Climate Analytics as a Service

John Schnase

Office of Computational and Information Sciences and Technology
NASA Goddard Space Flight Center
Provides an integrated high-end computing environment designed to support the specialized requirements of Climate and Weather modeling

- State-of-the-art high-performance computing, data storage, and networking technologies
- Advanced analysis and visualization environments
- High-speed access to petabytes of Earth Science data
- Collaborative data sharing and publication services

http://www.nccs.nasa.gov
Beyond the Data Deluge - Gordon Bell et al. (2009)

"Copying large amounts of experimental data from a data center to personal workstations or distributing data to numerous independent centers is no longer tenable without recourse to extreme - and thus expensive - networking.

"For research to be affordable, data analysis must increasingly be done where the data sets reside, leaving academic research networks to handle low-bandwidth queries and analytic requests, including visualization."

— Gordon Moore, 2009

Climate Analytics-as-a-Service

For research to be affordable, data analysis must increasingly be done where the data sets reside ...

— Gordon Moore, 2009
Climate Analytics-as-a-Service (CAaaS) is contributing to a global network of sector-specific data, driving innovation and discovery ...
What are the critical elements needed to deliver Climate Analytics-as-a-Service?

**Data**
- Relevance
- Co-location

*Data have to be significant, sufficiently complex, and physically or logically co-located to be interesting and useful...*

**Exposure**
- Convenience
- Extensible

*Capabilities need to be easy to use and facilitate community engagement and adaptive construction...*

**High-Performance Compute/Storage Fabric**
- Storage-proximal analytics
- Canonical operations

*Data can’t move, analyses need horsepower, and leverage requires something akin to an analytical assembly language...*
MERRA Analytic Services

Climate Data Services API

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MERRA Reanalysis

MapReduce
MERRA Analytic Services

Modern Era-Retrospective Analysis for Research and Applications

- Source: Global Modeling and Assimilation Office (GMAO)
- Input: 114 observation types (land, sea, air, space) into “frozen” numerical model. (~4 million observations/day)
- Output: a global temporally and spatially consistent synthesis of 26 key climate variables. (~418 under the hood.)
- Spatial resolution: 1/2° latitude × 2/3° longitude × 42 vertical levels extending through the stratosphere.
- Temporal resolution: 6-hours for three-dimensional, full spatial resolution, extending from 1979-Present.
- ~ 200 TB, but MERRA II is on the way …
The Basic MapReduce Paradigm ...

- MapReduce is a framework for processing parallelizable problems across huge datasets using a large number of computers.
- Computational processing can occur on data stored either in a filesystem (unstructured) or in a database (structured).
- MapReduce can take advantage of locality of data, processing data on or near the storage assets to decrease transmission of data.
- "Map" step: The master node takes the input, divides it into smaller sub-problems, and distributes them to worker nodes. A worker node may do this again in turn, leading to a multi-level tree structure. The worker node processes the smaller problem, and passes the answer back to its master node.
- "Reduce" step: The master node then collects the answers to all the sub-problems and combines them to form the output – the answer to the problem it was originally trying to solve.
"Canonical Ops" ...

- We're building in to our analytic services near-storage, early-stage analytical operations that represent a common starting point in many analysis workflows in many domains. For example, average, max, min, standard deviation, sum, count, and difference operations of the general form:

\[
\text{result} \leftarrow \text{average}(\text{var}, (t_0,t_1), ((x_0,y_0,z_0),(x_1,y_1,z_1)))
\]

that return, in this example, the average of a variable when given a variable name, temporal extent, and spatial extent.

- Built-in canonical ops exploit complexity stratification to optimize efficiencies along the workflow chain ...

- Large amounts of unstructured data
- Simple, common, general-purpose operations
- Highly structured, tailored, reduced, refined analytic products
- Specialized tools, models, operations
Domain Harmonized API

The Climate Data Services API...

- Based on the data flow interactions of the Open Archival Information System (OAIS) Reference Model
- Addresses climate science's "Big Data" challenge by integrating principals of archive data management with high-performance data analytics
  - Makes it easier to integrate high-performance analytics into existing digital preservation systems
  - Makes it easier to use high-performance analytics to create dynamically generated objects
- CDS API Methods
  - **Ingest** – Submit/register a Submission Information Package (SIP).
  - **Query** – Retrieve data from a pre-determined service request (synchronous).
  - **Order** – Request data from a pre-determined service request (asynchronous).
  - **Download** – Retrieve a Dissemination Information Package (DIP).
  - **Status** – Track progress of service activity.
  - **Execute** – Initiate a service-definable extension. Allows for parameterized growth without API change.
MERRA Analytic Services

MERRA/AS System

- Entire MERRA collection in a TRL 8 mission qualified analytic data service
- Virtual Hadoop Clusters
  - Three Hadoop clusters on the same hardware using containers: Test, Pre-Production, Production
  - Established agile protocols for testing new software and promoting the software changes into production
- Climate Data Services API
  - MERRA Analytic Service, Persistence Service, libraries, command interpreter, and client distribution package
- Documentation / Administrative Infrastructure
  - Using standard NCCS practices for configuration management and authentication
  - Complete documentation and system administrative infrastructure
- Established beta test user community

Hardware Configuration

- 36 node Dell cluster (11.7 TF Peak)
- 576 total cores (Intel 2.6 GHz SandyBridge)
- 2,304 GB of RAM (64 GB per node)
- 1,296 TB of RAW storage (36 TB per node)
- FDR Infiniband
Wei Experiment

An Estimation of the Contribution of Irrigation to Precipitation Using MERRA

Study Areas
- Nile Valley
- North China
- California Central Valley
- Northern India/Pakistan

Variables Needed
- Humidity
- Wind speed
- Temperature

Other Requirements
- 1979 – 2002
- 6-hr time steps
- 18 atmospheric levels

Data Wrangled:
- $23 \times 365 \times 4 \times 4 \times 18 \times 3 = 7,253,280$ layers ...

1. Introduction
Irrigation is an important human activity that has the potential to impact local and regional climate through the hydrological cycle and surface energy balance (e.g., Chase et al. 1999; Pielke et al. 2011). About two-thirds of the global freshwater withdrawals from surface and underground are used for agriculture (Shiklomanov 2000).
Wei Experiment

Traditional Approach
• 8.4 TB moved from archive (3 months)
• Clipping / averaging (days – weeks)

With MERRA/AS and the CDS API ...
• Clipping / averaging (2.5 minutes)
• 500 MB of final product moved to local workstation (8 minutes)
Nadeau Experiment

Temperature Anomaly
• Coverage: Global
• Period: 1 month
• Collection: instM_3d_ana_Np
• Time span: January — December 2011
• Levels: 1 – 42 (0.1 hPa – 1000 hPa)

Traditional Approach
• Find and order from archive (hours – days)
• Transfer ~10 GB (~3 hours)*
• Client-side clip/compute, GrADS (~1.5 days)

With MERRA/AS and the CDS API ...
• One line in a python script
• 3 minutes run time
• Final product ~0.5 GB (10 minutes to transfer)

* Assuming 10 Mbps average US internet speed with 25% overhead ...
MERRA/AS Beta Test Participants

- 21 individual testers across government, corporate, and university
- 10 projects using CDS API for access
  - NASA’s ABoVE Campaign
  - iPlant Collaborative
  - Iowa State University/ClimateMonkeys
  - DataNet Federation Consortium
  - George Mason University
  - RECOVER Wildfire Decision Support
  - Invasive Species Forecasting System

Usage Statistics
- Total Orders: 19,067
- Total Downloads: 35,673
- Total Status Checks: 427,425

Example MERRA/AS Beta Test Use Cases (Research and Applications)

<table>
<thead>
<tr>
<th>Project</th>
<th>Use Case/Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>NASA ABoVE Campaign</td>
<td>Using MERRA/AS to create historic climatology for the Arctic and Boreal region</td>
</tr>
<tr>
<td>NSF iPlant Collaborative</td>
<td>Leading collaborative effort between iPlant and MERRA/AS. Developer building an iPlant application within their Discover Environment that interfaces with our API</td>
</tr>
<tr>
<td>Iowa State University &amp; ClimateMonkeys</td>
<td>Using MERRA/AS to generate various averages pertaining to Brazil and Argentina</td>
</tr>
<tr>
<td>NSF DataNet Federation Consortium</td>
<td>NSF collaborative that’s building the data grid infrastructure for data driven science (<a href="http://datafed.org">http://datafed.org</a>) federation of MODIS data sets</td>
</tr>
<tr>
<td>George Mason University PhD Program</td>
<td>Uncertainty Quantification in Ensemble Atmospheric Reanalyses (C. Grieg)</td>
</tr>
<tr>
<td>Illinois Tech</td>
<td>Testing the interaction between Swift python script and CDS services</td>
</tr>
<tr>
<td>NASA / DOI RECOVER Project</td>
<td>Wildfire decision support system for BLM and USFS Burned Area Emergency Response (BAER) team post-wildfire remediation planning.</td>
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<tr>
<td>Invasive Species Forecasting System</td>
<td>Using MERRA/AS to generate habitat suitability maps based on 30+ key continental scale MERRA climatology variables</td>
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November 13, 2014
Copernicus Climate Data Store Workshop

The BiDS ‘14 Conference – Frascati, Italy
3-6 March 2015
Data Centric High Performance Computing

Data Sharing and Publication
- Capability to share data & results
- Supports community-based development
- Data distribution and publishing

DATA Storage & Management
- Global file system enables data access for full range of modeling and analysis activities

Code Development
- Code repository for collaboration
- Environment for code development and test
- Code porting and optimization support
- Web based tools

User Services
- Help Desk
- Account/Allocation support
- Computational science support
- User teleconferences
- Training & tutorials

High Performance Data Analytics
- Interactive analysis environment
- Software tools for image display
- Easy access to
- Specialized visualization support

Data Transfer
- Internal high speed interconnects for HPC components
- High-bandwidth to data center users
- Multi-gigabit network supports on-demand data transfers

Security

HPC Computing
- Large scale HPC computing
- Comprehensive toolsets for job scheduling and system monitoring

Data Archival and Stewardship
- Large capacity storage
- Tools to manage and protect data
- Data migration support
Discover Scalable Compute Unit 9

Summer 2013 Addition to the Discover Cluster (FY13)
- IBM iDataPlex
- 480 compute nodes
- Intel Xeon SandyBridge Processors
- 64 GB of RAM
- FDR Infiniband

Computational Capability
- Peak: 159,744 Gflops

Capable of additional Intel Phi coprocessors or NVIDIA GPUs
Discover Scalable Compute Unit 10

October 2014 Compute Upgrade
- SGI System
- Intel Xeon Haswell Processors
- 1,080 nodes; 30,240 cores
- 128 GB RAM per Node
- FDR Infiniband
- 1 PF peak Rmax Linpack

Storage Upgrades
- In procurement
- Target of 10 PB or more
- To be installed late 2014
Evolution to a Data Centric Environment

**Data**
- HPC Models
  - GEOS 5
  - ModelE
  - WRF
- Observations
  - Ground Based
  - Satellite
  - In Situ
- Reanalysis
  - MERRA
  - NOAA
  - Others
- HPC Computing and Storage
  - NASA NCCS
  - NOAA
  - Others

**Analytics**
- Data Services
  - Moving beyond just a file system and a storage repository.
  - NCCS and Data Services Projects
    - Dali Analysis Nodes
    - vCDS
    - Hadoop (HDFS)
    - Merra Analytic Service
    - Earth System Grid
    - Web Portals

**Discovery**
- Modelers/Scientists
- Downstream Users
  - Agriculture
  - Water Management
  - Health
  - Famine Prediction
- Commercial
  - Insurance/Reinsurance
  - Commodity Trading
- Public/Citizen Scientists

**Data Management System**
iRODS based management of federated data sets