

High Performance Computing (HPC) and Climate Model Data

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- Introduction to the NCCS
- Climate Models
- Growth of computing
- Growth of storage
- Toward exascale
- Analysis is different than HPC
- Need a different infrastructure
- ADAPT
- DASS
- Final Thoughts







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Provides an integrated high-end computing environment designed to support the specialized requirements of Climate and Weather modeling.

- High-performance computing, data storage, and networking technologies
- High-speed access to petabytes of Earth Science data
- Collaborative data sharing and publication services
- Advanced Data Analytics Platform (ADAPT)
- Data Analytics Storage System (DASS)

Primary Customers (NASA Climate Science)

- Global Modeling and Assimilation Office (GMAO)
- Goddard Institute for Space Studies (GISS)

High-Performance Science

- <u>http://www.nccs.nasa.gov</u>
- Code 606.2
- Located in Building 28 at Goddard





Takes in small input and creates large output

- Using relatively small amount of observation data, models are run to generate forecasts
- Fortran, Message Passing Interface (MPI), large shared parallel file systems
- Rigid environment users adhere to the HPC systems

Examples

- GMAO GEOS-5 High-Resolution Nature Runs for Observing System Simulation Experiments (OSSE)
- Evaluation of dynamical downscaling and • comparison of regional versus global models
- Extremely high-resolution global circulation models





10-km GEOS-5 meso-scale simulation for Observing System Simulation Experiments(OSSEs)



The Goddard Chemistry Aerosol Radiation and Transport (GOCART) model, Courtesy of Dr. Bill Putman, Global Modeling and Assimilation Office (GMAO). NASA Goddard Space Flight Center.

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Goddard Earth Observing System (GEOS) Model

- Dynamical Core uses a Cubed-Sphere which maps the Earth onto faces of a cube
- There are 6 faces of the cube and multiple vertical layers
- Total number of grid points
 X * Y * Z * 6 Faces of the Cube
- Current operational forecast is running at 27 KM resolution using about 27 million grid points
- Target operational resolution of 13 KM by the end of 2016
- Highest resolution research runs are at 1.5 KM global resolution





Dynamic Downscaling Assessment Narrow Scope – Focus only on 3 Impactful Phenomena



(cm) Nov 30, 2012

Northeast Wintertime Storms (NESs)

- Extreme precipitation/snowfall events
- Extreme wind events

Midcontinent Summertime MCSs

- Warm / Dry Climate Model Biases
- Extreme weather events

West Coast Wintertime Atmospheric Rivers (ARs)

- Crucial for water resources/availability
- Associated with most flooding events

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- Regional Climate Model
 - NASA Unified-WRF (NU-WRF) Based on WRF-ARW v3.5.1
- Initial/Boundary Conditions
 - MERRA-2 six-hourly re-analyses over CONUS
- Land Initial Conditions
 - Land Information System (LIS) 10-yr spin-up of Noah LSM
- Nudging (large scale forcing of certain variables to the synoptic scale)
 - Simulations with and without spectral nudging of p, t, and horizontal winds above the PBL





NASA Downscaling Models (Continued)

- MERRA-2 Replay at 12km M2R12K
 - Goddard Earth Observing System Model, Version 5 (GEOS-5) in replay mode at 12km resolution (global simulation)
- Boundary Conditions
 - MERRA-2 six-hourly re-analyses
- Land Initial Conditions
 - MERRA-2 CLSM
- Nudging
 - Replay capability adds a forcing term to constrain the 12km run to MERRA-2 p, t, winds, and humidity (q)



 Replay allows the model to develop its own internally developed mesoscale while following the large scale trajectory of the underlying MERRA-2 reanalysis (~50km)



- The highest resolution simulation performed with any US global model
 - Includes updated 2-moment micro-physics and interactive aerosols/chemistry with GOCART
 - Executed on 1,055 nodes of the NCCS 'Discover' SCU10 cluster (1,024 nodes for compute and 31nodes for IO)
 - 1.5km GEOS-5 completed ~1 simulated-day/wallclock-day
 - 0.87KM NICAM global simulation was run on the K-Computer (10.5 Petaflop system) with a throughput of ~0.5 simulated-days/wallclock-day



Total Aerosol Optical Thickness from GEOS-5 at 1.5-km, June 15, 2012 12:00z Global Modeling and Assimilation Office



Low clouds and column carbon monoxide from GEOS-5 at 1.5-km, June 17, 2012 23:00z, from wildfires throughout the western United States and from industrial emissions in the East (Global Modeling and Assimilation Office)

Clouds within Surface Low

Industrial Emissions wrapped up within a low pressure system and associated front

earl Peak, NV Fire

> Waldo Canyon, CO Fire

Tonoto Nat Forest, AZ

Croatan Nat'l Fores

Ocala Nat'l Forest, FL Fire

Marine Stratocumulus Clouds

and posting marine strateging of strate

Tropical Clouds











Calendar	Description	Decommission	Total Usable Capacity (TB)
2012	Combination of DDN disks	None	3,960
Fall 2012	NetApp1: 1,800 by 3 TB Disk Drives; 5,400 TB RAW	None	9,360
Fall 2013	NetApp2: 1,800 by 4 TB Disk Drives; 7,200 TB RAW	None	16,560
Early 2015	DDN10: 1,680 by 6 TB Disk Drives, 10,080 TB RAW	DDNs 3, 4, 5	~26,000
Mid 2015	DDN11: 1,680 by 6 TB Disk Drives, 10,080 TB RAW	DDNs 7, 8, 9	~33,000
Mid 2016	DDN11: 1,680 by 6 TB Disk Drives, 10,080 TB RAW	None	~40,000 (40 PB)





Requirements Continue to Grow: GMAO Science Portfolio

Forward Processing System	Satellite-Era Reanalysis 1979 - Present	EOS-Era Reanalysis 2000 – Present	Nature Runs (OSSEs)	Seasonal Forecast System	Coupled Simulations (Decadal, CMIP6)
3D-Hybrid Ensemble- VarMERRA (50km)1000000000000000000000000000000000000		M2R12K (12km) MERRA2 downscaled to 12 km Aerosols CO ₂ , CO, SO ₂ , O ₃ Non-Hydrostatic	$\begin{array}{c} \textbf{G5NR (7km)}\\ \text{Simulated 2005-2007}\\ \text{Aerosols, CO}_2, \text{CO, SO}_2,\\ \text{O}_3 \end{array}$	GEOS SFS (50km)GEOS CMIP (25km)MERRA-2 replay25km Atmosphere50km, 40L ocean25km 50L oceananalysisInclude aerosols	
Hydrostatic 1-Moment Cloud Microphysics Current GEOS-5 FP	MERRA-2 (50km) 3D-Var Aerosols and CO, SO ₂ , O ₃ 1-Moment Cloud Microphysics	1-Moment Cloud Microphysics	Non-Hydrostatic 1-Moment Cloud Microphysics 4 PB	31 members per month Include aerosols, CO, CO ₂ M2-driven EnOI ocean analysis	greenhouse gases Hydrostatic 2-Moment Cloud Microphysics
system 3D-Hybrid Ensemble- Var	~400 TB	IESA (12km) 3D-Hybrid Ensemble-Var 32 ensemble members	G5NR-CHEM (12km) Simulated 2013-2014 Replay to M2R12K	GEOS SFS (25km) Alignment with "MERRA-3"	Planning/alscussion and system evaluation in progress
(12km) 32 ensemble members Atmosphere, ocean surface Hydrostatic 2-Moment Cloud Microphysics Parallel FP stream in 1Q-2016	MERRA-2 GMI replay (50km) Replay GMI Chemistry 1 streams, 1,000 cores each 12 to 18 months ~ 1 PB	32 ensemble members atmosphere, land, ocean surface Aerosols, CO ₂ , CO, SO ₂ , O ₃ Non-Hydrostatic 2-Moment Cloud Microphysics 5,000 cores ; 40 simulation days/ day 150 days total wallclock ~3 to 4 PB of data	Full Reactive Chemistry Non-Hydrostatic 1-Moment Cloud Microphysics 1 PB of data 4Q-FY2016	25km, 50L ocean analysis System design under review <i>FY2019 target</i>	Will align with "MERRA-3" SFS and strategic direction of ESD
4D Ensemble-Var (9km) ~100 ensemble members Atmosphere, ocean surface	Coupled Reanalysis ("MERRA-3") Atmosphere-land-ocean- cryosphere	IESAR4K (4km) IESA Downscaled to 4km downscallng evaluation for NCA Aerosols, CO ₂ , CO, SO ₂ , O ₃ Non-Hydrostatic	G6NR (3km) Simulated 2015 Aerosols CO ₂ , CO, SO ₂ , O ₃ , CH ₄ Non-Hydrostatic	Core GMAO proje completed, in-prog	cts ress or planned.
Non-Hydrostatic(alignment with SFS and CMIP6)2-Moment Cloud Microphysics (The first GEOS-6 system)(alignment with SFS and CMIP6)		and 2-Moment Cloud Microphysics 2-Moment Cloud 5,000 cores ; 40 simulation days/ day ~4 PB 150 days total wallclock <i>Planning/evaluation</i> Pathfinding proj efforts. Proposed projec		Pathfinding project efforts. Proposed project	ts toward GMAO core
Parallel FP stream in 4Q-2016				SMD Reserve proj	ects. 16



- Target Run approximately 100 meter global resolution research runs in 10 to 15 years
- Each doubling of resolution requires 8x the grid points; hence, 8x the memory.

X Values	Grid Points	Resolution (meters)	RAM (PB)
5,760	14 x 10 ⁹	1,736	0.1
11,520	112 x 10 ⁹	868	0.8
23,040	896 x 10 ⁹	434	6.4
46,080	7,168 x 10 ⁹	217	51.2
92,160	57,344 x 10 ⁹	109	4,096

Bad News – This is only one component of the application (the atmosphere). To truly simulate the climate, we need a coupled model including Atmosphere, Ocean, Waves, Ice, and More; We expect the model to required much more memory pushing us toward a higher memory to flop ratio.



High Performance Computing

Takes in small amounts of input and creates large amounts of output...

- Using relatively small amount of observation data, models are run to generate forecasts
- Tightly coupled processing requiring synchronization within the simulation
- Simulation applications are typically 100,000's of lines of code
- Production runs of applications push the utilization of HPC systems to be very high
- Fortran, Message Passing Interface (MPI), large shared parallel file systems
- Rigid environment users adhere to the HPC systems

Data Analysis

Takes in large amounts of input and creates a small amount of output...

- Use large amounts of distributed observation and model data to generate science
- Loosely coupled processes requiring little to no synchronization
- Analysis applications are typically 100's of lines of code
- Require more agile development with many small runs; utilization can be low on average
- Python, IDL, Matlab, custom
- Agile environment users run in their own environments
- Steep learning curve for these users to take advantage of HPC resources

Data Analysis is inherently different than High Performance Computing applications.







Takes in large amounts of input and creates small output

- Using large amounts of observation or model data
- Python code of 100's of lines
- Easily run in parallel across multiple virtual machines



Processing work flow for the generation of the ABoVE water maps from Landsat scenes to ABoVE tiles.



AWM for 2001 and 2011 for Hay Lake and Beaver Hill Lake in Canada. Hay Lake has clearly expanded over this time frame while Beaver Hill Lake has diminished.

Taken from "ABoVE Water Maps: 30 meter spatial resolution surface water 1991-2011," M.L. Carroll, et. al, http://above.nasa.gov/pdfs/ABoVE_water_maps_user_guide_05102016.pdf



Reducing Data Friction Using MODIS Data

Goal: Build a cloud climatology record over the entire MODIS data record (TERRA & Aqua) for circumpolar Arctic 60 degrees north and above

Data Input requirements: Daily MODIS data from two sensors, 2003 to present. (36 tiles and approximate 56 TB)



NASA Different Infrastructure Needed for Analytics

- Big data analytics needs a different infrastructure than HPC
 - Analytics has traditionally used HPC resources, but it is beginning to limit its effectiveness and is causing issues within HPC
- An infrastructure that enables
 - Both the traditional use of data while enabling future analytics
 - Storage proximal analytics (dramatic reduction in data movement)
 - Builds towards emerging data analysis paradigms, such as deep learning
- NCCS is evolving its services using commercial Big Data technologies
 - Such as Virtualization, Hadoop and MapReduce, Object Store
- Major Challenge
 - These technologies were built for unstructured text data and do not easily integrate with structure scientific, binary data



Advanced Data Analytics Platform (ADAPT) Platform-as-a-Service (PaaS) Architecture

Compute systems are older, *repurposed high performance compute nodes*

- 100's of nodes currently with plans to expand over the next 6 months
- Capable of 1,000s of virtual machines

Persistent Data Services are long lived virtual machines specifically designed for data or web services. Examples include:

- Web Portals
- Web Map Service
- FTP
- OpenDAP
- Earth System Grid Federation (ESGF)
- ESRI ArcGIS

Itinerant purpose built virtual machines are customized for each user/project. These virtual machines are not persistent and can be spun up and down as needed.



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High Speed External Networks

Compute Cloud

Persistent Data Service

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Itinerant Purpose Built Virtual Machines

High Speed Internal Networks

Storage Cloud

- "Data Lake" concept storage is available as needed to all virtual environments
- Low cost, commodity based storage
- Multiple petabytes in size and easily expandable
- High performance file system using IBM GPFS

High speed external networks capable of 10 GbE and 40 GbE are available to transfer data into and out of ADAPT. In addition, remote mounts to external data sources, such as MODIS, are being served over these networks.

High speed internal networks use repurposed high performance Infiniband switches along with more traditional Ethernet switching.





- Not designed for Message Passing Interface (MPI)
 - These are highly coupled processes performing large amounts of data movement over high speed networks and synchronization
 - Recommend to use HPC systems for this
- ADAPT is designed more for inherently parallel processing of big data
 - Independent processes written to analyze large data sets
 - ADAPT has tools to assist users in submitting independent parallel scripts across multiple virtual machines
- ADAPT is not an archive
 - Large data sets relevant to multiple research projects can be made available, such as LandSat and NGA data
 - Remote access to commonly used data sets is also available, such as for MODIS
 - Projects must work with the NASA DAACs to provide long term data management for their products
- Publishing of data
 - Persistent data services created to provide a capability to share large data
 - NCCS can support this through a variety of technologies



- User directories: Home and Scratch (/nobackup) directories
- ADAPT has large volumes of relevant data that are locally stored for ABoVE researchers
- Data stored is driven by the science requirements
- NGA data data covers more than just the Arctic Boreal Vulnerability Experiment (ABoVE) study domain with more data coming in every day
- Will store the Digital Elevation Maps (DEMs) created both by the Polar Geospatial Center (PGC) and in the NCCS once those are created

Data Locally Stored in ADAPT	Volume
LandSat	101 TB
MODIS	252 TB
MERRA (Atmospheric Reanalysis)	200 TB
NGA	>1 PB



- ADAPT also has the ability to remotely mount data to a virtual machine to make it seem like it is local
- Uses the Lightweight Virtual File System (LVFS) developed by the MODIS team
- No need to download data; access what you need when you need it directly from OpenDAP and FTP sites as long as the application can tolerate the latency.

MODIS Data Example of ALL MODIS collection 5 and 6 data

• Local Directory: /att/pubrepo/MODIS/remote

NOAA Data Example of Global Brightness Temperature

- Remote Link: <u>ftp://ftp.cpc.ncep.noaa.gov/precip/global_full_res_IR/</u>
- Local Directory: /att/lvfs/ncep/data/precip/global_full_res_IR



- Artic Boreal Vulnerability Experiment (ABoVE)
 - Partnership with the Carbon Cycle Ecosystems Office to provide cloud services for ABoVE field campaign
 - Examples include comparing multiple, time displaced images of the same geographical area looking for changes in surface water extent using LANDSAT data; long-term multi-sensor record of fire disturbances in high northern latitudes using LANDSAT and MODIS
- NCCS Web Services
 - The NCCS is using ADAPT to host its own web services
- Asteroid Hunter
 - Evaluating design of next generation space-based telescope using a combination of asteroid projection modeling and simulated telescope
- National Geospatial Agency (NGA) High Resolution Image Processing
 - Examples include converting native NGA NTF to GTIFF (GeoTIFF); computing the vegetation index by counting trees, shrubs; computation of mosaics; digital elevation maps
- CALET Processing
 - Simulation of detectors for high energy particles



Data Analysis Storage System (DASS)





MPI, Open, Read, Write, etc.	Traditional HPC	Big Data Analytics	MapReduce, Spark, ML
Network, IB, RDMA	Classical Usage Patterns Data is moved to the process	Hadoop-Like Usage Analytics moved to the data	Cloudera, Horton, BDAS
GPFS	POSIX Interface	RESTful Interface	Hadoop Connector
IBM Spectrum Scale (GPFS)	Object Store/Posix Parallel File System Very large, scaling both horizontally (throughput) and vertically (capacity); permeated with compute capability at all levels		IBM Spectrum Scale (GPFS)
	Traditional HPC Storage	Server & JBOD Commodity-Based Hardware	



How do you make this work with NASA science data?

MPI, Open, Read, Write, etc.	Traditional HPC	Big Data Analytics	MapReduce, Spark, ML	
Network, IB, RDMA	Classical Usage Patterns Data is moved to the process	Hadoop-Like Usage Analytics moved to the data	Cloudera, Horton, BDAS	Spatiotemporal
GPFS	POSIX Interface	RESTful Interface	SIA Hadoop Connector	Indexing Approach (SIA)
IBM Spectrum Scale (GPFS)	Object Store/Posix Parallel File System Very large, scaling both horizontally (throughput) and vertically (capacity); permeated with compute capability at all levels		IBM Spectrum Scale (GPFS)	Working with GMU on this.
	Traditional HPC Storage	Server & JBOD Commodity-Based Hardware		

NASA

Spatiotemporal Index and Hadoop File System

- Use what we know about the structured scientific data
- Create a spatiotemporal query model to connect the array-based data model with the key-value based MapReduce programming model using grid concept
- Built a spatiotemporal index to
 - Link the logical to physical location of the data
 - Make use of an array-based data model within HDFS
 - Developed a grid partition strategy to
 - Keep high data locality for each map task
 - Balance the workload across cluster nodes







Test Clusters using decommissioned HPC servers

Test Cluster 1 SIA Cloudera HDFS	Test Cluster 2 SIA Cloudera Hadoop Connector GPFS	Test Cluster 3SIAClouderaHadoop ConnectorLustreAlmost completed
 20 nodes Cloudera HDFS Sequenced data Native NetCDF	 20 nodes Cloudera GPFS GPFS Hadoop	 20 nodes Cloudera Lustre Lustre HAM and
data Put only 	Connectors Sequenced data Put and Copy Native NetCDF Data Put and Copy 	HAL Sequenced data Put and Copy Native NetCDF Data Put and Copy





Initial Testing Results (No SIA at this point – sequenced data only)









Compute Where the Data Resides

CPU	On chip high bandwidth memory – think NVIDIA GPUs and Intel Phi architectures.
In Package Memory	High Bandwidth Memory on the chip.
Node Memory	NVME, emerging technologies, etc. Large quantities of persistent storage close to the CPU.
File System in Memory	Technologies to enable shared memory across many nodes as well as collective operations at the network level.
Network	Very fast reads and writes into and out of the network and the HPC environment.
High Performance File System	Large aggregate space and throughput designed for longer term persistent storage.
Tiered Storage Subsystems	Hierarchy of storage systems from SSD's to spinning disks to
Cloud	Ability to store data in the cloud and burst when appropriate for data analytics.

Challenge: Must be able to perform data analysis at EVERY layer. Be able to efficiently move the data to the appropriate layer for computation or move the thread to the data.



Future of HPC and Big Data at Exascale

•	Intensive
•	Analytics

ADAPT Virtual Environment HPC and Cloud ~1,000 cores 5 PB of storage Designed for Big Data Analytics	Environment Environment Merging of HPC and Big Data Analytics Capabilities Ability for in-situ analytics throughout the environment known analytics and machine learning	
Mass Storage Tiered Storage Disk and Tape 45 PB of storage Designed for long-term storage and recall; not compute	Discover HPC Cluster 80,000 cores 33 PB of storage Designed for Large-Scale Climate Simulations	
Computational Intensive		



- Let's start with the 5 V's of data that everyone knows...
- Volume, Velocity, Veracity, Variety, Value

Others are adding more V's ...

• Visualization, Variability, Viability



Here are a few more that we are keeping in mind as we move forward ...

Lifecycle of Data

- Viva La Data
- Vintage
- Vindictive
- Vicious

Data Security

- Vandalized
- Victimized
- Velociraptor
- Voldemort

Just for fun

- Vortex
- Vice
- Venomous
- Vivacious













NCCS Projections by Mid 2016 (traditional processors only)

- Peak Computing ~3,500 TF
- Total RAM ~403,968 GB and Total Storage ~54,667 TB

Ratio of Memory to Peak Computing

- Peak Computing ~3,500 TF
- Total RAM ~403,968 GB
- Ratio = $\sim 116 \text{ GB/TF} (0.1 \text{ Byte/Flop})$

Ratio of Storage to RAM

- Total Storage ~54,667 TB
- Ratio = ~ 138

Extrapolating to Exascale

- 1 EF Peak
- 100 PB of RAM
- 14 EB of Storage



- Start users with 1 to 4 virtual machines each with 4 cores and 9 GB of RAM
- Once the user has developed or ported their application, the system administrators will scale up the number of VMs
- Need to make sure the resources are available prior to scaling up
- Scheduling resources so far has not been a problem
- As is typical with virtual environments/clouds, utilization varies greatly over time



Snapshot of the Ganglia monitoring tool a summary of ABoVE virtual machine environment.

- 431 CPUs or cores
- 97 virtual machines



Software Stack (mostly open source)

External License Servers

Open Source Tools Python, NetCDF, R, etc.

Commercial Tools Intel Compiler (C, C++, Fortran), IDL (4 seats)

Operating Systems Linux (Debian, CentOS) and Windows

- Virtual machines can be set up to reach out to external license servers
- Time is needed to make requests to poke holes through various NASA firewalls

Open source tools:

- Very flexible
- If the open source tool does not need elevated privileges to install, the user can install the software in their home or scratch directories
- Commonly used tools may be installed in a shared directory for multiple users; the NCCS can assist with this as needed
- If the tool requires elevated privileges, users should submit a ticket to the NCCS for assistance. That tool will have to go through a security vetting process before it can be installed

Platform-as-a-Service

- Compute virtual machines are open souce Linux
 - Windows used for remote desktop and ArcGIS



Data Publication and Distribution Services



Future: Working on an architecture to support ArcGIS server, portal, and desktop.