

Cyberinfrastructure

10th Team Meeting
Berkeley, CA
January, 2011

John Helly



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

CIWG Agenda

- Current Status
 - NSF Architecture Planning Proposal (pending)
 - Teragrid Computing Allocations
 - Hugh Morrison's Experiments and Plans*
 - Community account for MMF runs
 - Exa-scale Data Transpose
 - Teragrid Allocation Calendar
- CMMAP CI Architecture (Roadmap)
 - Subversion MMF Development Repository (Mark B.)
 - iRODS web-browser and parallel data transfer service
 - MMF (SP-CAM) Community Account Portal
- Data Transportation
 - Parallel File I/O (Jeff Daily, Karen Schuchardt)
 - Data transpose project on Dash and Triton (prelim performance)
- Discussion



Current Status



Current Allocations

[Home](#)
[My TeraGrid](#)
[Resources](#)
[User Forums](#)
[Documentation](#)
[Training](#)
[Consulting](#)
[Allocations](#)

[Allocations/Usage](#)
[Accounts](#)
[Profile](#)
[Tickets](#)
[Registered DNs](#)
[Change Portal Password](#)
[Add/Remove User](#)
[Community Account](#)
[SSH Terminal](#)
[Citation Info](#)

Allocations/Usage

[Projects](#)
[Show Inactive Projects](#) | [Show Expired Allocations](#)

Modeling Global Climate Variability with the Multi-scale Modeling Framework

 New parameterizations of Cloud Micro-physics and Developing Community Accounts

 Portal for Running the MMF

[Show Project Details](#)

Allocations*

| Start Date | End Date | Resource | SUs Remaining | SUs Awarded | My Usage (SU) | % Remaining | Alloc. Type | State |
|---|------------|---------------------------------------|---------------|-------------|---------------|-------------|-------------|--------|
| 2010-07-01 | 2011-06-30 | abe-queenbee-steele-lonestar.teragrid | 2,307,000 | 2,307,000 | 0.0 | 100 % | new | active |
| Show Users on abe-queenbee-steele-lonestar.teragrid | | | | | | | | |
| 2010-07-01 | 2011-06-30 | NCSA Tape | 5 | 5 | 0.0 | 100 % | new | active |
| Show Users on NCSA Tape | | | | | | | | |

Data Transposition Development for Exa-scale Data in Memory

[Show Project Details](#)

Allocations*

| Start Date | End Date | Resource | SUs Remaining | SUs Awarded | My Usage (SU) | % Remaining | Alloc. Type | State |
|--|------------|--------------------|---------------|-------------|---------------|-------------|-------------|--------|
| 2010-05-04 | 2010-11-07 | dash.sdsc.teragrid | 29,970 | 30,000 | 30.0 | 100 % | supplement | active |
| Show Users on dash.sdsc.teragrid | | | | | | | | |
| 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 | 2010-09-30 | Ranger | 43,186 | 3,950,000 | 0.0 | 1 % | new | active |
| 2009-04-01 | 2010-09-30 | Spur | 397 | 500 | 103.0 | 79 % | 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 | 2010-09-30 | Steele | 103,900 | 950,000 | 0.0 | 11 % | new | active |
| Show Users on Steele | | | | | | | | |

Leveraging National & Partner Resources

| | Organization | Resource | 2007 | 2008 | 2009 | 2010 | 2011 |
|-----------------------|---|--|--------------|---------------|---------------|---------------|--------------|
| Data Allocations | San Diego Supercomputer Center (SDSC) | Disk | 15 Terabytes | 15 Terabytes | 30 Terabytes | 45 Terabytes | 45 Terabytes |
| | | BlueGene | | | 30,000 SUs* | | |
| | | Triton | | | | 30,000 SUs | 30,000 SUs |
| Computing Allocations | Teragrid (multi-institution) | SDSC DataStar (IBM SP4) | 600,000 SUs | 1,200,000 SUs | | | |
| | | Grid Roaming | | | 600,000 SUs | 2,703,000 SUs | |
| | | LSU Steele | | | 900,000 SUs | | 2,307,000 SU |
| | | SDSC (Dash) | | | | | 60,000 SU |
| | 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 | | |
| | | | | | | | |

TeraGrid Allocation Calendar



[TeraGrid Home](#) > [User Support](#) > [Access](#) >> [Allocations & Accounts](#) > Allocation Calendar

| | Startup/Educational Allocation | | Research Allocation (TRAC) | |
|---|--|---|--|--|
| Units Requested <i>Service Units (SUs) on compute resources (TeraGrid Resource Catalog)</i> <i>Terabytes (TBs) on Data Resources</i> | System size | Maximum compute request | 30,000 – Unlimited | |
| | < 100 TFLOPS | Up to 30,000 SUs | | |
| | >= 100 TFLOPS | Up to 200,000 SUs | | |
| | <ul style="list-style-type: none"> Aggregate request for multiple compute resources cannot exceed 200,000 SUs | | | |
| | | <ul style="list-style-type: none"> Storage on disk: 5 TB Storage on tape: 25 TB | | |
| Deadlines | N/A | | Open Submissions | Close Submissions |
| | | | Dec. 15 Mar. 15 ¹ Jun. 15 Sept. 15 | Jan. 15¹ 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 | |

CMMAP Architecture Roadmap





CMMAP Digital Library

DATA RESOURCES

- ◆ Data Collections Browser
- ◆ Search Metadata Catalogue

COMPUTING RESOURCES

- ◆ NSF Teragrid
- ◆ DOE INCITE

SOFTWARE

- ◆ Bulk Data Transfer Client
- ◆ Client software for accessing CMMAP data holdings.
- ◆ Model Development Team
- ◆ Multi-scale Modeling

Data Collections Browser now available from CMMAP Digital Library

This browser makes it possible to conveniently browse the data holdings of the CMMAP Digital Library. An account is so contact John Helly (hellyj@ucsd.edu) or Mark Branson (mark@atmos.colostate.edu) for access.

[hellyj's blog](#) [Add new comment](#)

Subversion repository account creation or password resetting.

Repository URL:

<https://svn.sdsc.edu/repo/cmmmap>

Obtaining or Re-setting a password.

1. To generate a new password from any unix host, please run the following:
`htpasswd -mn`
2. The output should look something like this: `jd:$apr1$L7wBD/..$.koeYBEZ3TfM.qOW6fXr0`
3. Copy and paste that output into an email to jd@sdsc.edu with the subject:

Please add or replace this user in the CMMAP subversion repository.

INCITE Resources & Allocations

Subversion Repository

The screenshot displays a Mac OS X desktop with several Subversion-related windows. The top menu bar includes 'Grab', 'File', 'Edit', 'Capture', 'Window', and 'Help'. The system tray shows various icons and the date 'Thu 7:12'.

Repositories Window: A table lists repository names and their URLs. The 'CMMAP' repository is highlighted.

| Name | Url |
|------------|---|
| Neptune | /Users/hellyj/Active/svn_repos |
| Geospatial | file:///Volumes/Geospatial001/svn_repos |
| CESM V1.0 | https://svn-ccsm-release.cgd.ucar.edu/model_versions/cesm1_0/ |
| CMMAP | https://svn.sdsc.edu/repo/cmmap |

Working Copies Window: A table lists working copy names and their paths. The 'DLF' working copy is highlighted.

| Name | Path |
|------------|--------------------------------------|
| DLF | /Users/hellyj/Active/svn_working/DLF |
| Geospatial | /Users/hellyj/svn_work/IcebergIII |

CMMAP Window: Shows the Subversion client interface for the 'CMMAP' repository. The URL is `https://svn.sdsc.edu/repo/cmmap/`. It features a search log field and a log table.

| Rev # | Date | Author | Log message |
|-------|-------------------|----------|---|
| 52 | 08/02/10 15:23:15 | u8753 | JNR 02 Aug 2010 4page version install file |
| 51 | 08/02/10 15:22:35 | u8753 | JNR Aug 02 4 page version |
| 50 | 07/29/10 19:27:25 | hellyj | First import |
| 49 | 07/29/10 19:20:39 | hellyj | Deleting DrupalModules |
| 48 | 07/29/10 18:47:13 | hellyj | Modules developed to integrate modeling servi |
| 47 | 07/28/10 15:07:12 | mbranson | Additions and fixes to allow the SPCAM to out |
| 46 | 06/02/10 15:28:20 | mbranson | Uncomment out the previously commented out li |

Below the log, the text 'JNR 02 Aug 2010 4page version install file' is displayed. The window also shows a file browser for 'Revision : 52' with a tree view of the repository structure:

- root
 - CAM
 - DrupalModules
 - SAM
 - SPCAM
 - branches
 - tags
 - trunk
 - form_spcam3
 - querym
 - querymv2

iRODS Web-browser

Terminal — irsync — bash — Big Kahuna's settings — ttys003 — 149x44

```
GATE_IDEAL_S_02250_057_to_070.nc
GATE_IDEAL_S_02250_071_to_084.nc
GATE_IDEAL_S_02250_085_to_098.nc
GATE_IDEAL_S_02250_099_to_112.nc
GATE_IDEAL_S_02250_113_to_126.nc
GATE_IDEAL_S_02250_127_to_140.nc
GATE_IDEAL_S_02250_141_to_154.nc
```

Terminal — bash — bash — Big Kahuna's settings — ttys001 — 149x36

```
--rw-r--r--@ 1 hellyj hellyj 1005584384 Jul 31 11:10 GATE_IDEAL_S_00450_001_to_014.nc
--rw-r----- 1 hellyj admin 0 Aug 3 08:43 GATE_IDEAL_S_02250_071_to_084.nc
drwxr-xr-x 7 hellyj hellyj 238 Sep 1 2009 Imeccoal
-rw-r--r-- 1 hellyj admin 508998 Aug 3 08:04 IntroToFRE.pdf
drwx-----@ 83 hellyj hellyj 2822 Apr 22 09:27 Library
drwx-----+ 7 hellyj hellyj 238 May 31 18:05 Movies
drwx-----+ 10 hellyj hellyj 340 Dec 14 2009 Music
drwx-----+ 309 hellyj hellyj 7104 Jun 3 15:29 Pictures
drwx---r-x* 6 hellyj hellyj 204 Jan 23 2008 Public
drwxr-xr-x 22 hellyj hellyj 748 Dec 14 2007 Shared
-rw-r--r-- 1 hellyj admin 3781 Apr 26 16:14 SomewhereOvertheRainbow.txt
drwxr-xr-x 6 hellyj admin 204 Nov 22 2009 bandwidthTest
lrwxr-xr-x 1 hellyj hellyj 33 Jun 11 2009 bin -> /Users/hellyj/Active/Projects/bin
drwxrwxrwx 10 hellyj hellyj 340 Mar 22 2009 cron
-rw-r--r-- 1 hellyj admin 75332 Apr 17 11:27 fm_user_coords.dat
drwxr-xr-x 5 hellyj admin 170 Aug 16 2009 grade_work
drwxrwxr-x 7 hellyj hellyj 238 May 11 2006 helly_family
drwx----- 3 hellyj hellyj 102 Mar 11 2009 iRODS_Vault
drwxr-xr-x 4 hellyj hellyj 134 Nov 17 2009 logs
drwxr-xr-x 3 hellyj admin 102 Jan 6 2010 mail.neptune
-rw-r--r-- 1 hellyj admin 679 Nov 3 2009 octave-core
drwxr-xr-x 6 hellyj hellyj 204 Oct 4 2008 odv_local
lrwxr-xr-x 1 hellyj hellyj 34 Jun 11 2009 perl -> /Users/hellyj/Active/Projects/perl
-rw-r--r-- 1 hellyj admin 234 Apr 3 22:11 pgadmin.log
drwxr-xr-x 3 hellyj admin 102 Apr 3 21:34 postgres
drwxr-xr-x 6 hellyj hellyj 204 Feb 22 07:20 python
drwxr-xr-x 7 hellyj admin 238 Apr 21 01:19 scratch
drwxr-xr-x 5 hellyj hellyj 170 Sep 22 2009 sites
drwxr-xr-x 15 hellyj hellyj 510 Aug 3 05:36 src
drwxr-xr-x 3 hellyj admin 102 Apr 11 01:08 svn_work
drwxr-xr-x 2 hellyj admin 48 Jul 21 13:48 untitled folder
drwxr-xr-x 3 hellyj hellyj 102 May 1 2009 workspace
neptunetravel:~#ls
/cnmap001/home/hellyj:
C- /cnmap001/home/hellyj/MODEL_RUNS
neptunetravel:~#
```

Macintosh HD
hellyj
DS_Store
AudiobooksSelect.xml
BeatlesMono.xml
BeatlesRemaster.xml
ConcertForGeorge.xml
Crossroads.xml
CSDI_workingGroupMeeting.pages



Update on Parallel Data I/O

Jeff Daily & Karen Schuchardt

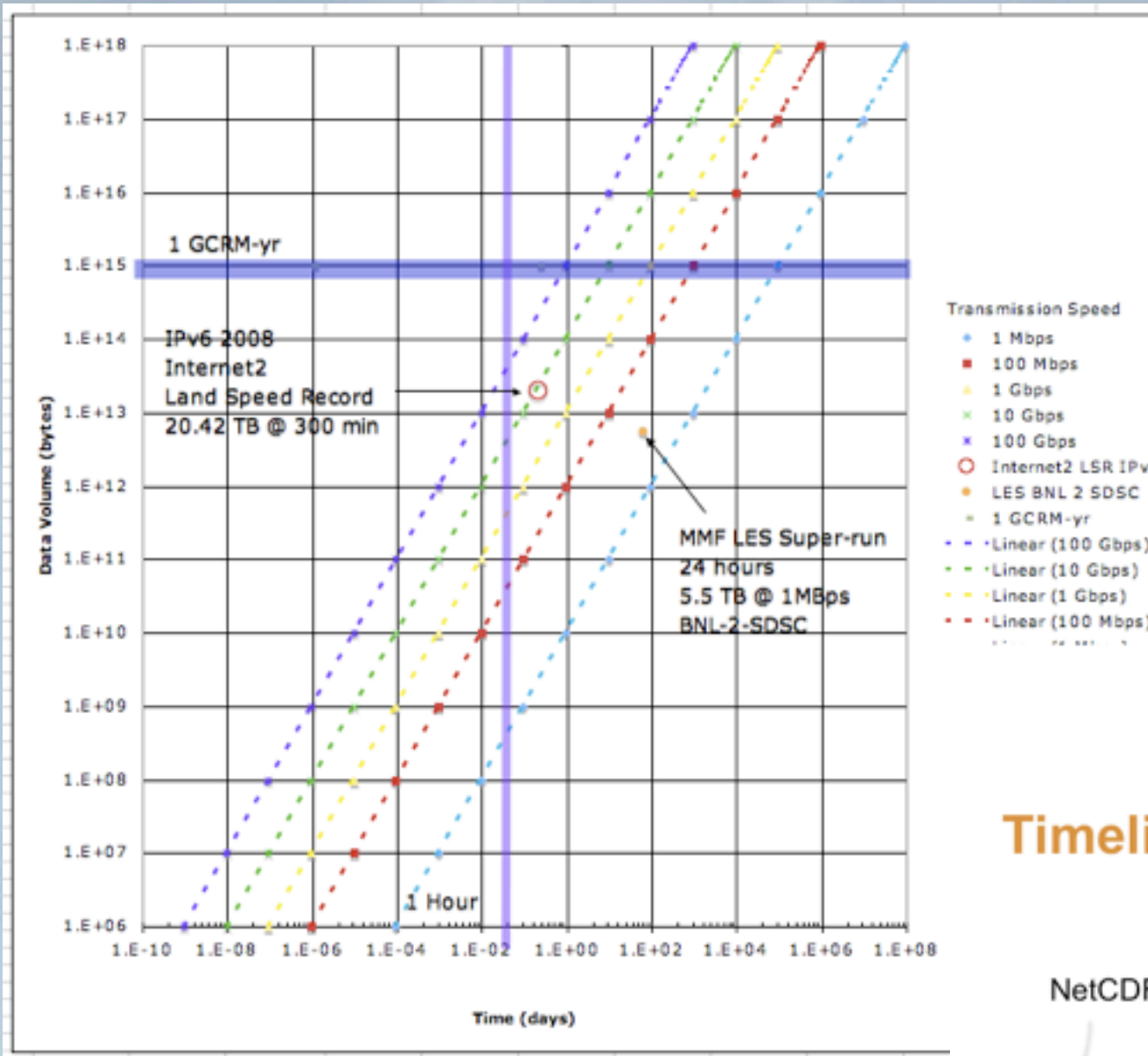
GCRM Data Problem

The GCRMs and Giga-LES models are conceptually complex, but in addition they pose problems that are technical, practical, and fiscal, rather than conceptual in nature. This is where the need for new infrastructure arises. Our proposed infrastructure project relates to data management, analysis, and visualization:

- GCRMs produce terabytes to petabytes of model output. The data is created at supercomputer centers. It must be archived, curated, and made available to users at remote sites.
- Many difficult choices must be made; for example, choosing which fields to output, and what subsetting spatial and temporal resolutions to save, are complex.
- Routinely saving global model output with high temporal resolution is not practical.
- A possible strategy is to save regional model output (for one or more selected regions) with high temporal resolution, and full spatial resolution, and global model output with lower temporal resolution and perhaps even reduced spatial resolution.
- Extraction of useful information from GCRM output is complicated by the sheer volume of data produced, the wide range of scales represented, and the diverse phenomena included. New methods are needed for comparison of model output with a variety of observations, including satellite data.
- New methods are needed for the efficient and effective visualization of GCRM results. The range of scales is so large that “zooming” capabilities are essential. New approaches are needed to visualize and analyze the time evolution of complex three-dimensional structures (such as large rotating convective clouds) that are associated with multiple interacting fields, including vector fields.

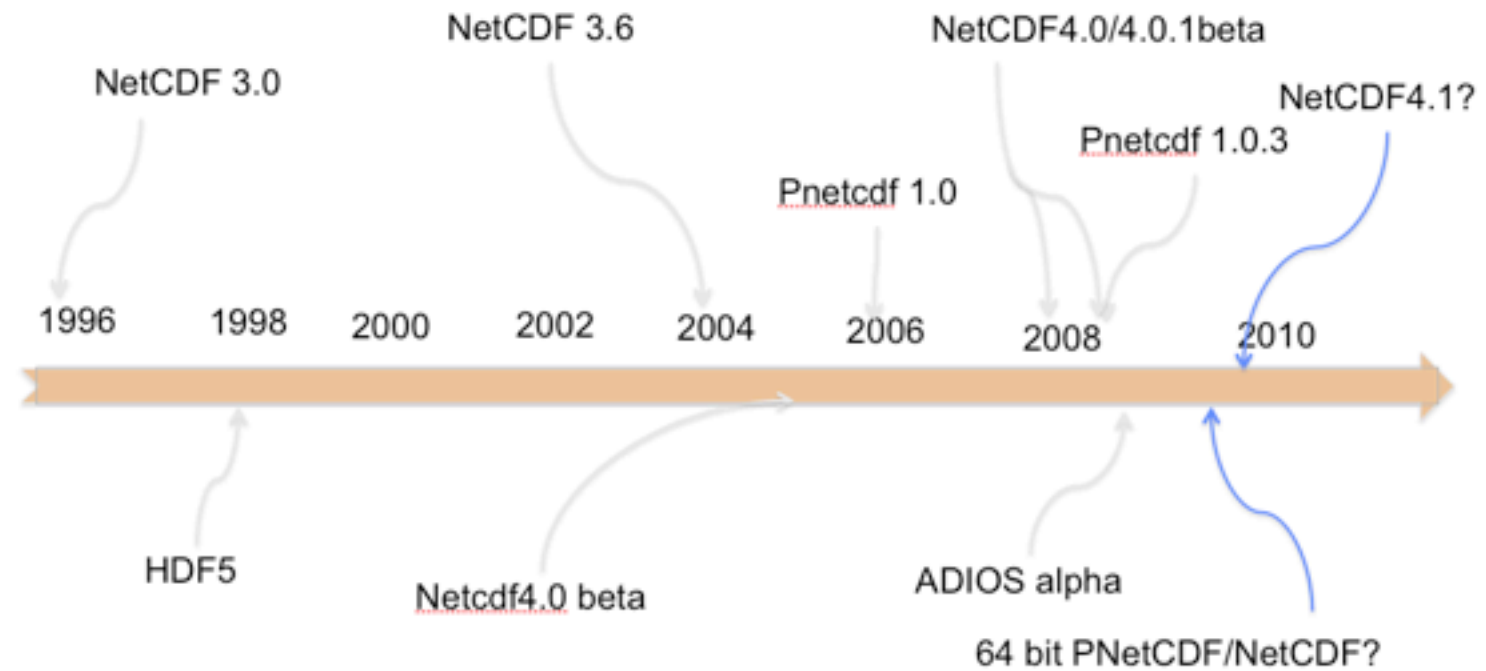
In short, *the very large models used in cloud-climate studies must be supported by a suitably designed infrastructure for data management, analysis, and visualization.* These needs are community wide and should be addressed in a coordinated fashion that serves the community as a whole.

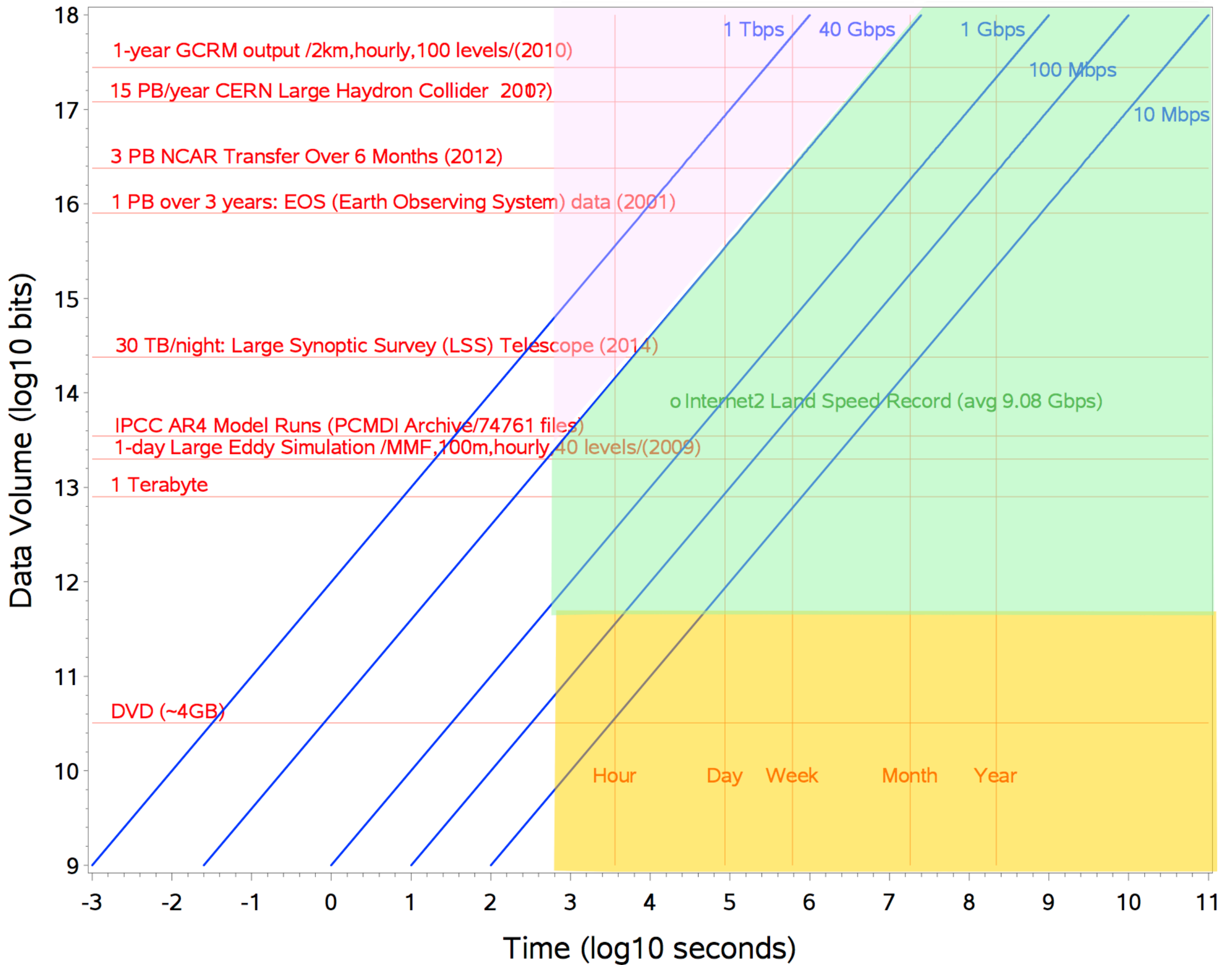
Internet Data Transfer Capacity



Parallel Input/Output Technology Progress

Timeline





CMMAP Data Services News

Karen Schuchardt
UC Berkeley
January 2011



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PNetCDF

- ▶ defines cdf5 format based on cdf3 with fixes for large variables
- ▶ New psuedo non-blocking IO that improves performance
- ▶ Support for setting the header padding size (important for basic metadata editing)
- ▶ Integers are 4 bytes; no longs
- ▶ In theory, can be specified as the mechanism to use via the NetCDF4 interface
- ▶ Up to 10GB/s franklin (of possible 16GB)
- ▶ **Pretty robust and good performance** (version 1.2)
- ▶ **Data can only be processed with pnetcdf-based analysis tools**
 - Future support model not clear

NetCDF4

- ▶ Based on widely used HDF5 data model
 - HDF5 format is a rich data format with filesystem-like constructs
 - Lots of tunable features like compression, chunking
 - Can be restricted to netcdf data model constructs
- ▶ Fortran interface (still) has 32bit restriction
- ▶ Not stress tested
- ▶ Performance currently lags PNetCDF
- ▶ New DOE Exascale project to optimize HDF5
 - ▶ LBNL (Prabhat – PI), HDF5 Group, PNNL
 - Being done in context of real applications
 - GCRM
 - ▶ Pore scale simulators (groundwater, physics)

Runs

- ▶ Z anelastic model (run to date)
 - 15km, 26 interfaces, 18 days, 3 hourly
 - Jablonowski test case, 10000 processors on franklin

 - About 8 variables \approx 44GB

- ▶ Z anelastic model (by spring/summer)
 - 4 or 7 km (or both), 36? interfaces, 18 days, 3? hourly
 - Initial conditions TBD, \sim 10000/40000 processors on hopp2
 - ▶ Will have physics added (Don Dazlich)
 - 8? variables \approx **TBD**

NOTE: time free only until April

Analysis - ParCal

- ▶ New DOE Project for Parallel Data Analysis Tools
- ▶ ANL (Rob Jacob PI), NCAR, PNNL, Sandia
- ▶ Major outcomes
 - Version of NCL which transparently turns current NCL data arrays and operations into parallel operations
 - Climate specific compression to be tested in PNetCDF

Cyber-infrastructure Working Group: Pagoda

Jeff Daily and Karen Schuchardt, PNNL



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Parallel Analysis of Geodesic Data

- ▶ a.k.a Parallel Analysis of Geoscience Data
- ▶ C++ API for developing custom analysis
 - Most similar to Java NetCDF API
- ▶ Data-parallel command-line tools
 - Mimics the NetCDF Operators (NCO)

| NCO | pagoda |
|----------|--------|
| ncks | pgsub |
| ncra | pgra |
| ncea | pgea |
| ncbo | pgbo |
| ncflint | <soon> |
| ncwa | <soon> |
| ncrcat | |
| ncrename | |
| ncatted | |
| ncpdq | |



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Pagoda Design

- ▶ Focus on parallel IO and large variables
 - Do what NCO does but when your data is too large for your workstation
- ▶ Handles regular and geodesic grids
 - Geodesic grids are described using an explicit topology
 - Explicit topology needed for analysis/visualization e.g. VisIt
- ▶ Reads and writes classic NetCDF via Parallel NetCDF
- ▶ Reads and writes NetCDF4
- ▶ Runs on workstations, clusters, HPC systems e.g. hopper

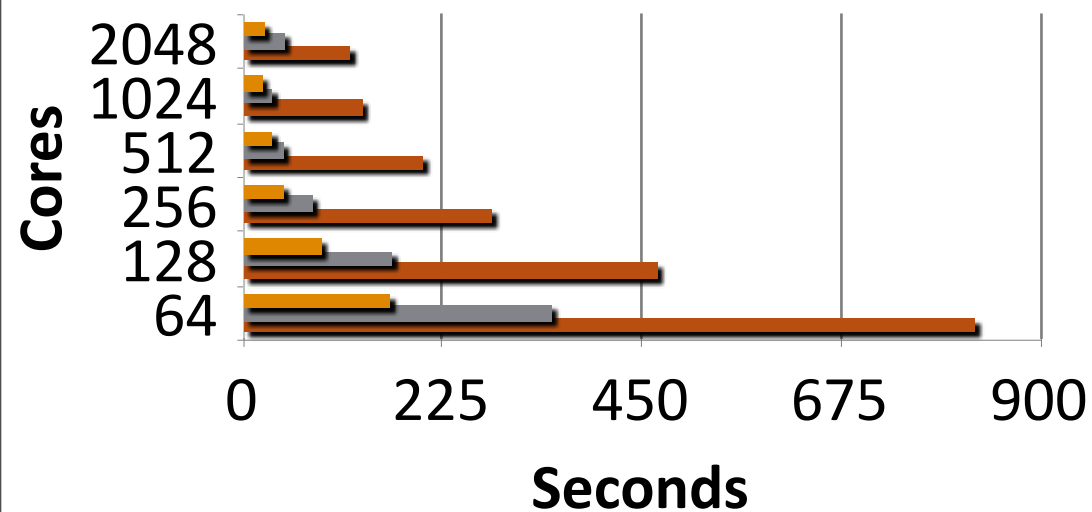


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pgsub Strong Scaling

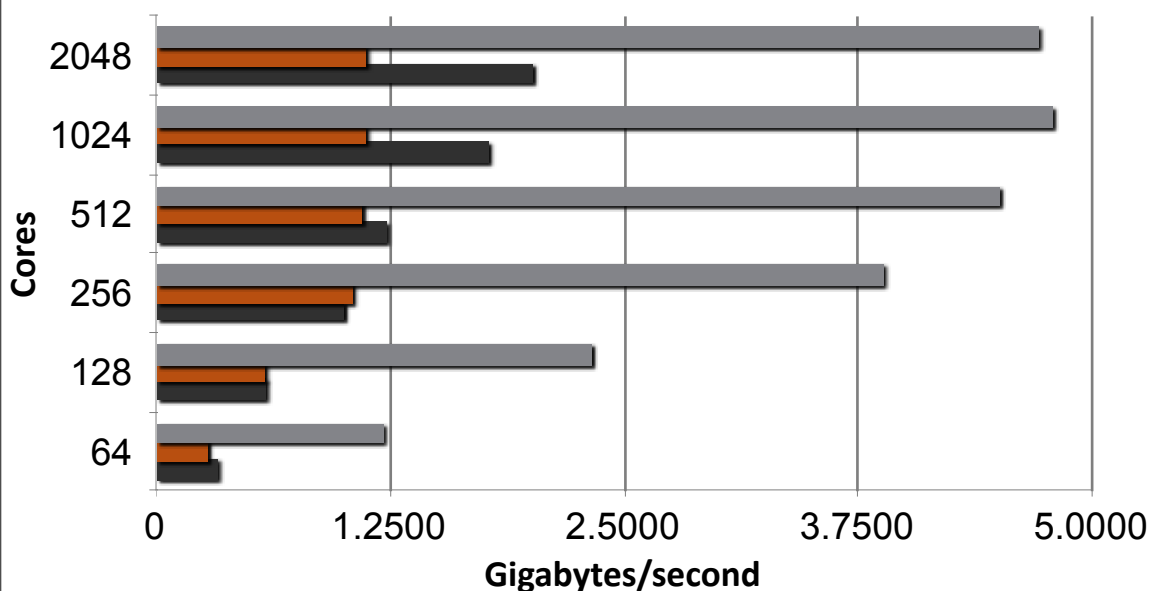
Strong Scaling - Wall Time



- ▶ Shown to scale up to 2K cores
- ▶ Shows that IO is a major bottleneck
- ▶ Write bandwidth nearly 5GB/s on franklin
- ▶ Our first optimization shows importance of efficient use of IO

■ Non-IO
■ Optimized
■ Subsetting

Strong Scaling - IO Bandwidth



■ Write
■ ReadOpt
■ Read

Future Directions

- ▶ “make it easy” – A higher level API
- ▶ New language bindings? Python? Fortran?
- ▶ Handle additional conventions e.g. missing_value
- ▶ Finish pgflint (ncflint), pgwa (ncwa)
- ▶ Grid interpolation
- ▶ Other operators?
 - What if header isn't big enough and data is too large?
 - What if pnetcdf's “CDF5” format is used?
- ▶ We need more users and user input on what's needed
 - Already in use/testing by CSU, ANL, NCAR



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Thanks

- ▶ <http://svn.pnl.gov/gcrm/wiki/pagoda>
- ▶ pagoda-dev@googlegroups.com



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Model Run Management App

Safari File Edit View History Bookmarks Window Help

CMMAP Digital Library

http://cmmmap-dev.sdsc.edu/

Q* how do clouds tr...

CMMAP

CMMAP Digital Library

NEW FORUM TOPICS

- Subversion Management
- data format conversion
- What software should we use to produce the SUPERLES derivatives?
- We have identified nedCDF as the default format for data products. Any discussion needed?

more

ACTIVE FORUM TOPICS

- Subversion Management
- What software should we use to produce the SUPERLES derivatives?
- We have identified

Subversion repository account creation or password resetting.

Repository URL:

<https://svn.sdsc.edu/repo/cmmmap>

Obtaining or Re-setting a password.

1. To generate a new password from any unix host, please run the following:
`htpasswd -mn`
2. The output should look something like this: `jd:$apr15L7w8D/...$l.koeYBEZ3TFM.qOW6FXr0`
3. Copy and paste that output into an email to jd@sdsc.edu with the subject:

Please add or replace this user in the CMMAP subversion repository.

INCITE Resources & Allocations

2010 INCITE Call for Proposals

[Add new comment](#) [Read more](#)

Teragrid Resources & Allocations

Model Run Management App

Safari File Edit View History Bookmarks Window Help (100%) Thu Jan 13 7:30

Experiment with SPCAM | CMMAP Digital Library

http://cmmap-dev.sdsc.edu/Run_SPCAM

CMMAP Digital Library

NAVIGATION Experiment with SPCAM

Experiment with SPCAM

Welcome hellyj!(Please avoid browser "back" button. TAI)

What would you like to do?

[Run SPCAM](#) [Check Status](#) [Process Results](#)

NEW FORUM TOPICS

- Subversion Management
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more

ACTIVE FORUM TOPICS

- Subversion Management
- What software should we use to produce the SUPERLES derivatives?
- We have identified

Macintosh HD
hellyj
HellyVault001
DS_Store
AbWorkOut.mp3
ArakawaTalk
Audiobook1Select.xml
EachProfileWork
CalCOFI_2010.ppt
Combined...rofiles.mov
Combined...nolin.mov
CombinedQuarterly.mov
Downloads alias
gmt
gmt_work
HDFView
IntroToFRE.pdf
mathworks_downloads
Music alias
MusicMP3
MV1102
NavyReports
Notes.pages
SDSC_Geos...01028.key
SLR_SERDP...ucts.pages
test.txt
Transfer
UCMexus_201007
UCMexus...otes.pages
Why.pages



Introduction to FRE: The Flexible Modeling System Runtime Environment

Developed at GFDL, 2002-2010, by:

Amy Langenhorst Amy.Langenhorst@noaa.gov

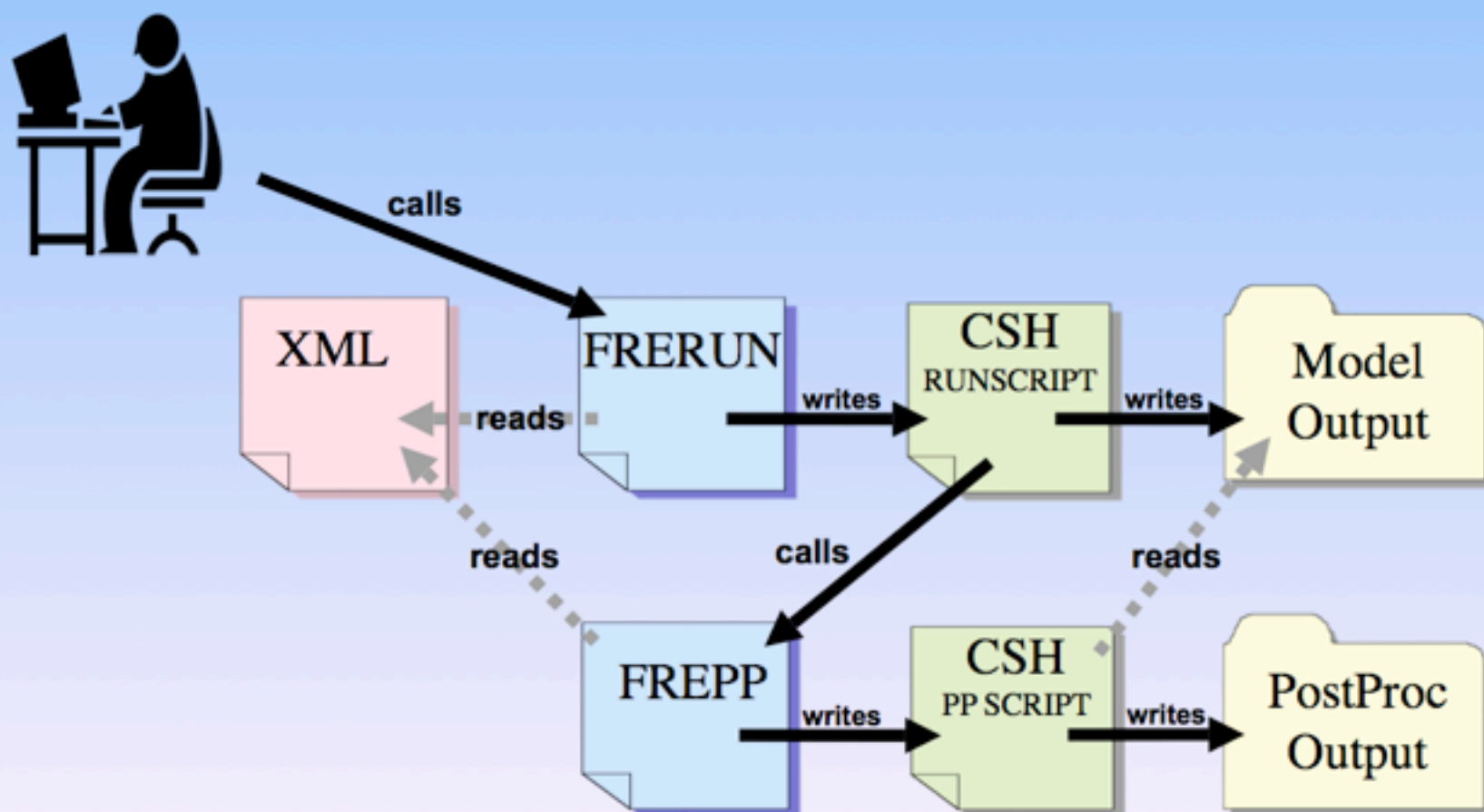
Aleksey Yakovlev Aleksey.Yakovlev@noaa.gov

V. Balaji V.Balaji@noaa.gov

Introduction to FRE

- The FMS Runtime Environment (FRE) is a toolset for managing experiments from start to finish
 - acquire source code, compile (*fremake*)
 - launch jobs to run models (*frerun*)
 - postprocessing the output (*frepp*)

The Mechanics of FRE





Hugh Morrison

Proposed tests of microphysics in MMEF using Teragrid

- Recent request for large Teragrid allocation was reviewed and accepted (allocation through July 2011)
- Broadly, goal is to address two separate but related issues: 1) sensitivity to key parameters in scheme, 2) tuning
 - anticipate ~ 50 sensitivity runs (1 week spinup + 4 additional weeks) for initial tests, ~ 10 tuning runs (2 year runs + 1 month spin up) based on configurations identified from sensitivity tests, and a ~25-year AMIP- type run – total of 633 months simulation time, coupled run?
 - anticipate tests using 1.9 x 2.5 degree fv core, 64 CRM columns per large grid

- Based on timing tests from Mike Pritchard on Purdue Steele cluster, 3.5 million SU's were requested

• ~ 2.5 x more expensive using 2-moment microphysics compared to standard SpCAM, estimated cost is 5600 SU per month simulation.

- Tests to focus on:

1) Reducing costs of microphysics

- larger microphysics timestep**
- reduced # of prognostic (advected) variables**

2) Sensitivity to new microphysics developments and parameter settings

- Morrison and Grabowski (2008) ice microphysics (has 6 prognostic variables versus 9 in M2005 → improved cost)**
- Parameter settings identified as being important in CRM tests (e.g., graupel density and fallspeed)**

3) Tuning

Next steps:

Tests in stand-alone SAM (for significant code changes, such as reduction in # of prognostic variables)

**Working with GUI interface to compile/run SpCAM
- approaches for modifying/testing code (e.g., svn)**

Analysis of output

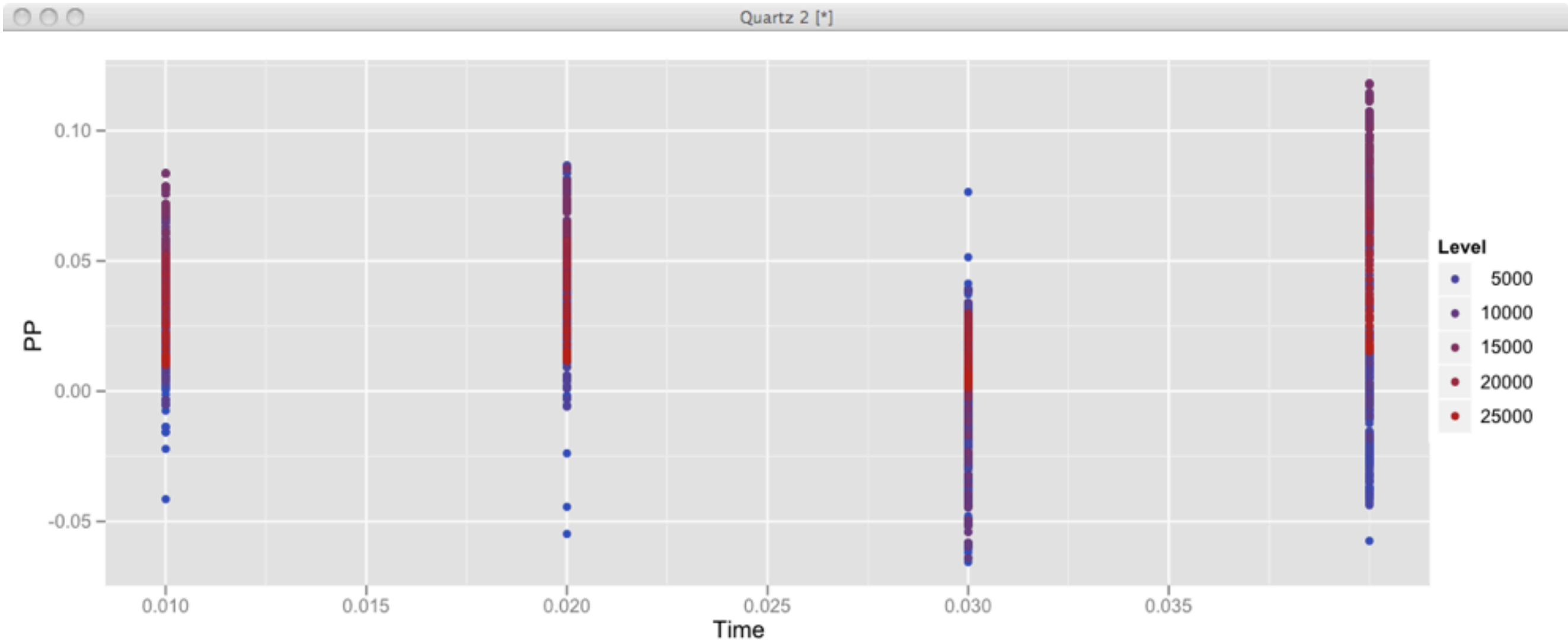
- do we want to develop a “standard” diagnostics package, a la the CAM diagnostics?

CMMAP Data Transposition Code

Overview of Code

- LES (SP-CAM) Data files in NETCDF format.
- OpenMP code setup to read one file per core simultaneously.
- Each file corresponds to a spatial partition at a given time. The code reads in all the files into memory to do the transposition.
- Tested on
 - Triton regular [8 core, 24GB] and large memory nodes [32 cores, 512GB] w/ data oasis [lustre].
 - Dash regular [8 core, 48GB] and vSMP node [128 cores, 650GB] w/ GPFS-WAN.

Initial Recovery of Time-series



Triton Results

- Code tested with 76 files. Total size of data read : 128GB.
- Run times are dominated by I/O performance.

| No. of Cores | 8-core node [2 Quad Nehalems] | 32-core node [8 Quad Shanghais] |
|--------------|----------------------------------|------------------------------------|
| 1 | 347s | 505s |
| 2 | 197s | 222s |
| 4 | 122s | 118s |
| 8 | 105s | 154s |

Dash Results

- Tested on regular compute nodes w/ GPFS-WAN.
vSMP node testing in progress.

| No. of Cores | 8-core compute node (w/GPFS-WAN) |
|--------------|----------------------------------|
| 1 | 838s |
| 2 | 496s |
| 4 | 301s |
| 8 | 245s |

Summary and Future Work

- OpenMP code tested and results verified on Triton and Dash.
- Current performance limited by I/O performance of filesystem on given node.
- Achieved ~1.2GB/s w/ lustre on Triton node. The maximum achievable is 1.25GB/s [Myrinet card peak]. GPFS-WAN performance on Dash node is lower due to network setup. Lustre testing on Dash is in progress.
- Peak performance achieved using 4 cores on 32-way node => it might be useful to limit number of threads reading. Can still use more threads for analysis part.
- Developing hybrid (MPI + OpenMP) code to make use of more nodes and get better I/O performance [Lustre on Triton can do over 7GB/s on reads].

Discussion

- Upcoming allocation proposals (new LES run?)
- Additional model runs for digital library
- High-volume data visualization
- Time-series data recovery from model runs for validation support

Backup



Proposal to the National Science Foundation for

**Community Infrastructure Planning:
Cyber-Infrastructure for the Cloud-Climate Community**

Prepared in response to
CISE Computing Research Infrastructure (CRI) Program Solicitation 08-570

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NSF Planning Proposal

4. Planning process

Our goal is to submit the CI proposal in the summer of 2011.

Planning will begin at CMMAP's Team Meeting in August 2010, the same week that this planning proposal will be submitted to NSF. We will also take advantage of CMMAP's Team Meeting in January 2011, in Berkeley, California, where we systematically collect ideas from the CMMAP team, and also engage the local talent at NERSC, including the developers of ViSIT. The planning activity will be a major component of the January 2011 meeting.

The tasks to be completed before the submission of the CI proposal include:

- Scoping the hardware and software systems, including the determination of expected life-cycle cost to operate over its useful lifetime.
- Developing a plan for maintaining and enhancing the proposed infrastructure up to and beyond the sunset of the planned CI grant.
- Outreach to solicit input from the CMMAP community and the national HPCC centers on the design of the hardware and software components and external and internal interfaces of the proposed infrastructure.
- Soliciting input from the CMMAP community on the design of the education and outreach activities that will be associated with the proposed infrastructure.
- Developing a site plan for the hardware, in cooperation with the CSU administration, including the university's Facilities office.

13

- Developing an operations plan, which must take into account the education and outreach activities. Initiation of a planning process to determine hardware and software configuration and a likely data loading model to size the system against

5. Management Plan

- Many difficult choices must be made; for example, choosing which fields to output, and what subsetted spatial and temporal resolutions to save, are complex.
- CMMAP standard?

The Program Planning Prism

- Management
 - CIWVG (Cyberinfrastructure Working Group)
 - Data Policy
 - Software Policy
- Resource Planning
 - Computing
 - Data
 - People
- Community Support
 - Data interoperability
 - Model code portability

R: Analysis and Plotting

Click to **LOOK INSIDE!**

Use R!

Hadley Wickham

ggplot2

The R Project for Statistical Computing

http://www.r-project.org/

Q: R download

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[Contributors](#)
[Screenshots](#)
[What's new?](#)

Download, Packages
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R Project
[Foundation](#)
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[Bug Tracking](#)
[Developer Page](#)
[Conferences](#)

PCA 5 vars
prcomp(x = data, cor = cor)

Clustering 4 groups

Factor 1 [41%]

Factor 3 [19%]

Getting Started:

- R is a free software environment for statistical computing and graphics. It compiles and runs on a wide variety of UNIX platforms, Windows and MacOS. To [download R](#), please choose your preferred [CRAN mirror](#).
- If you have questions about R like how to download and install the software, or what the license terms are, please read our [answers to frequently asked questions](#) before you send an email.

News:

RGL - 3D Real-Time Visualization Device System for R

http://rgl.neoscientists.org/download.shtml

Q: 3d visual

RGL

3D Real-Time Visualization Device System for R

News

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Get it from [CRAN](#)

rgl package details at <http://cran.r-project.org/src/contrib/Descriptions/rgl.html>

Get it from our local [Archive](#)

Checkout the latest revision

See [Developer](#) section for details.

GSP's Guide to netCDF and R

http://www.image.ucar.edu/GSP/Software/Netcdf/

Q: netcdf R

UCAR | NCAR

Statistics Software Data Publications Projects

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GSP's guide to netCDF format data and the 'R' package 'ncdf'.

netCDF is a common, self-describing, portable binary format for geophysical data. GSP made an executive decision earlier this year (i.e. Tim and Doug talked after lunch) to use this format as much as possible when creating or manipulating data sets. For the statistical readership we should note that there are contributed packages for R that allow for the efficient reading and writing of netCDF files and part of the intent of this web page is to provide some simple [examples](#) to get users started. Some advantages of this format are:

- The netCDF libraries to create and access files for many (all?) architectures are free and available through [UNIDATA](#).
- A netCDF file not only contains the "data" but also a description of the variables, the creation history, and any other important attributes about the data set.
- A netCDF file is a reasonably compact **portable** binary format. i.e. You can make one on a 'supercomputer' and read it on a PC.
- The netCDF interface can extract parts of a large data file without having to read the entire record. Since many netCDF files are 0- Gigabytes, this is important.
- netCDF is a standard format not only for geophysical observational data but also for numerical model output, such as the NCAR community climate system model.
- A contributed package in R, [ncdf](#) is free, readily available, and simplifies the interface to the otherwise gory low-level routines available in the Unidata library.

A brief description of netCDF

With regards to netCDF, a little philosophy goes a long way. A netCDF file is intended to provide all the information needed to interpret the data, as well as the data itself. The information about the length of each dimension, how many dimensions, the units of the quantity, etc. are all contained in a netCDF file. They are intended to be **self-describing**. The netCDF format is flexible enough to allow for a tremendous variety of incarnations. Some netCDF files contain the data for (a set of) radiosonde instruments, some represent the output of a General Circulation Model (GCM), or a set of observations taken at a weather station, for example. All three cases will be explored in the following discussion.

The netCDF file can be broken down into logical parts. To that end, lets take a look at the **header** of a very simple netCDF file.

netCDF example ↵

Citable Publication of Scientific Data

John Helly
Scripps Institution of Oceanography
San Diego Supercomputer Center
University of California, San Diego



Optiputer@SDSC

http://cmmmap.sdsc.edu/

CMMAP Digital Library

Active forum topics

- Allocation Proposal Schedule (as of: 2008-07)
- Computing Time
- Proposals
- Fortran90
- Data

hellyj

- Create content
- Login
- Search Data Catalogue
- My account
- Recent posts
- Administer
- Log out

Allocation Proposal Schedule (as of: 2008-07)

Tue, 07/29/2008 - 2:46pm — hellyj

Latest summary schedule

Add new comment 1 attachment CIWG

2008 Annual Meeting

Tue, 07/29/2008 - 1:02pm — hellyj

First blog entry

hellyj's blog 2 comments

Developer Tools

- Migrating code to Future NSF resources (<http://www.sdsc.edu/us/consulting/migration.html>)
- Script automation (<http://www.ibm.com/developerworks/aix/library/au-satbuildscript.html>)
- Compiler quirks (<http://en.wikipedia.org/wiki/Compiler>)

Read more

Recent blog posts

- 2008 Annual Meeting

Recent comments

- Model Taxonomy has been updated 2 min 7 sec ago
- ECMWF Multi-grid modeling idea 2 hours 44 min ago

Who's new

- mikepritchard
- kelly
- mbranson
- leoners56
- jasonc

Who's online

RSS

CMMAP Digital Library - Reach for the sky - RSS (8 messages, 3 unread)

| Date Received | From | Subject |
|---------------------------|---|---|
| Today 2:46 PM | CMMAP Digital Library - Reach for the sky | Allocation Proposal Schedule (as of: 2008-07) |
| Today 1:02 PM | CMMAP Digital Library - Reach for the sky | 2008 Annual Meeting |
| Today 10:18 AM | CMMAP Digital Library - Reach for the sky | Developer Tools |
| Today 10:01 AM | CMMAP Digital Library - Reach for the sky | Visualization Resources |
| Today 9:54 AM | CMMAP Digital Library - Reach for the sky | Computing Allocation Resources |
| July 26, 2008 8:57 PM | CMMAP Digital Library - Reach for the sky | Example of Creating HTML from External Editor |
| July 26, 2008 7:52 PM | CMMAP Digital Library - Reach for the sky | How to Create Drupal Content |
| February 11, 2008 6:51 PM | CMMAP Digital Library - Reach for the sky | Preparing for Track 2 NSF Systems |

CMMAP Digital Library - Reach for the sky

Developer Tools

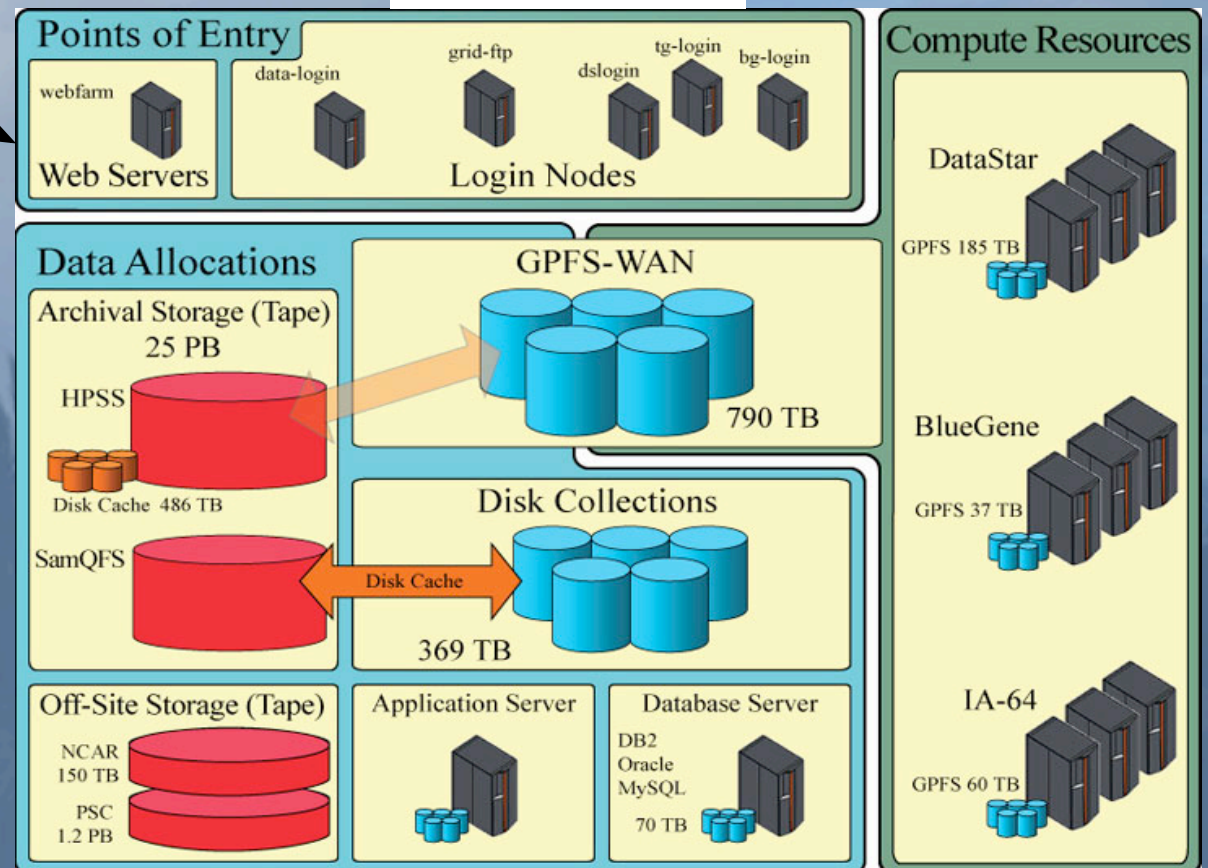
July 29, 2008 10:18:40 AM PDT

- Migrating code to Future NSF resources (<http://www.sdsc.edu/us/consulting/migration.html>)
- Script automation (<http://www.ibm.com/developerworks/aix/library/au-satbuildscript.html>)
- Compiler quirks (<http://en.wikipedia.org/wiki/Compiler>)

read more

Read more...

SDSC
SAN DIEGO SUPERCOMPUTER CENTER



URL data retrieval

OAI metadata



Management Data Policy



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

Community Support

Data Interoperability





Resources

Visualization of Very Large Datasets



File Edit View Sources Filters Animation Tools Help

Navigation toolbar with icons for file operations, view manipulation, and animation. Includes a 'Time: 0' display on the right.

Toolbar for object manipulation, including 'Result' and 'Surface' dropdowns, and various movement and rotation icons.

Secondary toolbar with icons for calculator, zoom, and other utility functions.

Pipeline Browser

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

Object Inspector

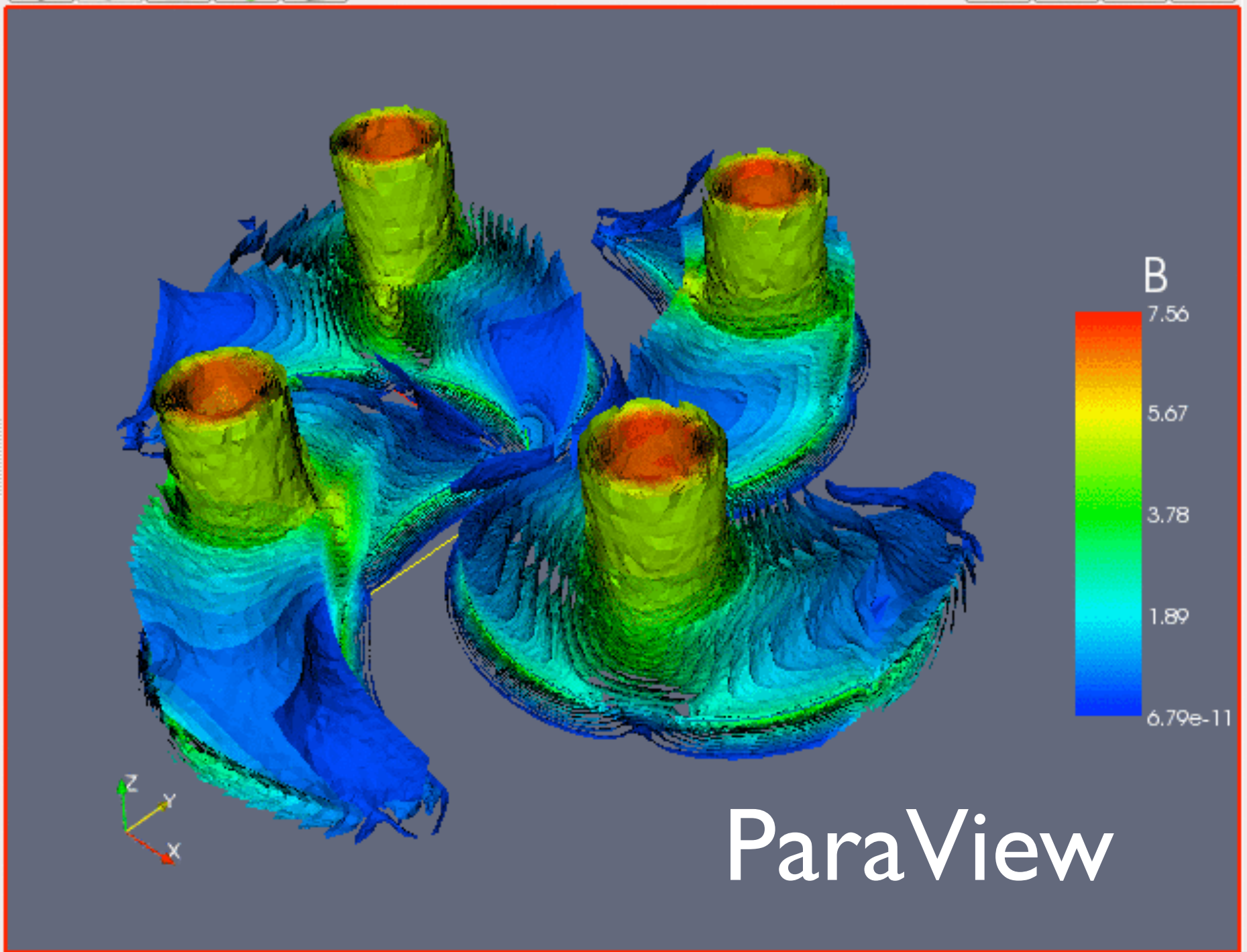
Properties | Display | Information

Apply | Reset | Delete

Isosurfaces

Value Range: [6.79195e-11, 7.55638]

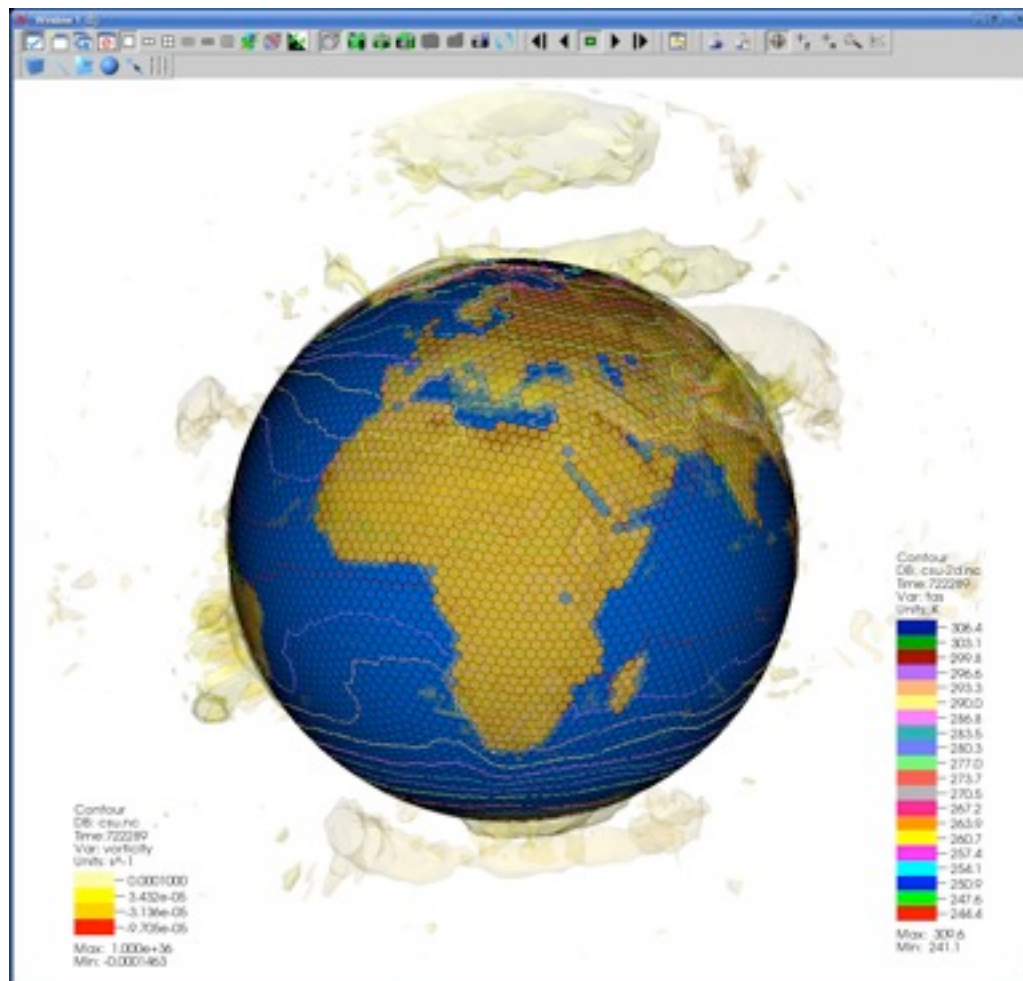
| | |
|----------|-------------------------------------|
| 6.79e-11 | Delete |
| 0.329 | Delete All |
| 0.657 | New Value |
| 0.986 | New Range |
| 1.31 | <input type="checkbox"/> Scientific |
| 1.64 | |
| 1.97 | |
| 2.3 | |
| 2.63 | |



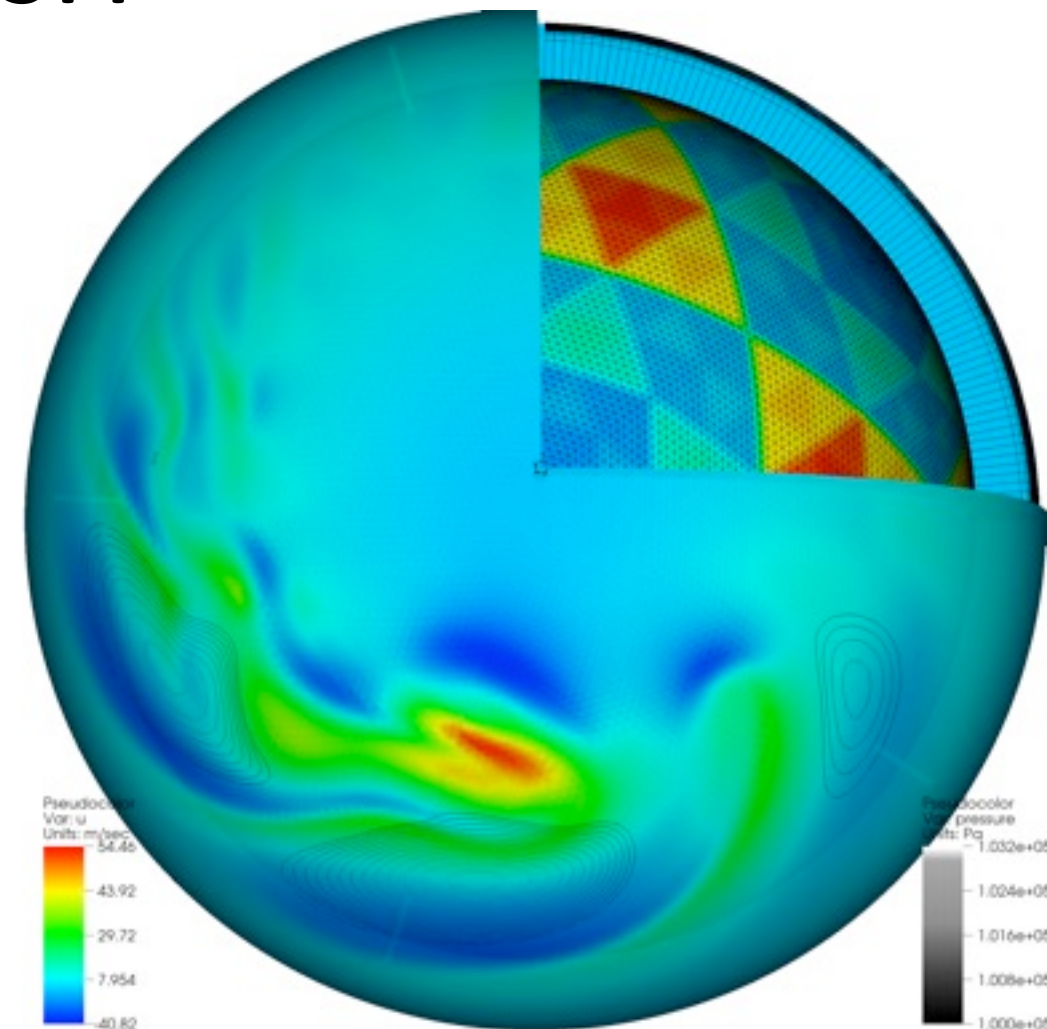
ParaView

3D visualization of geodesic data

VisIT



3D isocontours of vorticity.

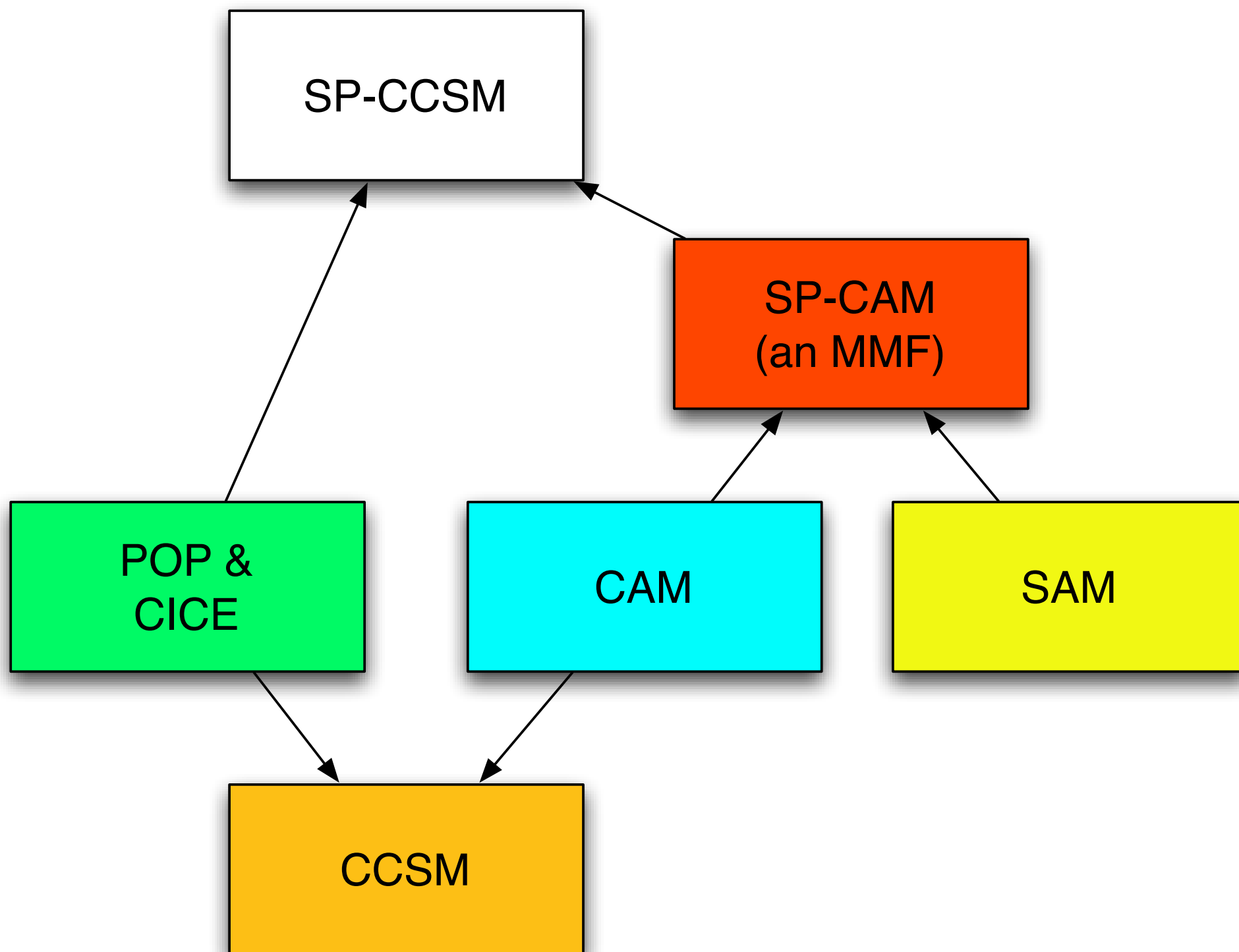


Composite plot of multiple mesh types and variables in the geodesic grid. Cell area (2D cell-centered data) and wind velocity (3D corner-centered on layers) data is shown by pseudocolor plots. Pressure (3D cell-centered on layers) is shown by contour lines.



Community Support Model Code Portability





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?