8th Team Meeting
La Jolla, CA
January, 2010

John Helly

CMMAP
Reach for the sky

Outline

- Management
  - CIWG (Cyberinfrastructure Working Group)
  - Data Policy
  - Software Policy
- Resources
  - Computing
  - Data
- Community Support
  - Data interoperability
  - Model code portability

Objective 6

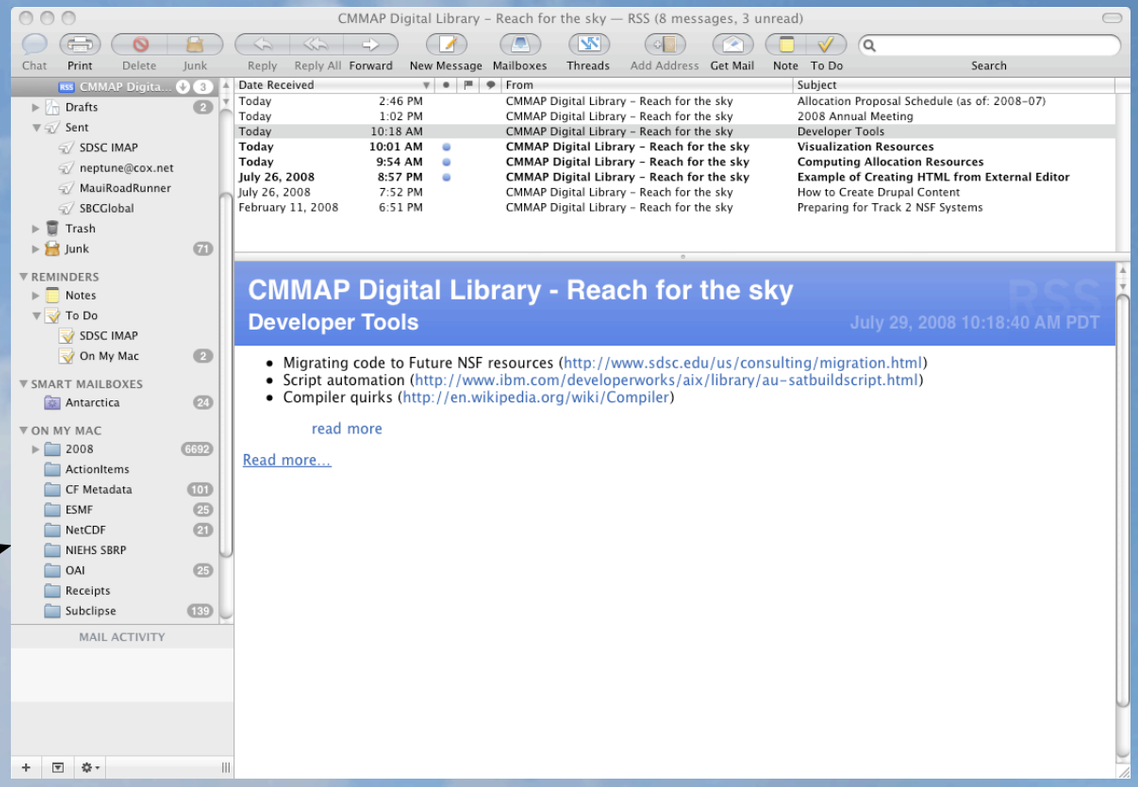
- Management, analysis and visualization of very large model output datasets - creation of infrastructure
  - Resource procurement & distribution
  - Data management
  - Analysis and visualization of model results

Management CIWG

CIWG Objectives

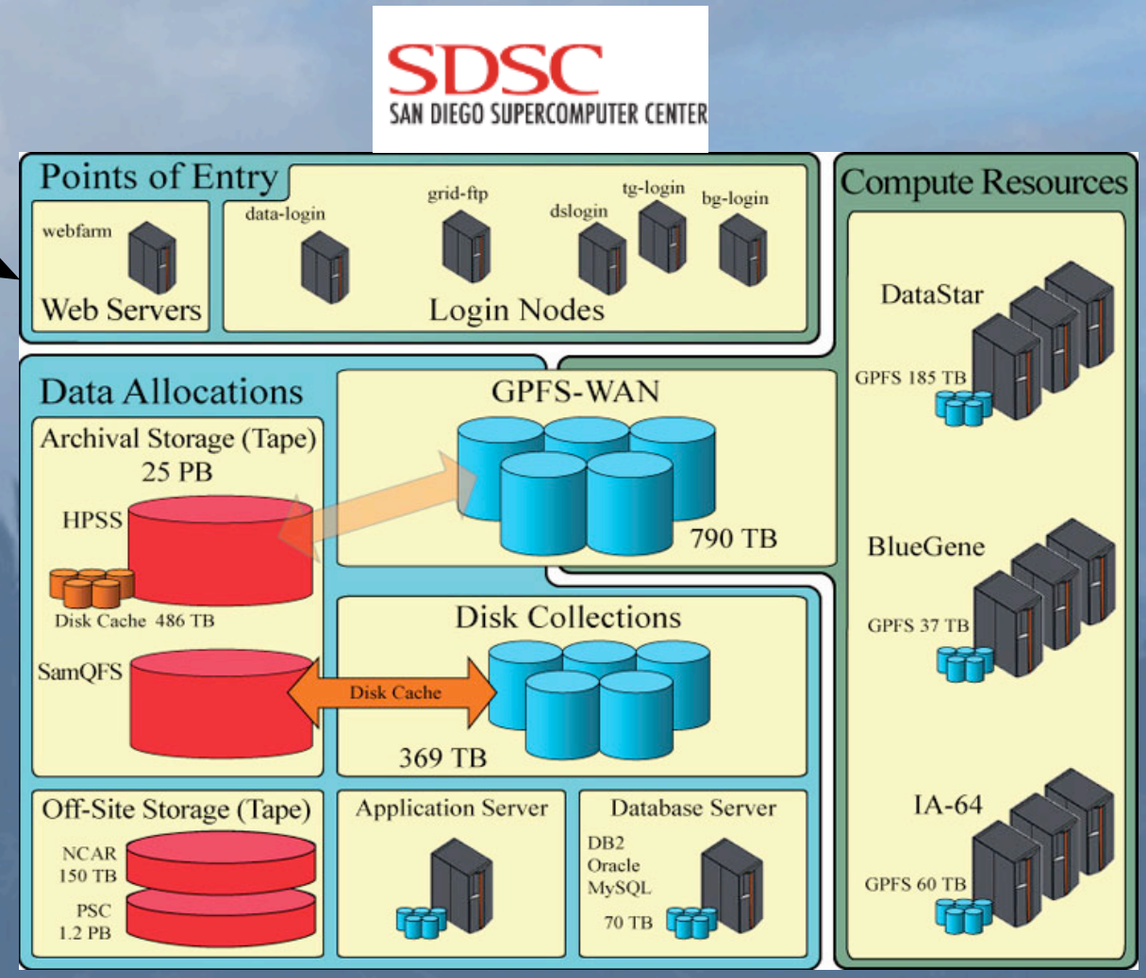
- Make efficient use of computing and data resources
  - acquire resources
  - coordinate resource utilization
  - collaborate to leverage joint efforts
- Provide technology look-ahead
- Validate goals and provide advice and consent to Executive Committee

RSS



URL data retrieval

OAI metadata



200 GB/snapshot=1/2 hr

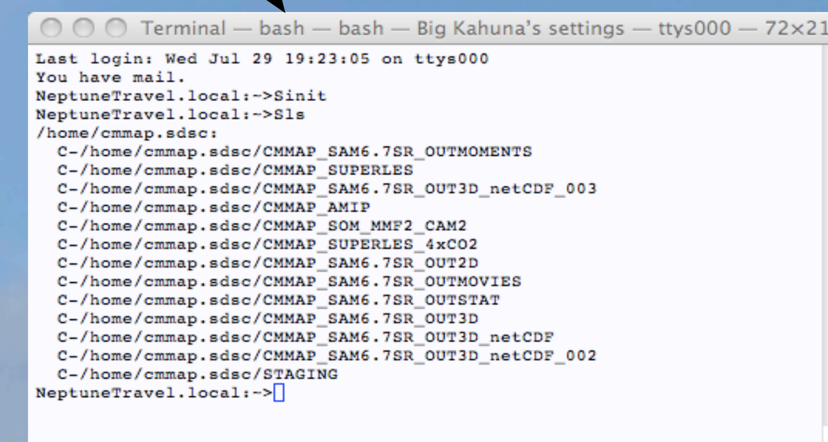
MMF-LES Model Data Output Budget

20 TB/day

Simple Methods of Data Download (2) and Upload (1)

Selective
Data Transfer

Bulk Data Transfer
SRB Client



Storage Resource Broker (SRB)

SAM–QFS has 16 tape drives, an 304–TB disk cache

– Meta Data Servers: 2 x Sun x4600

– Data Login Servers: 2 x Sun v40z /

6 x 1GbE connections to the TeraGrid/HPC network

– Tape Drives

16 STK 9940–B tape drives

– 24 IBM J2 3592 tape drives

The GCRM Tsunami

2 km, 100 levels, hourly data

- ~4 TB / simulated hour
- ~100 TB / simulated day
- ~35 PB / simulated year

4 km, 100 levels, hourly data

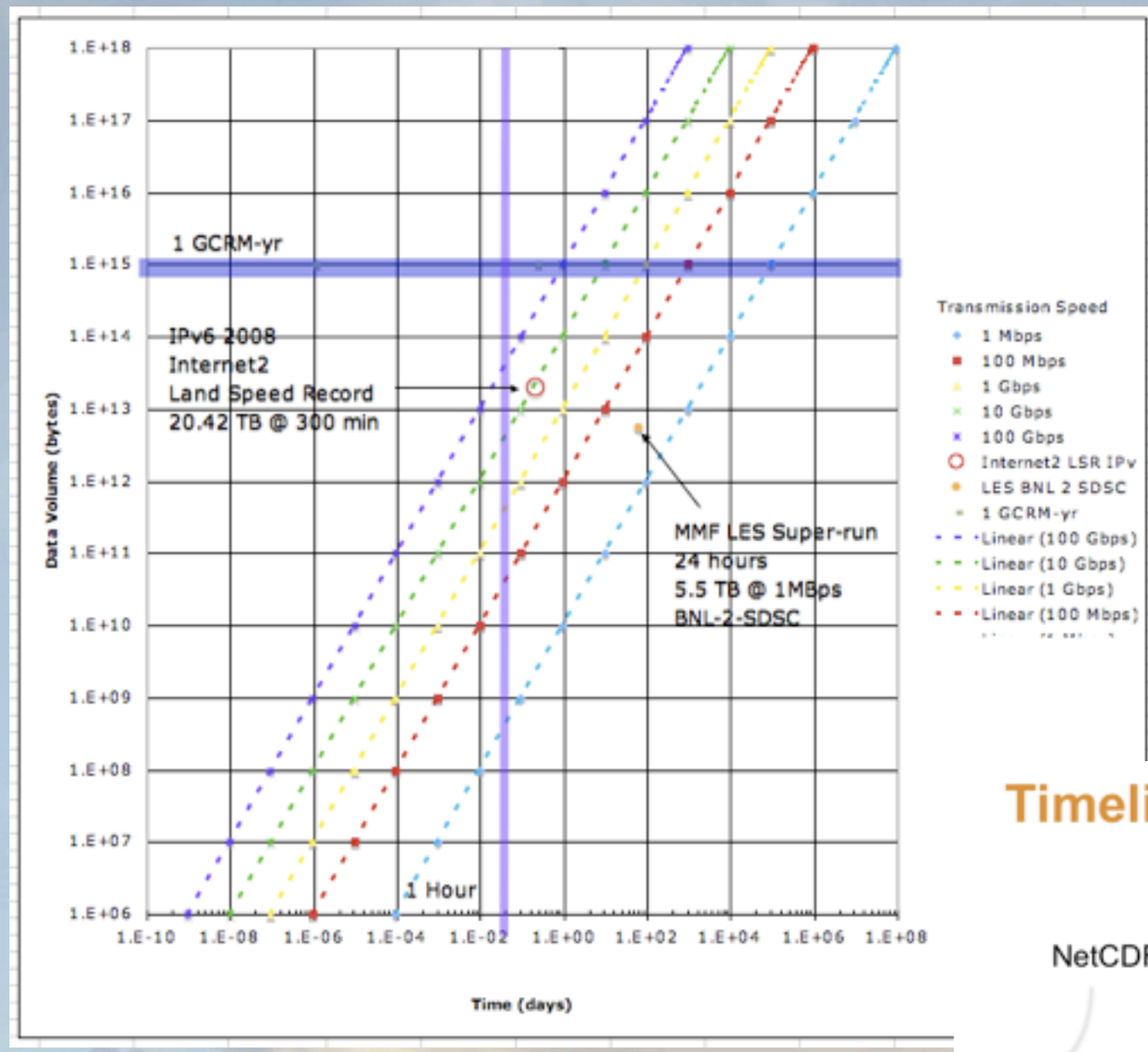
- ~1 TB / simulated hour
- ~24 TB / simulated day
- ~9 PB / simulated year

Other Data Tsunamis

- 30 TB/night: Large Synoptic Survey (LSS) Telescope (2014)
- 15 PB/year: CERN's Large Haydron Collider (May 2008)
- 1 PB over 3 years: EOS (Earth Observing System) data (2001)

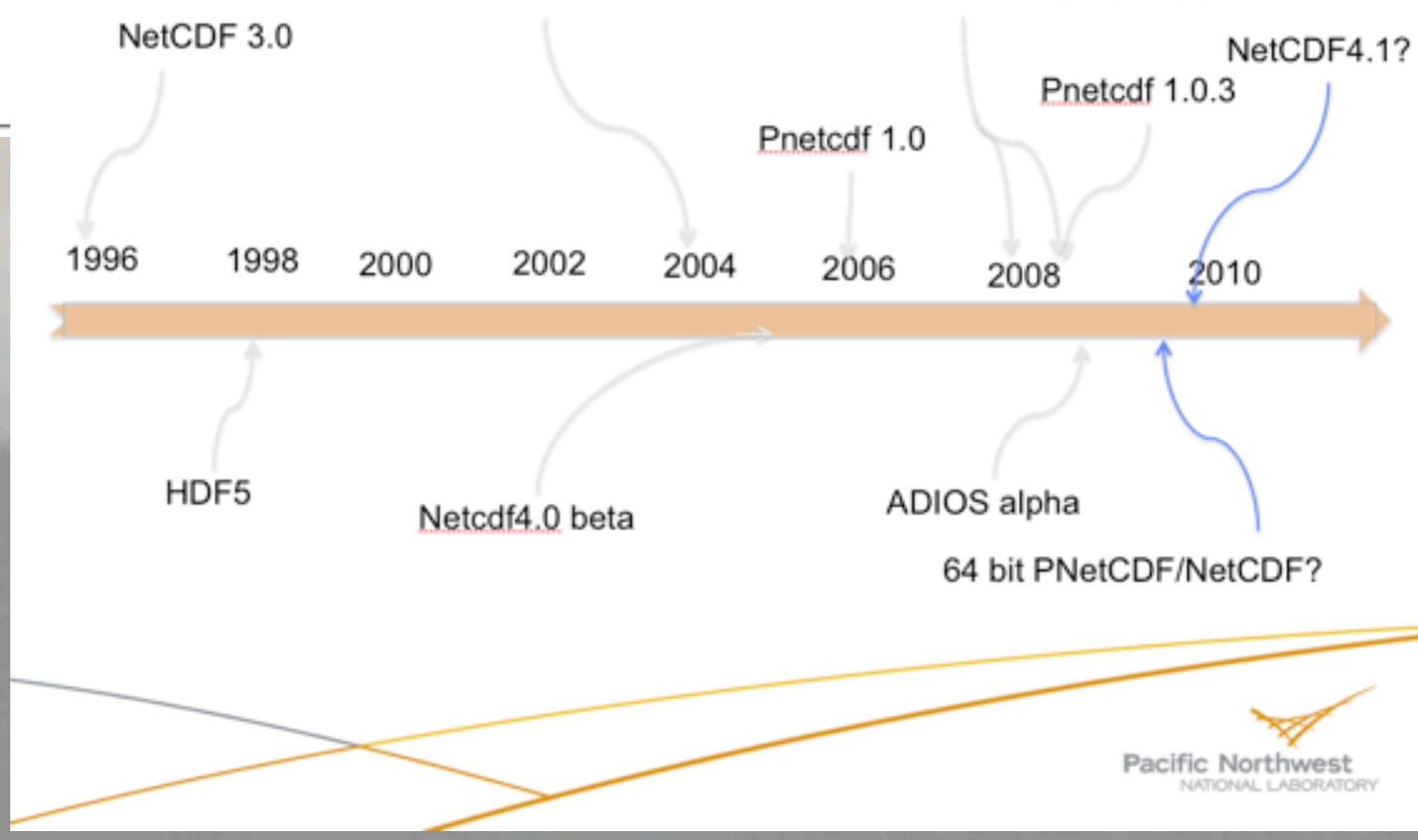
(from K. Schuchart presentation January, 2008)

Internet Data Transfer Capacity



Parallel Input/ Output Technology Progress

Timeline



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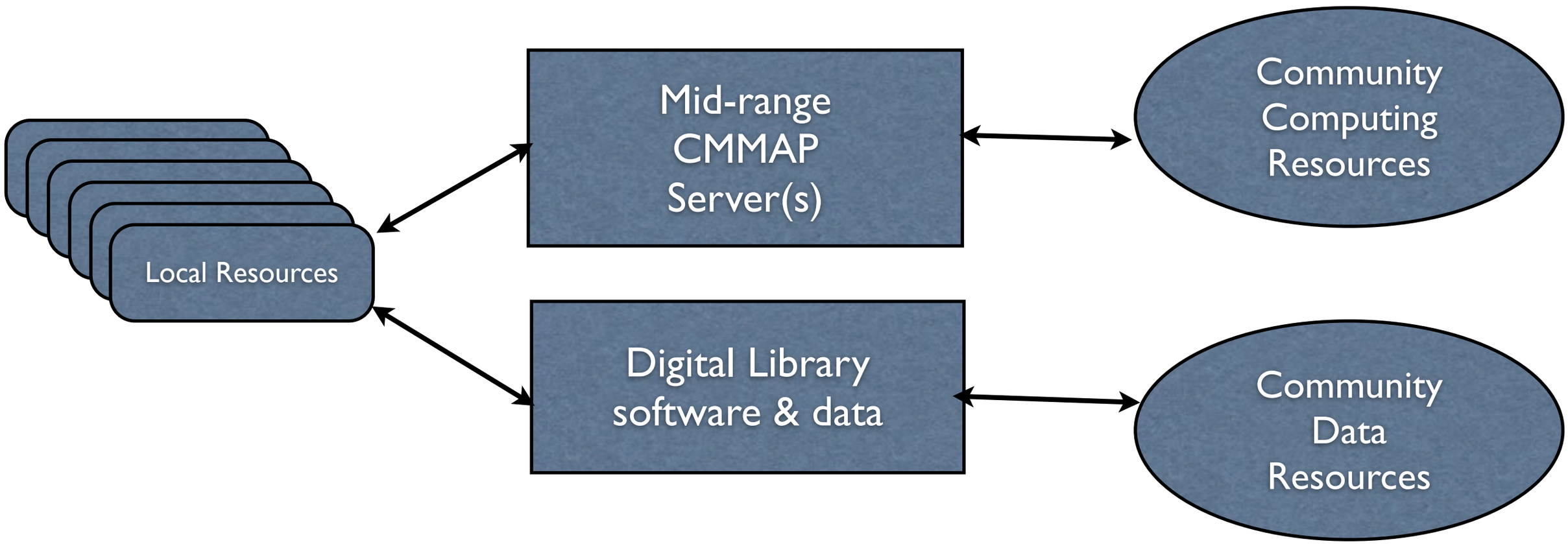
Architectural Goals



Home Institution

CMMAP Machine Room

External Resources

Management

Data Policy

Wednesday, January 13, 2010

Data Policy

- Data published on the CMMAP Digital Library is in the public domain but registration and authorization required to access it
  - this is to prevent hacking and bot-crawling and
  - provide tracking of who is accessing the data
- All metadata is public
  - will be published via a new OAI (Open Archive Initiative) service to be instituted this year
  - CF metadata conventions are followed
- We are investigating the use of DOIs (digital object identifiers) for data consistent with the scholarly publication process

CMMAP Digital Library

Edit primary links

Search

Computing Resources

- NSF Teragrid
- DOE INCITE

Data Resources

- Search for Data

Software

- Bulk Data Transfer Client
- Multi-scale Modeling Framework (MMF)

hellyj

- My blog
- Create content
- Search for Data
- My account

INCITE Resources & Allocations

Mon, 05/18/2009 - 23:25 — hellyj

2010 INCITE Call for Proposals

Add new comment Read more Computational Resources

Teragrid Resources & Allocations

Mon, 05/18/2009 - 23:14 — hellyj

Add new comment Read more Computational Resources

Sample Fortran program to read GIGALES netcdf 3D snapshot data

This program will read one variables for a subset of the horizontal domain for all vertical levels of a given 3D snapshot time.

1 attachment

Data Conversion Tools

Thu, 11/27/2008 - 20:54 — hellyj

Management

Software Policy

Wednesday, January 13, 2010

Software Policy

- Software developed with CMMAP funding is covered by an intellectual property agreement between CSU and CMMAP partners
- MMF code is controlled by the author of the code
- GCRM code is very new and developed under SCIDAC funding
- Subversion source control system has been provisioned but has not yet been required
- CCSM coding conventions are encouraged

Community Sea Ice Model (CSIM) Developer's Guide
Code Reference for Version 5.0

Released with CCSM3.0

Julie Schramm
Cecilia Bitz
Bruce Briegleb
Marika Holland
Elizabeth Hunke
Bill Lipscomb
Dick Moritz

Subsections

5.1 Style Guidelines

General Guidelines

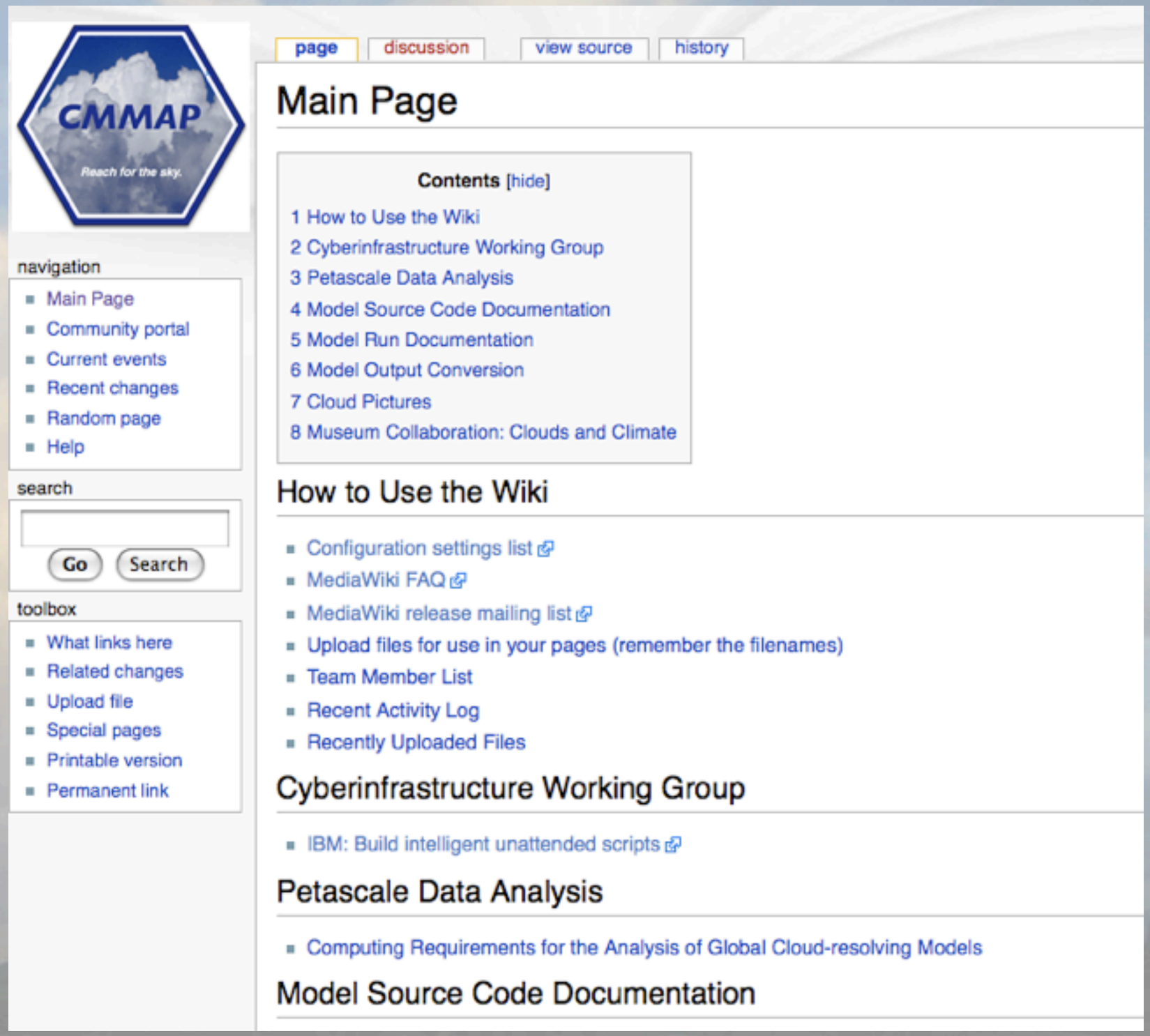
- **Fortran 90 Standard** CSIM uses the F90 standard.
- **Preprocessor** The C preprocessor is required as the macro processor (cpp). All tokens should be uppercase to distinguish them from fortran code. The use of ifdef constructs should be avoided wherever possible. The option should be set in the namelist instead.
- **Fixed-Form Source** Fixed-form source will be used for readability. Columns 7 to 72 of a line may contain a Fortran statement, while columns 1 to 6 are reserved for special purposes. Blanks may be used freely anywhere. Exclamation marks should be used to denote comments. A statement may include a maximum of 19 continuation lines.
- **Bounds Checking** All code should be able to run when the following compiler options are set:
  - Array bounds checking
  - Automatic variables are initialized to NaN
  - Floating point exception conditions: overflow, division by zero, and invalid operations

Modules

- The use of modules is strongly encouraged since they provide global access to variables.
- Modules must have the same name as the file in which they reside, due to dependency rules used by "make" programs. This implies that multiple modules are not allowed in a single file.
- Module names must begin with "ice_". This will provide unique module names when CCSM is released as a single executable version.
- Related subroutines and variables should be placed in a single module/file rather than keeping a single routine per file.

Documentation

http://cmmap.sdsc.edu/wiki/



Resources

Computing

NSF Teragrid

Allocation Types, Limits, and Deadlines

	Startup/Educational Allocation	Research Allocation (TRAC)	
Units Requested *Service Units (SUs) on Compute Resources* *Terabytes (TBs) on Data Resources*	**Maximum compute request** • Most systems have a limit of 30,000 SUs, though some may be as high as 200,000 SUs. Please see the Resource Catalog for specific resource limits. • Maximum Startup request for TeraGrid Roaming: 50,000 SUs • Aggregate request for multiple compute resources cannot exceed 200,000 SUs. • Storage on disk: 5 TB • Storage on tape: 25 TB	30,000 – Unlimited	
Deadlines	N/A	**Open Submissions** Dec. 15 Mar. 15 [1] Jun. 15 Sept. 15	**Close Submissions** **Jan. 15** [1] **Apr. 15** **Jul. 15** **Oct. 15**
Allocations Begin	Two weeks after submission	April 1 July 1 October 1 January 1	
Review Cycle	Within one week	Quarterly [2]	
Typical Use	Classroom or training accounts and startup accounts requiring small amounts of time	Experienced users with research projects	

[1] The TRAC Meeting schedule is available for reviewers on the POPS Review page.
[2] See the Past Allocations for a list of previous awards.

DOE Earth System Grid

Leveraging National & Partner Resources

	Organization	Resource	2007	2008	2009	2010
Data Allocations	San Diego Supercomputer Center (SDSC)	Disk	15 Terabytes	15 Terabytes	30 Terabytes	45 Terabytes
		BlueGene			30,000 SUs*	
Computing Allocations	Teragrid (multi-institution)	SDSC DataStar (IBM SP4)	600,000 SUs	1,200,000 SUs		
		Grid Roaming			600,000 SUs	
		LSU Steele			900,000 SUs	
	Lawrence Berkeley National Laboratory (LBNL)	National Energy Research Scientific Computing Center (NERSC)			700,000 SUs	
	Oak Ridge National Laboratory (ORNL)	Cray XT			2,000,000 hrs	3,000,000 hrs
	National Center for Atmospheric research (NCAR)	BlueIce IBM Power5			500,000 SUs	
	IBM Watson Research Center	BGW - eServer Blue Gene Solution			TBD	
	Stonybrook				TBD	

Resources

Data

ari File Edit View History Bookmarks Window Help (100%) We

Search for Data | CMMAP Digital Library

http://cmmap.sdsc.edu/querym

teragrid community accounts

SAIC VPN Solo Guitar ...Blues Guitar Post to CiteULike IODP Site S...Bank — SSDB Adobe Photoshop CS Help SAS OnlineDoc, Version 8 .Mac Automated S...ite Imagery

arch for Data | CMMAP Digital L...

CMMAP Digital Library

Edit primary lin

Home

Search

Computing Resources

- NSF Teragrid
- DOE INCITE

Data Resources

- Search for Data

Software

- Bulk Data Transfer Client
- Multi-scale Modeling Framework (MMF)

hellyj

- My blog
- Create content
- Search for Data
- My account
- Recent posts
- News aggregator
- Administer
- Log out

Search for Data

Search Parameters

- CMMAP_AMIP
- CMMAP_SAM6.7SR_OUTMOMENTS
- ✓ CMMAP_SAM6.7SR_OUTMOVIES
- CMMAP_SAM6.7SR_OUTSTATa
- CMMAP_SAM6.7SR_OUT2D
- CMMAP_SAM6.7SR_OUT3D
- CMMAP_SAM6.7SR_OUT3D_netCDF
- CMMAP_SUPERLES
- CMMAP_SUPERLES_4xCO2

Navigation

North:
South:
East:
Wast:

Submit Query

Filename	Collection	Subject	Keywords	Description	Type
GATE_IDEAL_S_2048x2048x256_100m_2s_cldtop.raw	metadata		CMMAP_SAM6.7SR_OUTMOVIES	MMF Output for the SUPERLES project	
GATE_IDEAL_S_2048x2048x256_100m_2s_cwp.raw	metadata		CMMAP_SAM6.7SR_OUTMOVIES	MMF Output for the SUPERLES project	
GATE_IDEAL_S_2048x2048x256_100m_2s_iwp.raw	metadata		CMMAP_SAM6.7SR_OUTMOVIES	MMF Output for the SUPERLES project	
GATE_IDEAL_S_2048x2048x256_100m_2s_mse.raw	metadata		CMMAP_SAM6.7SR_OUTMOVIES	MMF Output for the SUPERLES project	
GATE_IDEAL_S_2048x2048x256_100m_2s_qvsfc.raw	metadata		CMMAP_SAM6.7SR_OUTMOVIES	MMF Output for the SUPERLES project	
GATE_IDEAL_S_2048x2048x256_100m_2s_sfcprec.raw	metadata		CMMAP_SAM6.7SR_OUTMOVIES	MMF Output for the SUPERLES project	

Conversion of SAM6.7SR com3D to netCDF

Published in Digital Library

Stored in Archival File System

jitterbug:/archive/science/cmmap-staging>du -kh

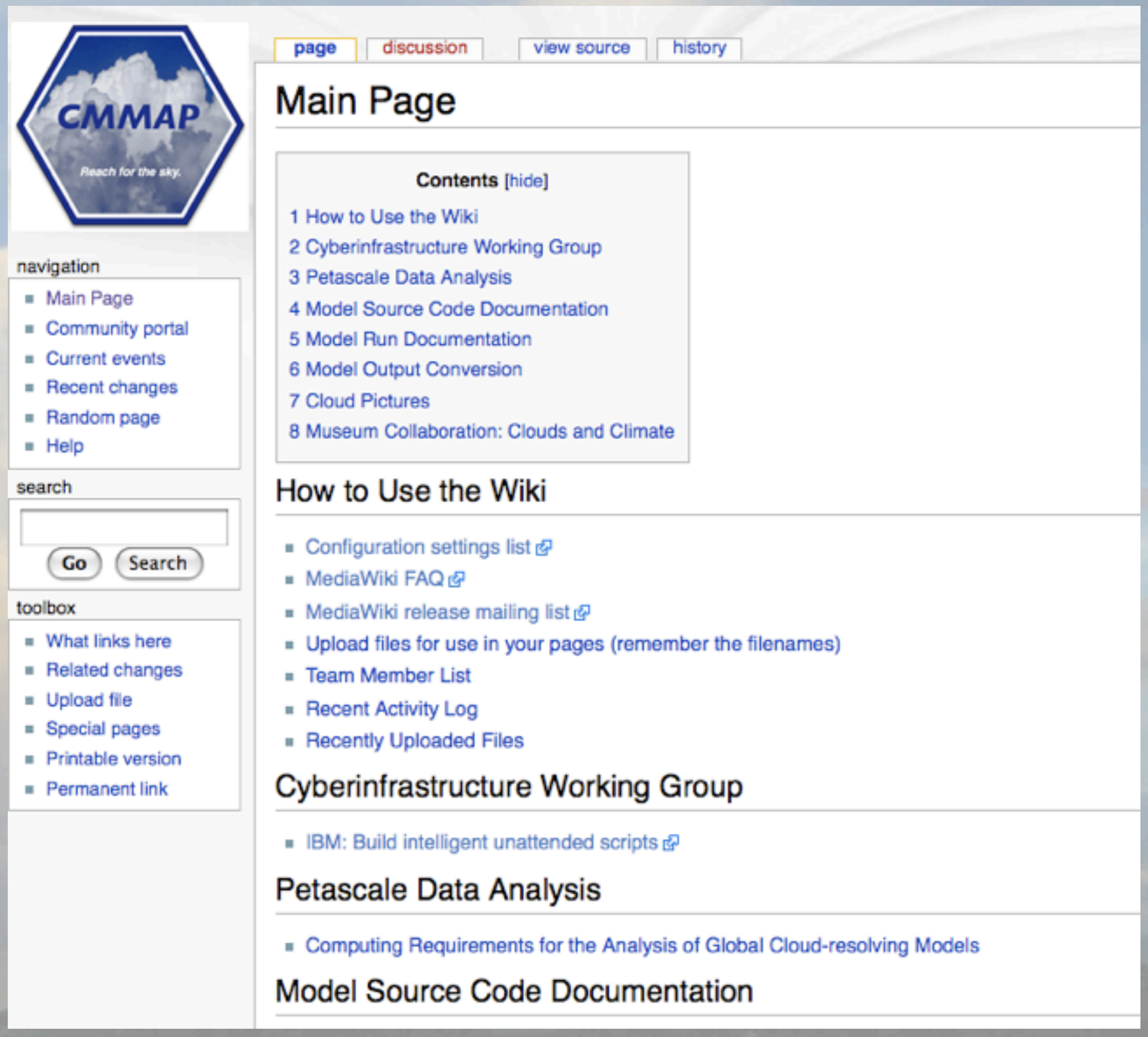
```
114G ./staging/CMMAP_AMIP
91G  ./staging/CMMAP_SUPERLES_4xCO2
92G  ./staging/CMMAP_SUPERLES
14G  ./staging/CMMAP_SAM6.7SR_OUT2D
3.7T ./staging/CMMAP_SAM6.7SR_OUT3D
113G ./staging/CMMAP_SAM6.7SR_OUTMOMENTS
51G  ./staging/CMMAP_SAM6.7SR_OUTMOVIES
137M ./staging/CMMAP_SAM6.7SR_OUTSTAT
4.2T ./staging

781G ./source/PRITCHARD
114G ./source/CMMAP_AMIP
92G  ./source/CMMAP_SUPERLES
91G  ./source/CMMAP_SUPERLES_4xCO2
14G  ./source/CMMAP_SAM6.7SR_OUT2D
113G ./source/CMMAP_SAM6.7SR_OUTMOMENTS
51G  ./source/CMMAP_SAM6.7SR_OUTMOVIES
137M ./source/CMMAP_SAM6.7SR_OUTSTAT
2.1T ./source/CMMAP_SAM6.7SR_OUT3D_com3D
3.1T ./source/CMMAP_SAM6.7SR_OUT3D_netCDF
6.3T ./source
11T  .
```

*AI: Rename SUPERLES to SPCAM

http://cmmap.sdsc.edu/wiki/

Same as Wikipedia



Community Support

Data Interoperability

CMMAP Digital Library

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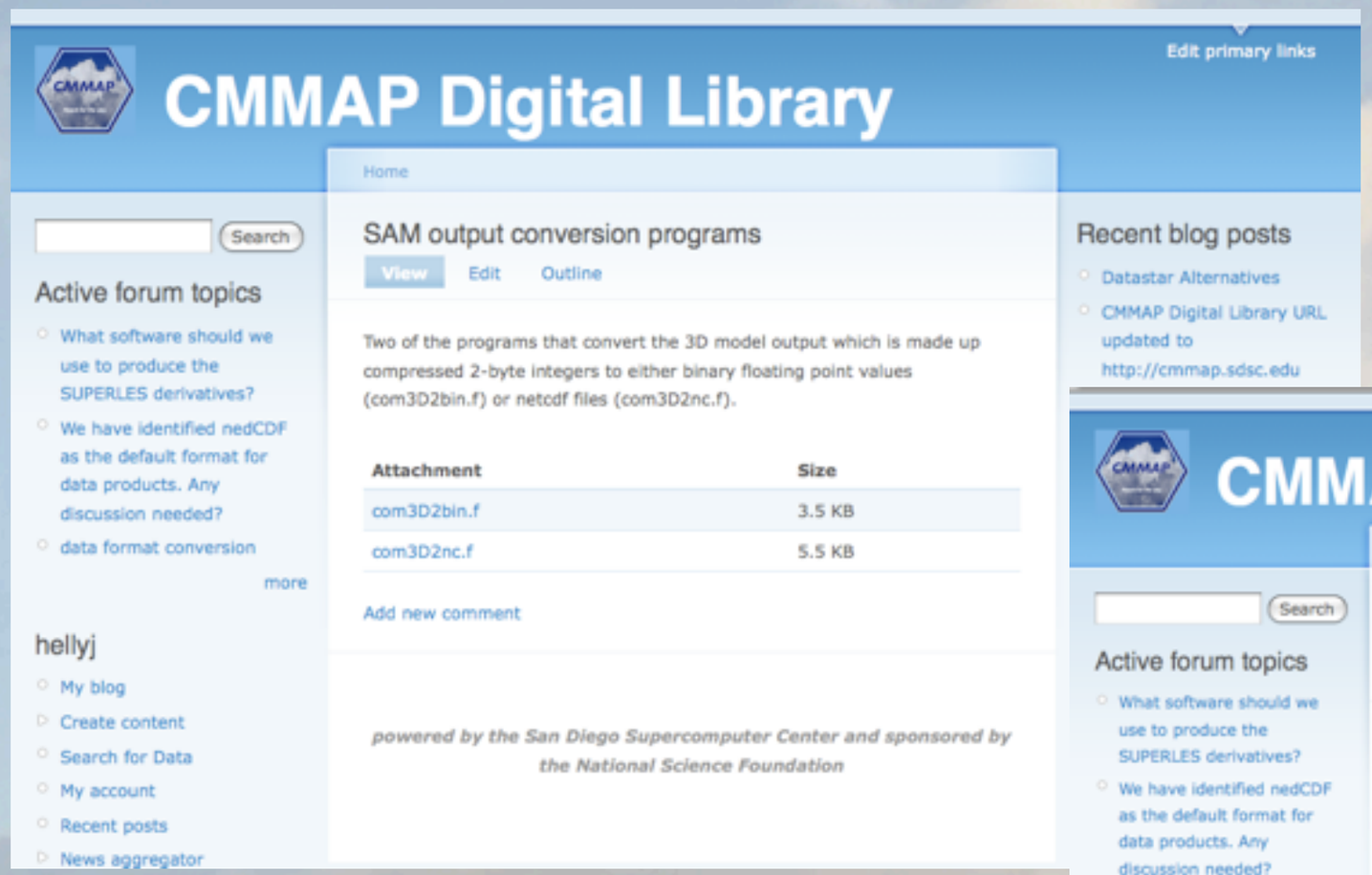
1 attachment

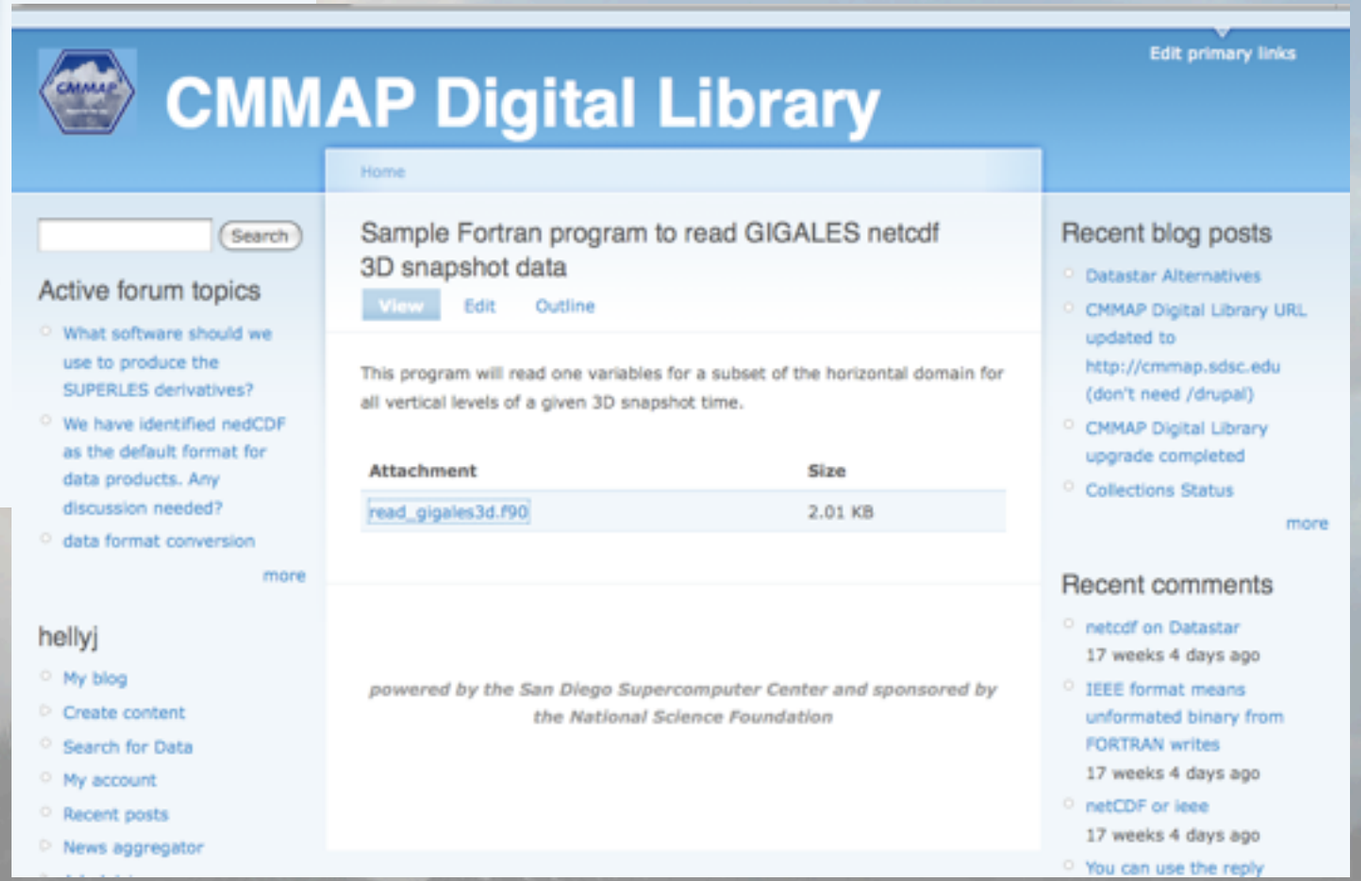
Data Conversion Tools

Thu, 11/27/2008 - 20:54 — hellyj

Data Conversion (com3D->netCDF)

by Mark Branson/CSU





Circulating External Disk Drives

- FAT32 volume format
- USB 2.0 connector

- SRB-client can also bet used for non-web data transfer ala rsync
- List-base scripts are also possible if they are desired

Resources

Visualization of Very Large Datasets

Testing (preliminary data point)

- Remote viz on Teragrid
  - –TACC (UT Austin) / SPUR
  - –Super-LES data
  - –ParaView (client-server, remote X-session over ssh)
- TACC<-->Cox Cable (residential ~10Mbps)
  - –‘works’ but not usable
- Need better bandwidth for both data transfer and interactivity

Kitware ParaView 3.2.0

File Edit View Sources Filters Animation Tools Help

Time: 0

Result Surface

Pipeline Browser

cs://mpc1074:11111
comet_p4.pvtu
Calculator2
Contour2

Object Inspector

Properties Display Information

Apply Reset Delete

Isosurfaces

Value Range: [6.79195e-11, 7.55638]

6.79e-11
0.329
0.657
0.986
1.31
1.64
1.97
2.3
2.63

Delete
Delete All
New Value
New Range
Scientific

B
7.56
5.67
3.78
1.89
6.79e-11

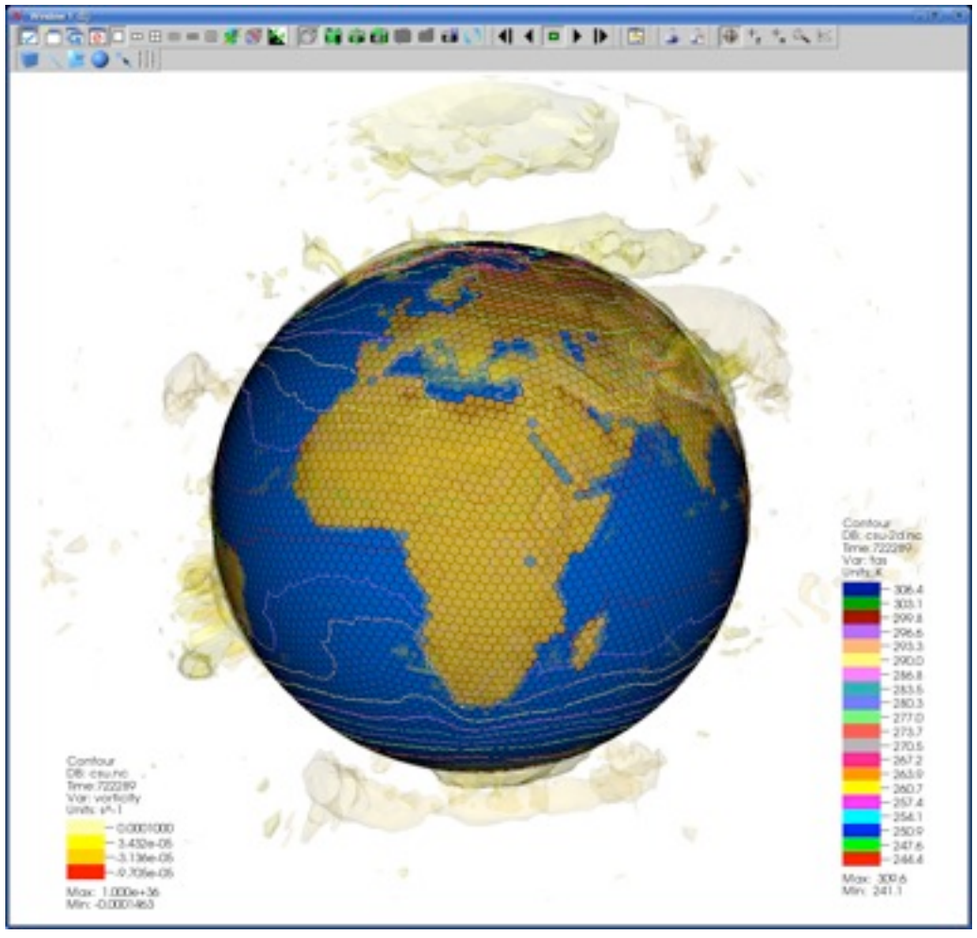
Z Y X

ParaView

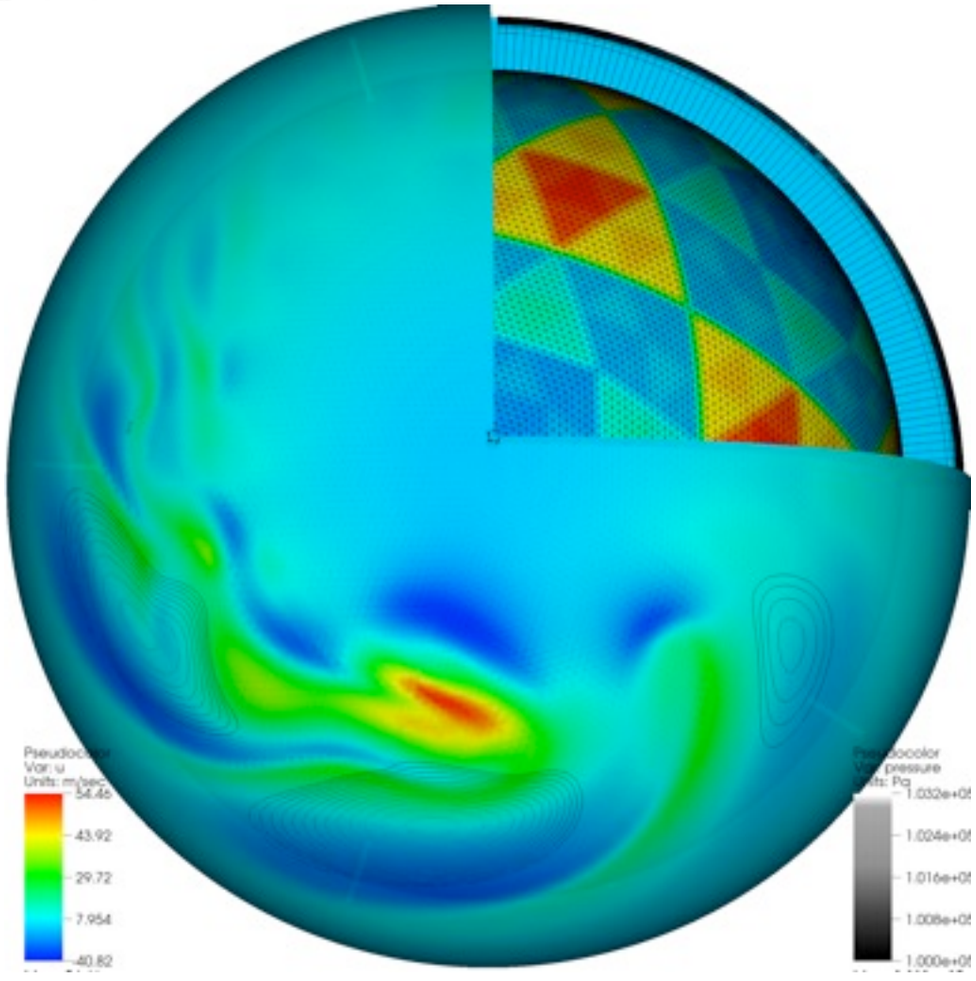
Wednesday, January 13, 2010

3D visualization of geodesic data

VisIT



3D isocontours of vorticity.



Composite plot of multiple mesh types and variables in the geodesic grid. Cell area (2D cell-centered data) and wind velocity (3D corner-centered on layers) data is shown by pseudocolor plots. Pressure (3D cell-centered on layers) is shown by contour lines.

Plots and movies courtesy of Prabhat (lbnl)

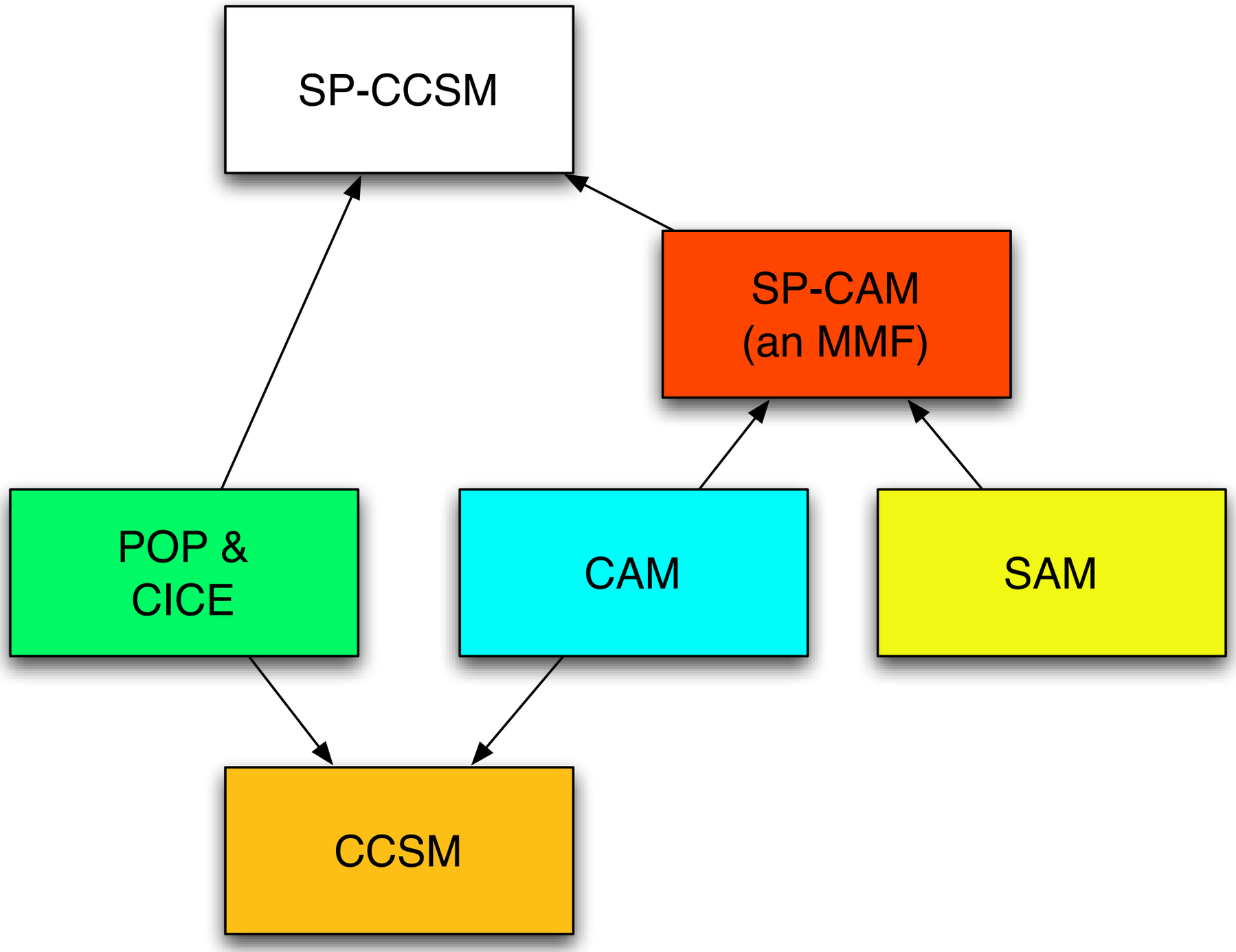
Future Testing

- Remote viz on Teragrid
  - –TACC (UT Austin) / SPUR
  - –Super-LES data
  - –ParaView (client-server, remote X-session over ssh)
- UCSD Cave
- SDSC high-capacity network connections
- CSU network connections
- Other interested parties?

Community Support

Model Code Portability

Wednesday, January 13, 2010


SP-CCSM
SP-CAM
(an MMF)
POP &
CICE
CAM
SAM
CCSM

Model Taxonomy & Software Configuration Management

- Model codes
- Utility codes

Mark Branson

CMMAP User Support

Connecting to TeraGrid

Community Accounts

To address scalability issues, many gateways provide access to TeraGrid resources through a community account rather setting up unique TeraGrid accounts for each gateway user.

A community account has the following characteristics:

- Only a single community user account (i.e., a TeraGrid username/password) is created.
- The Science Gateway uses the single TeraGrid community user account to launch jobs on the TeraGrid.
- The gateway user running under the community account typically has privileges to run only a limited set of applications.

The chief difference between an individual and a community account is that a community account is essentially a single username on the TeraGrid shared by many (human) users. While this eliminates the need for individual gateway users to request their own TeraGrid accounts, it places additional accounting and security burdens on the gateway developers. To distinguish one gateway user from another, the gateway developer has to institute a user registry and gateway authentication mechanism.

User Support & Documentation

Advanced Support for TeraGrid Applications (ASTA)

Home > User Support > ASTA

Advanced Support for TeraGrid Applications (ASTA) provides collaboration between Advanced User Support (AUS) staff and users of TeraGrid resources. The objective of the program is to enhance the effectiveness and productivity of scientists and engineers. As a part of the ASTA program, guided by the allocation process, one or multiple AUS staff will join the principle investigator's (PI's) team to collaborate for up to a year, working with users' applications.

AUS staff from TeraGrid resource provider sites have expertise and experience in many areas of high performance computing, domain sciences, data management, and grid computing. Collaborative work can include any of the following:

- Porting applications to new resources
- Implementing algorithmic enhancements
- Implementing parallel math libraries
- Improving the scalability of codes to higher processor counts
- Optimizing codes to efficiently utilize specific resources
- Providing help for portal and gateway development
- Assisting with visualization, workflow, and data analysis/transfer

In addition to requesting ASTA at the four quarterly allocations meetings, ASTA can also be requested throughout the year, as a Startup or Supplemental request, via POPS. Please visit the ASTA Project List page to view a list of current ASTA projects.

On this page

- How to Apply
- ASTA Selection Process

Related Links

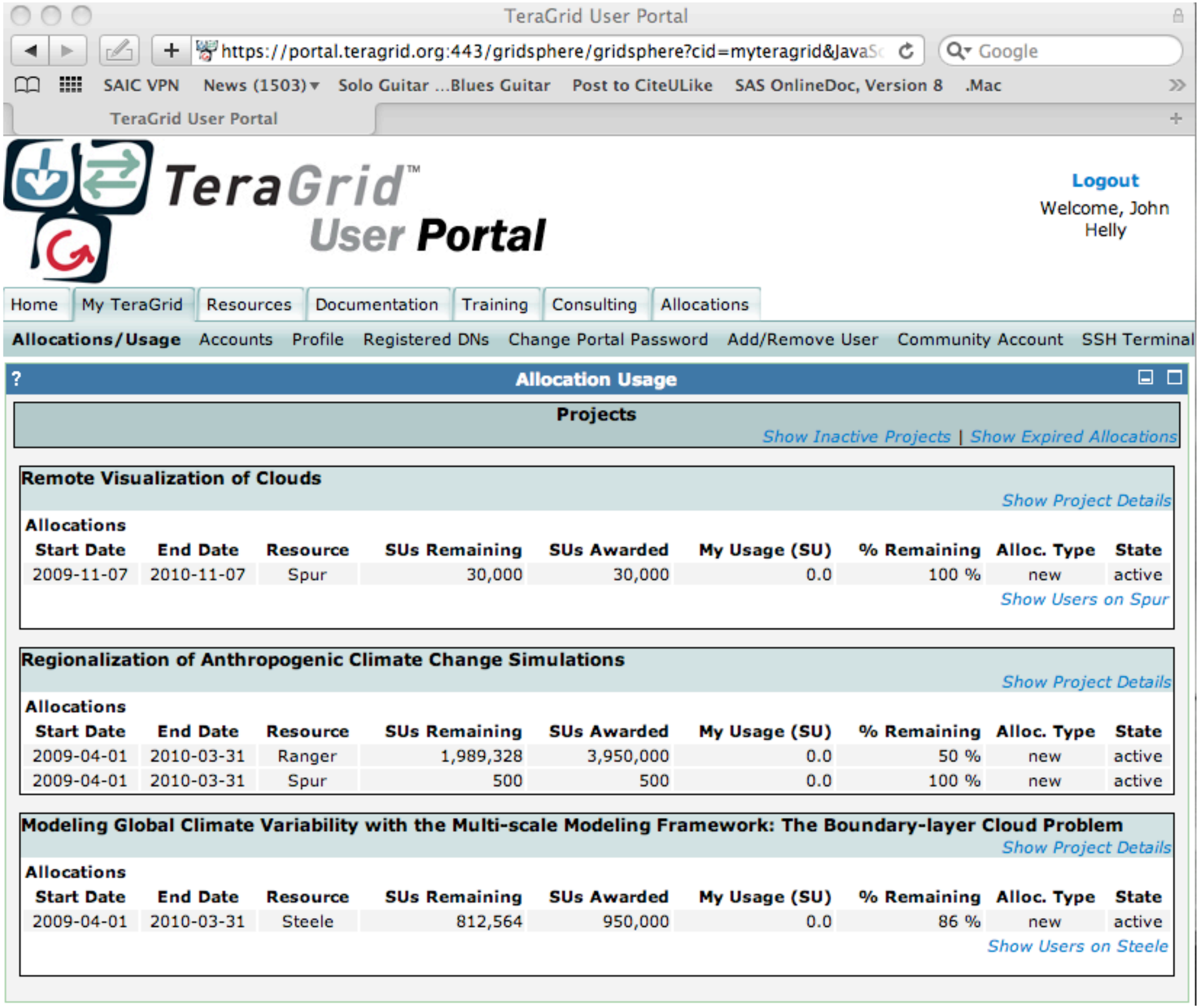
- ASTA Project List
- Allocations Information

Need Help?

- Phone Toll-free 1.866.907.2383
- Submit a Ticket (online form -- *fastest*)
- Submit a Ticket via email
- TeraGrid Knowledge Base

Wednesday, January 13, 2010

Backup


TeraGrid User Portal
https://portal.teragrid.org:443/gridsphere/gridsphere?cid=myteragrid&JavaS
Google
SAIC VPN
News (1503)
Solo Guitar ...Blues Guitar
Post to CiteULike
SAS OnlineDoc, Version 8
.Mac
TeraGrid User Portal
TeraGrid™ User Portal
Logout
Welcome, John Helly
Home
My TeraGrid
Resources
Documentation
Training
Consulting
Allocations
Allocations/Usage
Accounts
Profile
Registered DNs
Change Portal Password
Add/Remove User
Community Account
SSH Terminal
Allocation Usage
Projects
Show Inactive Projects | Show Expired Allocations
Remote Visualization of Clouds
Show Project Details
Allocations
Start Date | End Date | Resource | SUs Remaining | SUs Awarded | My Usage (SU) | % Remaining | Alloc. Type | State
2009-11-07 | 2010-11-07 | Spur | 30,000 | 30,000 | 0.0 | 100 % | new | active
Show Users on Spur
Regionalization of Anthropogenic Climate Change Simulations
Show Project Details
Allocations
Start Date | End Date | Resource | SUs Remaining | SUs Awarded | My Usage (SU) | % Remaining | Alloc. Type | State
2009-04-01 | 2010-03-31 | Ranger | 1,989,328 | 3,950,000 | 0.0 | 50 % | new | active
2009-04-01 | 2010-03-31 | Spur | 500 | 500 | 0.0 | 100 % | new | active
Modeling Global Climate Variability with the Multi-scale Modeling Framework: The Boundary-layer Cloud Problem
Show Project Details
Allocations
Start Date | End Date | Resource | SUs Remaining | SUs Awarded | My Usage (SU) | % Remaining | Alloc. Type | State
2009-04-01 | 2010-03-31 | Steele | 812,564 | 950,000 | 0.0 | 86 % | new | active
Show Users on Steele

Data Challenges of GCRM

- Extremely high volumes of data
  - 10 GB/ variable / step
  - 1-10 petabytes / simulated year
  - Can’t just move data to local systems
  - Data will have to be on-offline
  - 4 byte offsets exceeded
  - Huge number of files per simulation
  - Model for running analysis on the entire data set needed

Data Challenges of the GCRM (cont)

- Geodesic Grid
  - Preliminary (but not sufficient) support in some analysis tools
  - Standards for complete description not defined
  - Hyperslab-ing on coordinate values not supported and very costly
  - Grid itself is large (~ 2GB)

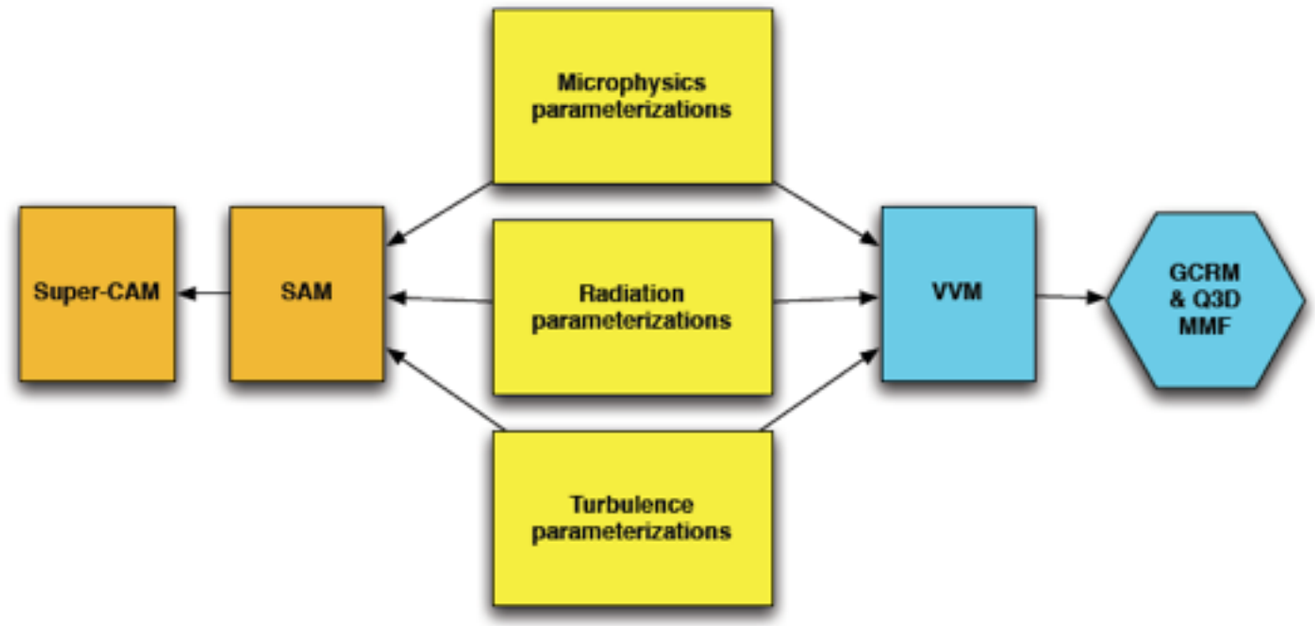
CMMAP's Stable of Models

- Current
  - Super-CAM
  - SAM
  - VVM
- Under development
  - GCRM
  - Q3D MMF

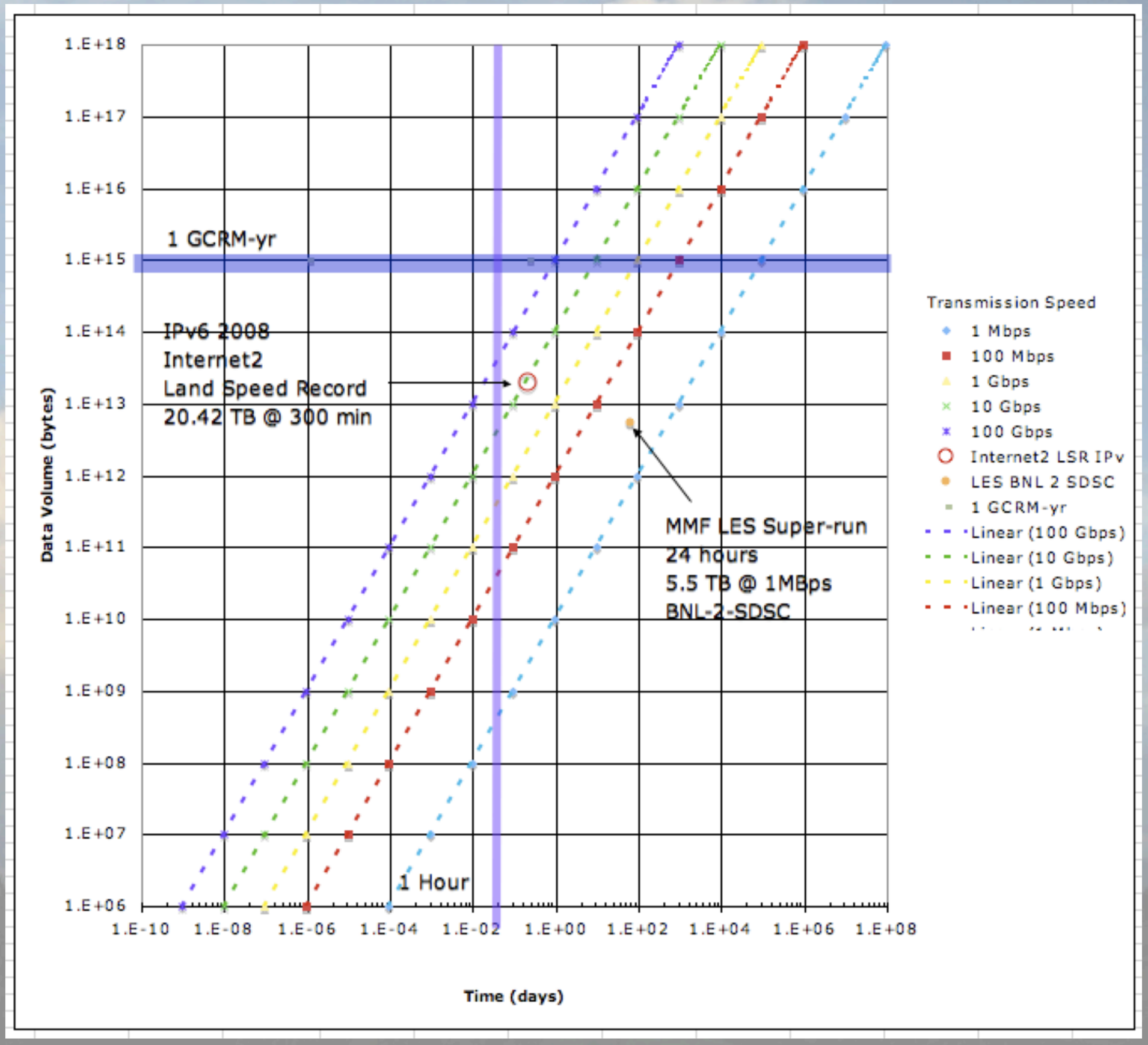
What do we mean when we say we '...are running the MMF'

Who's using what and what modifications are being made?

Testing parameterizations



Internet Data Transfer Capacity



Conventions for Naming Datasets

- spcam_climo_-3C-12C_1e-5_re7-10_vt01---> CMMAP_SUPERLES

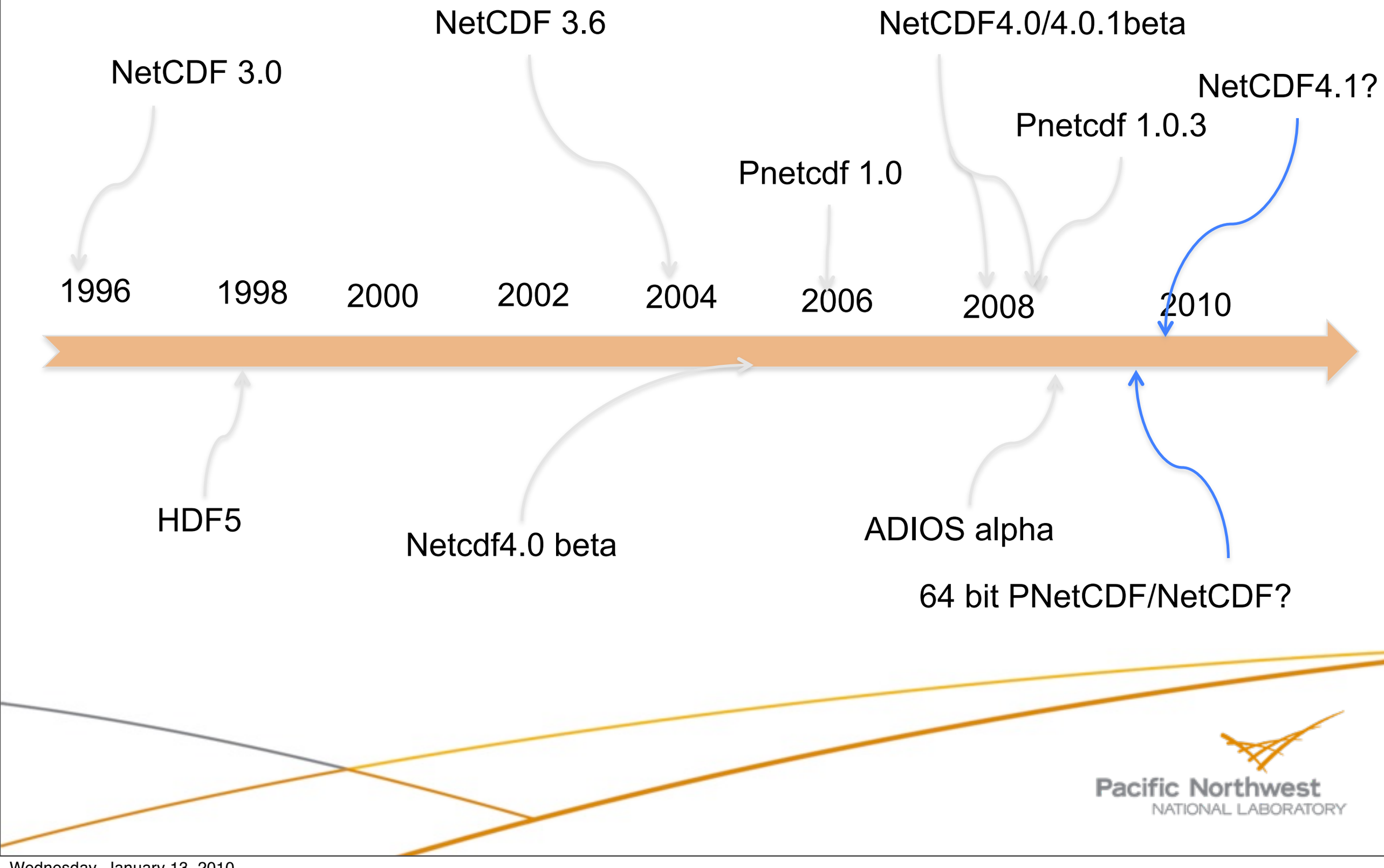
- Standardized names aid communication and data management
  - current convention is adapted from oceanographic collections done for SIO and IODP
  - none apparent for climate modeling (e.g., AMIP, CF)
  - DOI (digital object identifiers) are used in the publishing world)
  - this is similar to a DOI and we may add a DOI if a DOI authority emerges for atmospheric data
  - In the meantime we should have something equivalent

CMMAP_SUPERLES_20080725014445402_20080725014445402_	spcam3.clm2.r.0003-01-01-00000.mif

Standardized prefix is added to facilitate search and identification

Original filename is untouched

Timeline



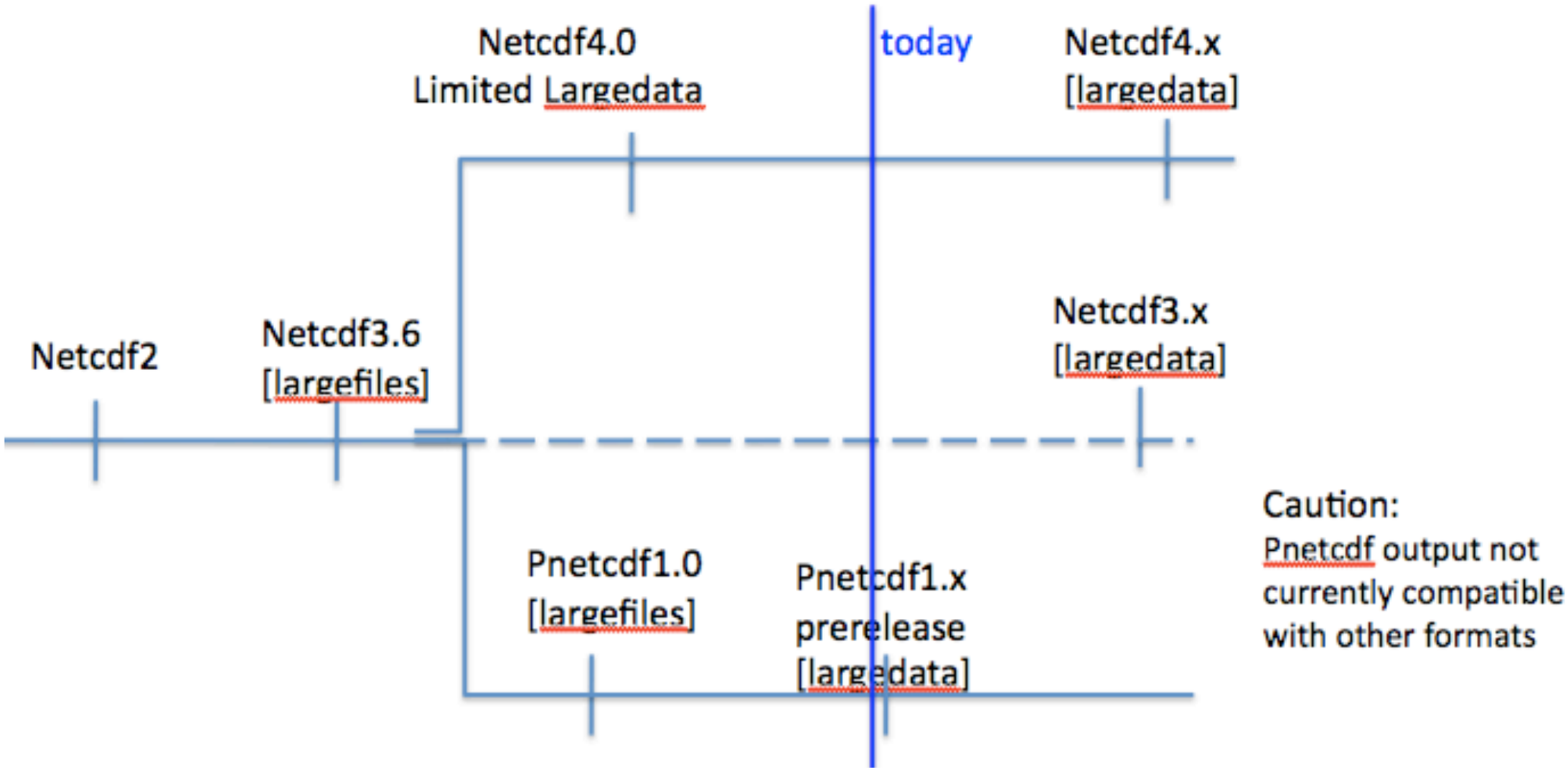
Pacific Northwest
NATIONAL LABORATORY

Action Items

- Data conversion code: com3d-netCDF (Helly, Branson)
  - add sample dataset
- Data Distribution of LES dataset (Helly)
- NSF LRAC Allocation Proposal w/technical support (Helly, Randall, Ackerman/Bretherton, Krueger)
- Digital Library search interface extension (Helly)
- OAI metadata server for external interoperability (Helly)
- Intercalibration observations for digital library (Helly, Ackerman)
- Prepare version control for MMF 2.0 and GCRM

NetCDF Status

Real large data support coming soon!



Model Taxonomy