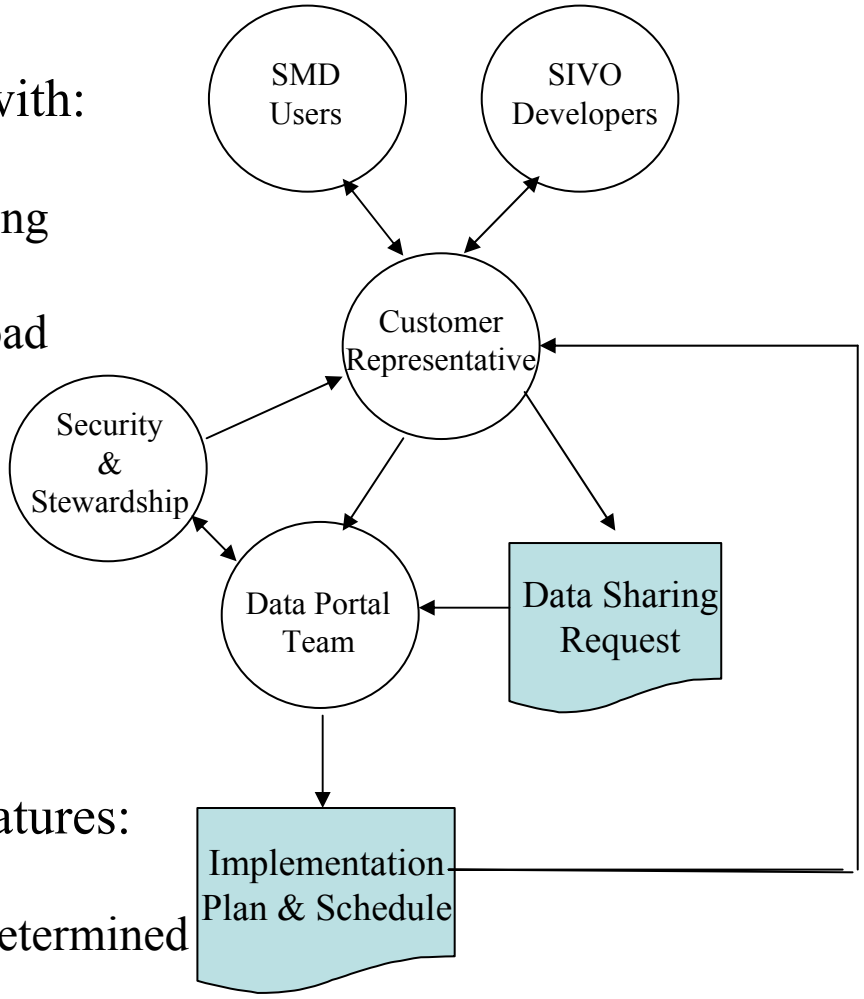
- Systems administration support
- System security administration & monitoring
- Agency required data sharing paperwork
- Development tools – web, display, download

NCCS will manage user requirements to completion:

- Coordinate internal development
- Establish user development area
- Support your customer needs

NCCS will assist in establishing standard features:

- Support assessment
- Promote features to standard services, as determined
- Maintain underlying services



NCCS Data Portal Features

- Architecture
  - Selective portal disks mounted to NCCS archive to facilitate data movement from mass storage
  - GPFS based to serve data for multiple sharing services
    - Data files can be used by Web Mapping Services (WMS),
    - OpenDAP/GrADS Data Server
    - Anonymous ftp

- Disk Upgrade, February 2008
  - 120 TB (4X previous capacity) to host more data
  - Improved disk technology for more reliable storage
  - Additional data paths between the portal CPUs and the storage array for improved I/O performance

Discussion

- Let us know if you have a project that could benefit from data sharing services – so we can plan for it.

- Contact us if you want to explore opportunities.

- Your Points of Contact are:

  Harper.Pryor@nasa.gov 301-286-9297

  And

  User Services: support@nccs.nasa.gov

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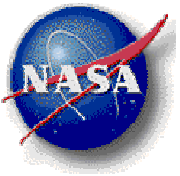
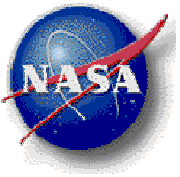


The Modeling Guru

- New “knowledge base” to support scientific modeling within NASA
  - Commercial package, customized by ASTG, hosted by NCCS
  - Moderated discussions/forums
  - Document repository
  - Questions and support
- Goal is to leverage and share community expertise
  - New paradigm for level 2 support provided by SIVO to the NCCS
  - Topics/Communities include
    - HPC systems
    - Programming languages (e.g. SIVO F2003 Series)
    - Models: GEOS-5, GMI, modelE, etc
- Access: https://modelingguru.nasa.gov
  - Most categories publicly visible
  - Posting requires login
    - All NCCS users have login by default
    - Anyone with relevant interest can request an ID

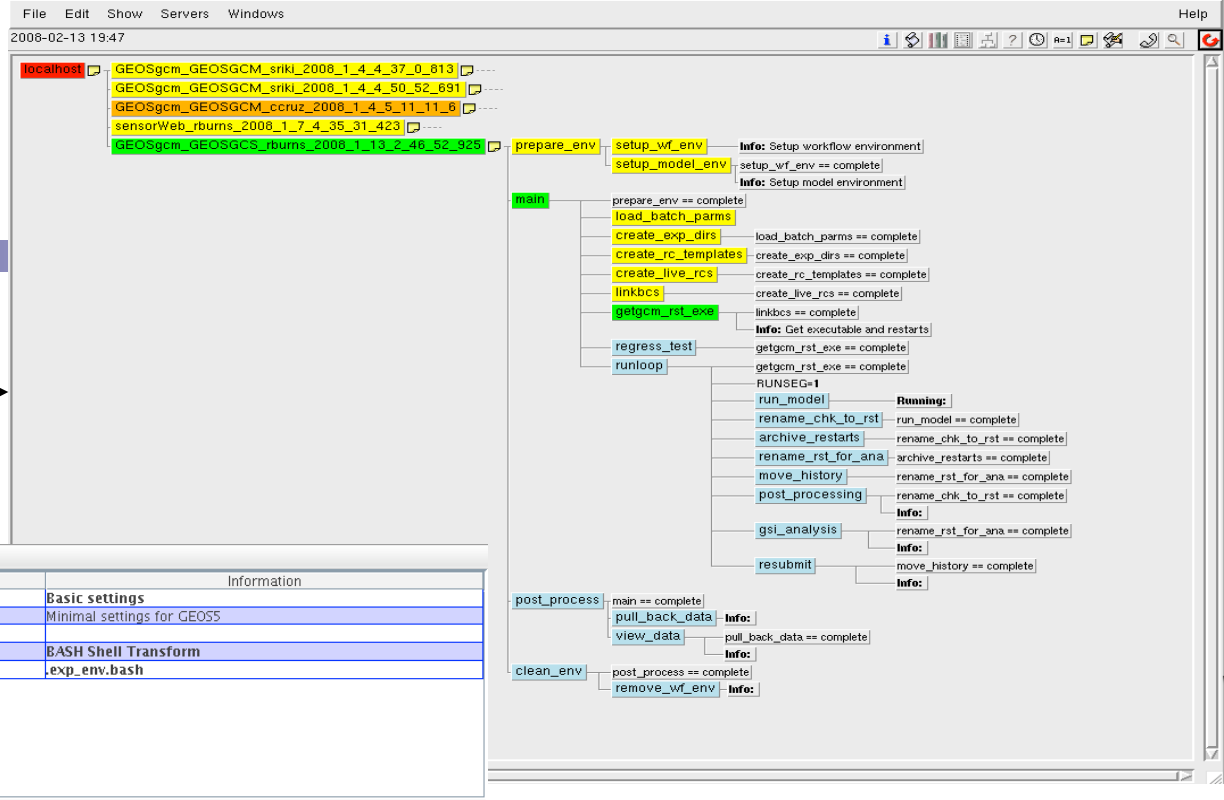
NASA Modeling Guru: Clearspace: NASA Modeling Guru
https://modelingguru.nasa.gov/clearspace/index.jspa
Google
Published Articles
RSS Feeds
SAX
Guru
ASL Browser
DOUG development pages
Exchange
National We...e - Oakland
Web Paint-by-Number
CAF
GSFC Exchange
Id hint
Bibtex
NASA Modeling Guru: Cl...
Web Paint-by-Number
+ Modeling Guru Home
Modeling Guru
BETA
Welcome, clune (Log out)
New
Your Stuff
History
Browse
Enter Search Term
NASA Modeling Guru
Modeling Guru is a research and collaboration resource for all those concerned with NASA scientific models or NASA's HPC systems.
Communities
Space Science Models
DYNAMO
Atmospheric Dynamic Models
GEOS-DAS
GEOS
MERRA
GCE
GISS ModelE
Climate@Home
fvCore
Atmospheric Chemistry Models
GEOS-CHEM
GMI
Ocean Models
Poseidon
MOM4
MIT OCCM
Solid Earth Models
MAP Modeling Environment Workflow Tool
Languages, Libraries & Tools
Software Development
Computing Systems & Technologies
Modeling Guru FAQs, Feedback & General Questions
SIVO Internal
Welcome NASA Modelers
Modeling Guru's combined forums and knowledge base is becoming a repository for the accumulated expertise of NASA's scientific modeling community. All NASA modelers and associates are encouraged to participate and help us fill the "holes" in our modeling knowledge.
Disclaimer: While this is a government resource, it is not totally screened for content. By accessing this site, you agree to use it at your own risk.
Become a Registered Member Today!
Registration offers you a number of benefits, including being able to view restricted material, ask questions, contribute your expertise and more. View registration instructions in the Modeling Guru Registration FAQ.
New to Modeling Guru?
This site offers a number of powerful features, including "wiki" documents, RSS feeds, search tools, and more. For a brief intro, see Modeling Guru Basics or take the more-detailed Quick Tour.
Important Links
How To Register
Frequently Asked Questions
Posting Policy
What's New
All Content
Your View
Go to: Discussions Documents Blog Posts
ANNOUNCEMENT:
Edit
Expire
Delete
SIVO Seminar Series on Fortran 2003
by clune at Jan 29, 2008 9:02 AM
SIVO is hosting a biweekly series on the Fortran 2003 standard. The next session on "Interoperability with C" will be on Tuesday February 12th. Materials for the seminars will be available here in Modeling Guru. Participants are also encouraged to use Guru's Languages, Libraries & Tools community for further discussions on the standard.
Modeling Guru text editor issue
39 minutes ago in Modeling Guru FAQs, Feedback & General Questions
by rsyed

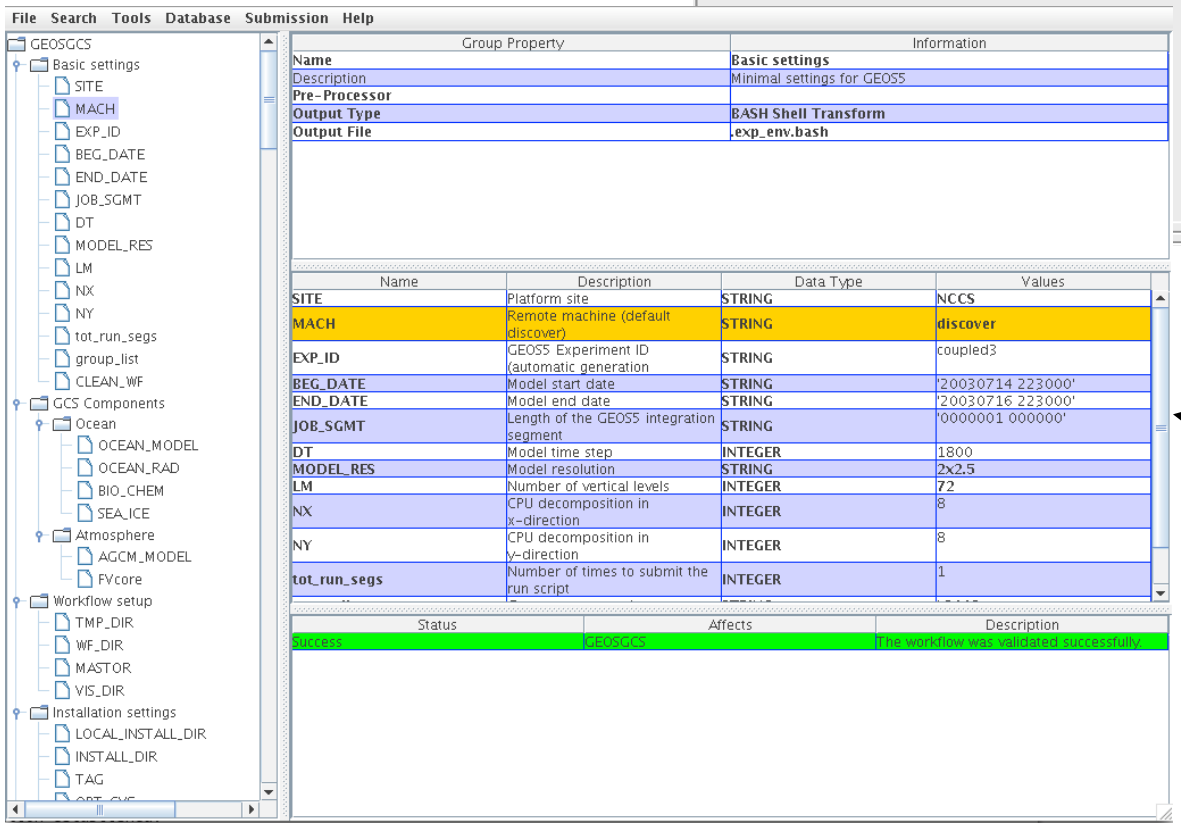


GUI-Based Workflow Tool

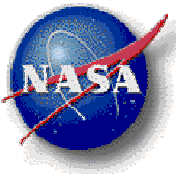
- Streamlines process of building and running complex models such as GEOS-5 and GMI
  - Provides different views to different categories of users
    - Narrow set of options for external users
    - Wide set of options for developers and internal users
  - Enables SIVO and NCCS to propagate patches to entire community quickly and efficiently
  - Streamlines management of input and output data sets
  - Manages batch jobs and provides visual feedback about execution progress
  - Enables sharing/comparing of experiments with other users
- Built on top of tools from ECMWF

Monitoring progress of experiment





Configuring experiment

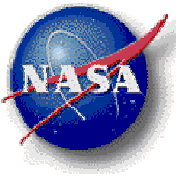


ASTG Services - Software

- ASTG help scientists to extend modeling capabilities
  - Cubed-sphere finite-volume dynamical core
  - ESMF/MAPL support
    - Coupling modelE - FV dynamical core
    - Componentization of biogeochemistry model
    - Componentization of GMI model
    - Coupling of LIS with NOAA forecasting system
  - Optimization
    - Parallelization of GISS modelE via MPI
    - Tuning GMAO next generation 4Dvar assimilation
    - MPI implementation of Gigaparticles
  - Stewardship for GMI model
- ASTG develops tools to improve developer productivity
  - pFUnit: Fortran framework for Test Driven Design
  - FFTT: Fast Fortran Transformation Toolkit for refactoring legacy Fortran code

Training

- ASTG provides training on a variety of topics
  - Programming languages
  - Software best practices
  - Tools
  - Parallelization: MPI, OpenMP, hybrid
  - Optimization
- Training formats include
  - Tutorials, including hands-on workshops
  - Consulting
  - Seminars
  - Written materials
  - Possible summer school this year: “Boot Camp for Modelers”



Level 2 Ticket Support

- ASTG provides Level 2 Ticket Support
  - Application level questions, problems, and requests
  - Support NASA centralized computing resources both at NCCS and NAS
  - Porting between platforms
  - Installing 3rd party software libraries
  - Optimization/parallelization
  - Training
- Develop and maintain benchmark suite to assess computing platforms

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- *Lots of help from Tom Bridgman , Randy Jones, Alex Kekesi , Kevin Mahoney, Marte Newcombe, Lori Perkins, Greg Shirah, Stuart Snodgrass , Eric Sokolowsky, Cindy Starr, Joycelyn Thomson, Jim Williams*

- *Most of the visuals in this talk are available at svs.gsfc.nasa.gov*

There are 3 Basic Types of Visualization

- Visualization as a communication tool:

  The public face of NASA science relies on these visuals.

  SVS - *About 60%-70% of SVS projects are communication-related, with a growing emphasis on specialized products: show booth visuals, museum exhibits, dome shows, Science on a Sphere, etc.*

- Visualization as a research & analysis tool:

  Tools are decided upon based on cost and local utility, not future requirements - very little visualization R&D.

  SVS - *Tiled Hyperwall displays for analyzing complex simulation models*

- Visualization as an operational tool:

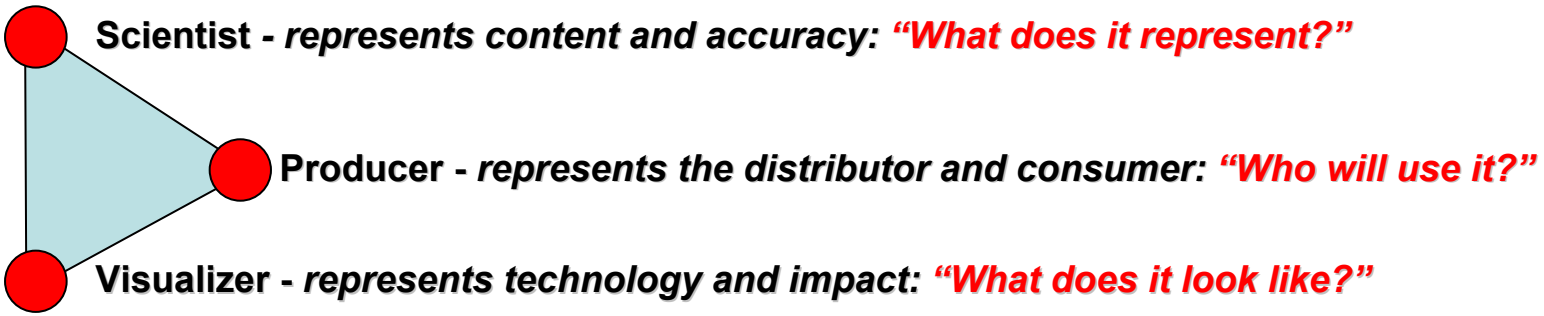
  Operational projects deliver data, browse images, satellite status displays.

  SVS - *Web-based delivery to visualizations through GIS systems and geo-browsers:* Google Earth, WorldWind, etc.

It Takes Three Legs to Make a Tripod Stable

Goal: *To weave NASA Science images into the everyday fabric of American life*

Our unique approach was to use a tripod of individuals for each project, each of whom could represent an important aspect of the outreach process.



Practice Makes Perfect

Example: In 1997, *NASA was about to launch a satellite (TRMM) that would take 3D rainfall measurements.*

Question: *What would excite the public?*

Answer: *3D Hurricanes, of course*

1997 - Preliminary Design Test Data (weeks)	1998 - Hand Design Hurricane Bonnie (days)	2003 - Automatic Design Hurricane Isabel (hours)

We often work towards well-planned products that can be produced automatically (pipelines) and delivered to the media.

- *40 Hurricane, cyclones, and storms produced in 5 years*

Scientific Visualization Studio

Go **Time (UT) and Forecast Selection**

Date: 2007 - 05 - 28 Time: 12 Forecast: 0.5

NOTE: Actual time of each image is shown beside legend

Go **Map Size**

Magnify: 100%

Width: 720

Height: 360

Go **Bounding Box (degrees)**

Top: 90

Left: -180 Right: 180

Bottom: -90

Go **Map Layers**

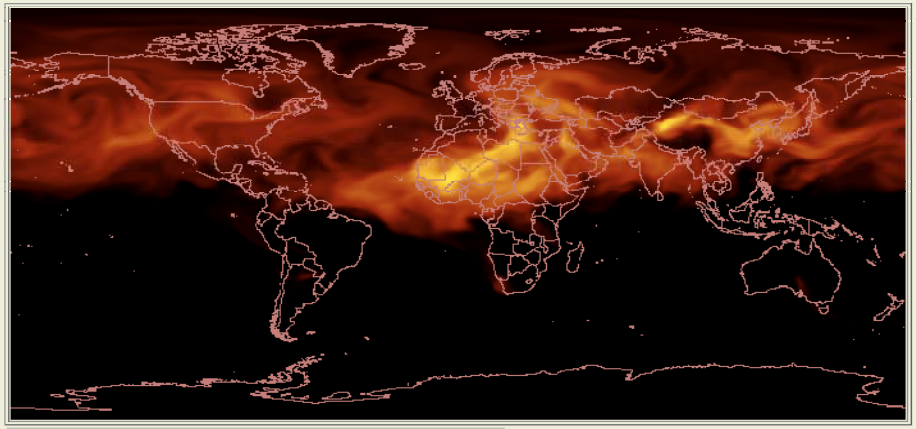
- [x] National Boundaries
- [x] Dust Aerosol Optical Thickness
- [ ] USA State Boundaries 1:20M scale
- [ ] Lat/Lon Grid
- [ ] Sea Salt Aerosol Optical Thickness
- [ ] Sulfate Aerosol Optical Thickness
- [ ] Black Carbon Aerosol Optical Thickness
- [ ] Organic Carbon Aerosol Optical Thickness
- [ ] Organic+Black Carbon Aerosol Optical Thickness
- [ ] Total Aerosol Optical Thickness
- [ ] Sea-Level Pressure
- [ ] Ozone Total Column
- [ ] Carbon Monoxide - Global
- [ ] Carbon Monoxide - North America Anthropogenic
- [ ] Carbon Monoxide - Central America Anthropogenic
- [ ] Carbon Monoxide - Western Hemisphere Biomass
- [ ] Carbon Monoxide - Asian Anthropogenic
- [ ] Carbon Monoxide - Northern Asia Biomass
- [ ] Carbon Monoxide - Southern Asia Biomass
- [ ] Carbon Monoxide - Mexico City Anthropogenic
- [ ] Aqua MODIS 1km true-color imagery
- [ ] Terra MODIS 1km true-color imagery
- [ ] GOES-12 full-disk long-wave infrared imagery
- [ ] CPC global infrared composite
- [ ] Blue Marble 2002 - MODIS composite land image

Select Project: Aerosol Forecasting

Aerosol WMS Viewer

WMS Viewer / NASA / GSFC / GMAO / ACDB /

Viewer development courtesy of NASA GSFC Software Integration and Visualization Office and Scientific Visualization Studio.
WMS Server development courtesy of NASA Geosciences Interoperability Office.
Software Developer: Jeff de La Beaujardiere, GSFC 610.3, 301 286 1569
Responsible NASA Official: Michael Seablom, GSFC 610.3, 301 286 8580
Privacy Policy and Security Notice / Software Version: 2007-05-04 13:57:33Z



Click on map to: Zoom ◉ In ○ Out by 2 , or ○ Recenter Google Earth KML file [?]

National Boundaries

National Boundaries. Metadata.

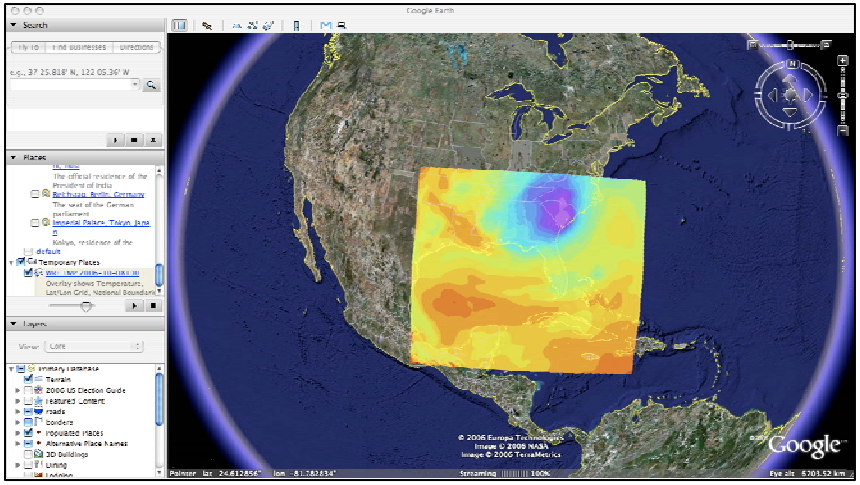
Dust Aerosol Optical Thickness

0.02 0.05 0.1 0.2 0.5 1.0 2.0

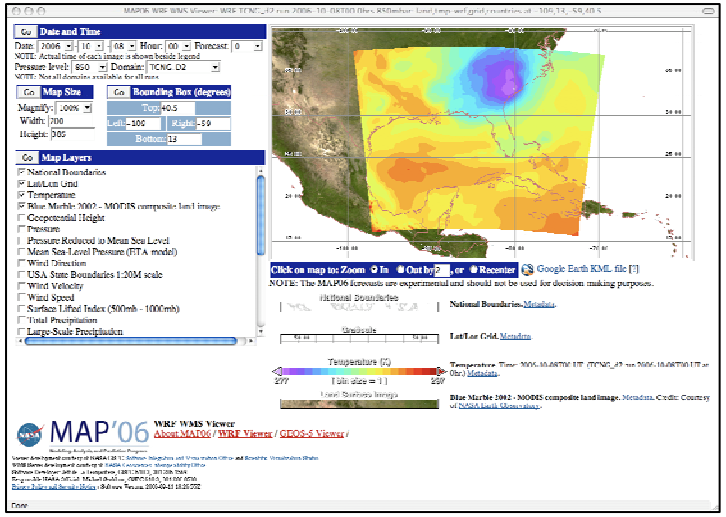
Dust Aerosol Optical Thickness. Time: 2007-05-28T12:30 UT. (run 2007-05-28T12 UT at 0.5hr.) Metadata. GeoTIFF. NetCDF. MPEG animation (5.8 MB). Credit: Courtesy of NASA GSFC Global Modeling and Assimilation Office and Atmospheric Chemistry and Dynamics Branch.

Scientific Visualization Studio

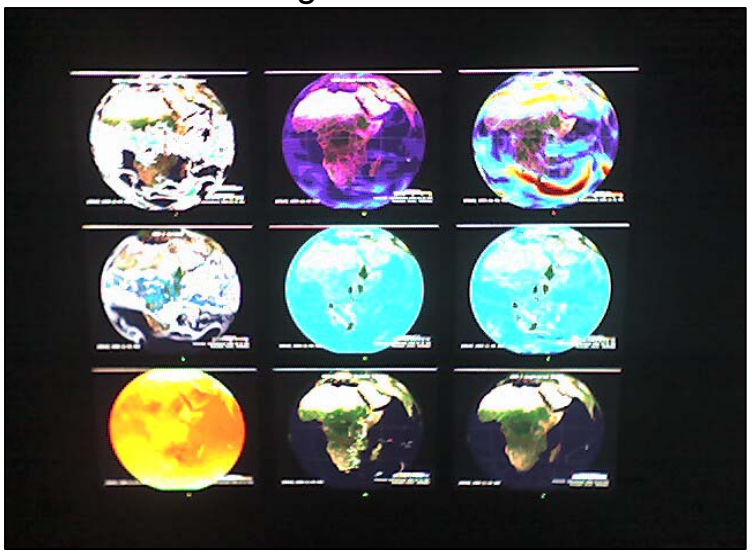
Modular system design allows Visualization as a Web Service across many different Geo-browsers



Google Earth



NASA WMS Viewer



Hyperwall

Agenda

Welcome & Introduction
Phil Webster/NCCS, Mike Seablom/SIVO

About the NCCS

Cluster Upgrade	*Dan Duffy*
Data Sharing Services	*Harper Pryor*

About SIVO

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Scientific Visualization Studio	*Horace Mitchell*
ESD Education & Public Outreach	***David Herring***

Questions / Comments	*Phil Webster & Mike Seablom*
Tour of NCCS Facility	*NCCS Staff*

NASA Earth Observations (NEO)

Kevin Ward • 503-977-2970 • kevin_ward@ssaihq.com
David Herring • 301-614-6219 • david.d.herring@nasa.gov

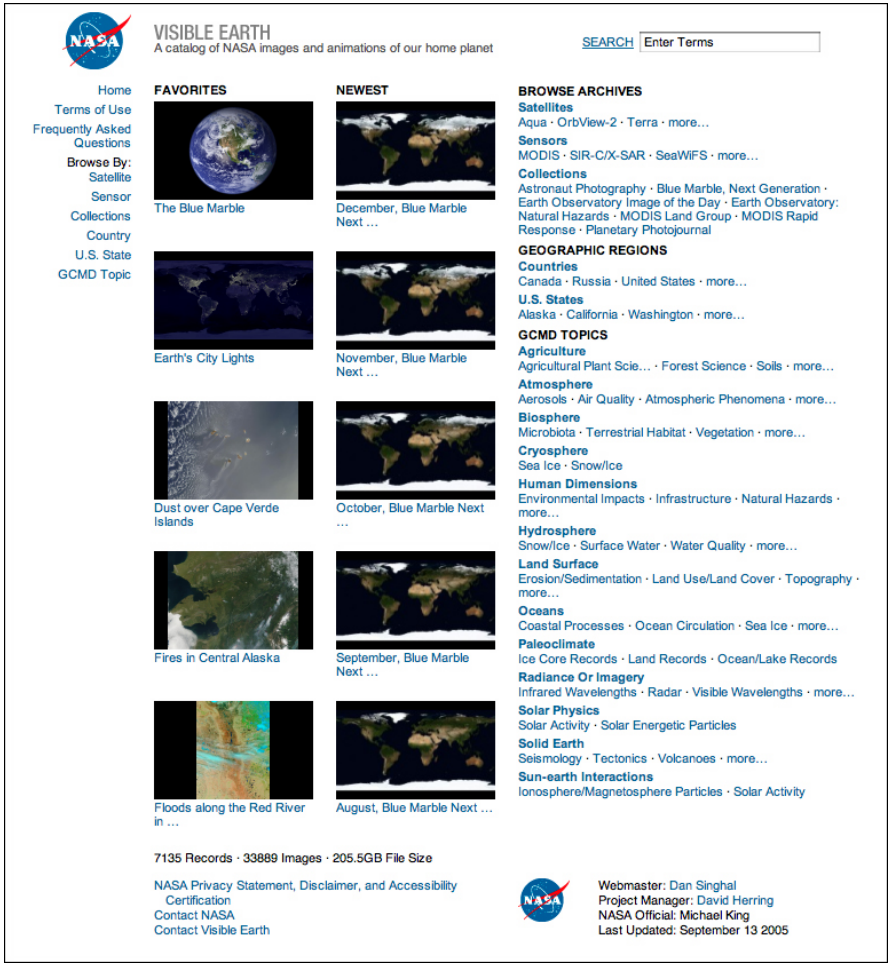
http://neo.sci.gsfc.nasa.gov

- **Easy access to NASA remote sensing imagery**
- **Designed for educators, communicators, & citizen scientists**
- **Why visit NEO?**
  - Obtain Earth images for articles, posters, kiosks, etc.
  - Access data & analytic tools for educational lessons
  - Export images to geobrowsers (e.g., GoogleEarth, WorldWind)
  - Export images for display in virtual globes (e.g., Magic Planet, Science on a Sphere)
  - Browse scenes and then order matching data

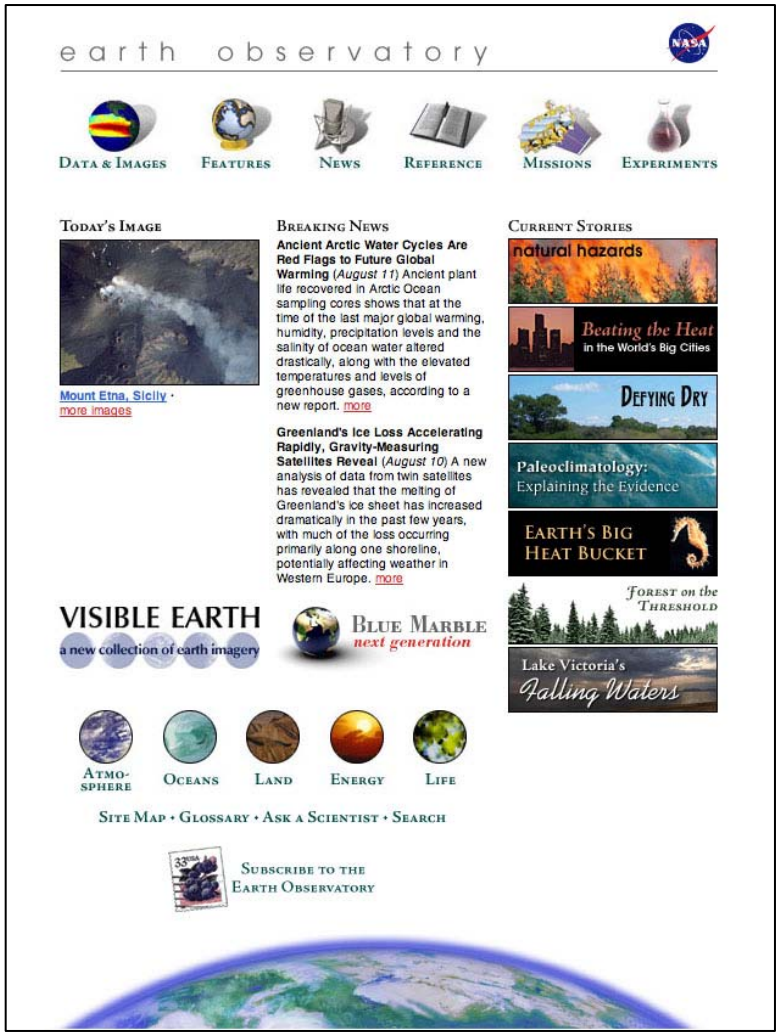
NASA's Visible Earth

- Digital image library of NASA Earth images, animations & data visualizations for public release
- More than 20,900 image records (~103,000 images) & growing!
- One of the 3 most-visited Web sites at GSFC
  - Serving ~35 Gb per day
  - 1.1 Terabytes last month
- Just rebuilt the entire system & database
  - XML database will allow scripted queries & content syndication
  - Simple forms will allow content authoring by colleagues from across the agency

http://visibleearth.nasa.gov



NASA's Earth Observatory



http://earthobservatory.nasa.gov

- Interactive Web-based magazine
  - First published April 29, 1999
- Recipient of numerous awards
  - Webby People's Voice Award ('06)
  - NASA Group Achievement Award ('05)
  - Webby Award in Education ('03)
  - Webby People's Voice Award ('03)
  - Webby People's Voice Award ('02)
  - Selected "50 Best of the Web" by *Scientific American ('02)*
  - NASA Group Achievement Award ('01)
  - GSFC Public Service Achievement Award ('01)
  - Selected "50 Best of the Web" by *Popular Science ('00)*

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- Questions?
- Comments?

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NCCS Facility

- Explore
- DICE
- Data Portal
- Discover
- Archive