CISL HPC and allocations update

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Outline

- Yellowstone updates
- Procurement process update
- HPC Futures lab
- NCAR Data Sharing Service
- Application efforts
  - SPOC, IPCC-WACS, Data Workflows
- Google Apps update
- Allocations and usage updates
- Climate Simulation Laboratory changes
Resource Upgrades
January – March 2014

• Completed major RHEL operating system upgrade to Yellowstone, GLADE, Caldera, Geyser, Pronghorn
  – From RHEL 6.2 to RHEL 6.4

• Completed addition of 5 PB to the GLADE file systems, bringing the total usable capacity to 16 PB
  – New capacity being added to project and work spaces

• Installing new tape drive technology that will bring the archive capacity to 160 PB

• New GPU testing underway for upgrade of Caldera (from Fermi Tesla M2070 to K40) and Geyser (from Fermi Quadro 6000 to Quadro K5000)
Yellowstone Cable Health

• Since the full cable replacement in October 2013, Mellanox identified a second failure mode that impacts approximately 300 cables.

• CISL and Mellanox are closely monitoring the issue.

• Potentially faulty cables are identified preemptively and replaced before they fail.
Procurement Updates

- High-level NWSC-2 timeline has been developed that shows a production date of January 1, 2017.
- Yellowstone production will be extended for one year to give an overlap of the two systems.
- Rough order of magnitude power estimates are being used to scope NWSC Module A build-out.
- Archive procurement will start in about 2 years. This follows a recent extension of the existing Oracle contract and a review of technology roadmaps.
HPC Futures Lab

• CISL HPC Futures Lab is infrastructure for the hosting and testing of future HPC architectures and software
  – Processors, storage, interconnect, file systems, compilers, etc.

• Access to emerging technology for mitigating risk in future deployments and for the development of applications that may need these.

• Location: Primarily ML, but also NWSC depending on the system (e.g., storage we want closely coupled to Yellowstone for testing)
NCAR Data Sharing Service

- Share files with external persons, no need to get them a UCAR username or token
- Based on Globus Plus extension to Globus data transfer
  - Ideal for sharing large data sets
- Any NCAR user can set up an endpoint for specific colleagues or custom groups
- Contact cislhelp@ucar.edu to get started
Data Service I/O Networks

GLADE 16.4 PB
- 6Gb SAS
- nsd1
- nsd20

10 Gb Ethernet

HPSS

Data Transfer Services
- Globus, GridFTP, scp, sftp, bbcp, HSI/HTAR
- 4 nodes
- 10 GB/s

FDR14 InfiniBand
- > 90 GB/s

DATASHARE 1.5 PB
- FDR IB
- nsd1
- nsd4

Yellowstone
Geyser
Caldera

Cheyenne
Boulder

Thanks to Pam Gillman

data-access.ucar.edu
Data Sharing How-to

- Data recipient only needs a free Globus account—no token or other local access
- Data sharers are provided a location within ncar#datashare endpoint
- Data owner controls access via Globus features
  - Create your own endpoints, e.g. davidlhart#2b_shared
  - Create groups for access control
  - Share ‘read-only’ or ‘read-write’
  - Create custom access interfaces via CLI or REST API
- Data owner moves/copies files to shared space
  - Via Globus interface, or
  - By logging into data-access.ucar.edu and using *nix commands, HSI, or HTAR into /data/share/your-space
Strategic Parallel and Optimization Computing — SPOC

• A new initiative to improve the development of NCAR models and their use on production NCAR HPC environments

• Objectives
  – Help developers be more efficient in development, profiling, and debugging
  – Improve the job throughput by identifying and fixing application, software, and system issues
  – Implement tools for rapid validation of code changes.
  – Develop and disseminate best practices for running jobs efficiently

• Benefits
  – More productive science completed on Yellowstone today
  – Prepare CISL and the models for future systems at NCAR and elsewhere
SPOC structure and governance

Project Management & Tech Team

- CESM, WRF, MPAS Development Teams
- TDD/ASAP
- USS/CSG
- IMAGe (verification Project)

Advisory Committee

IPCC Weather and Climate Simulation (WACS)

CISL/OSD
CGD?
MMM?
NCAR?
New Grants

New Monies

Tools, Knowledge
Intel Parallel Computing Center

- Officially, “IPCC-WACS’ — Intel Parallel Computing Center for Weather and Climate Simulation
- Partnership of NCAR & CU Boulder
- Announced April 22, 2014
- Intel-funded effort focused on developing tools and knowledge to help improve performance of CESM, WRF, and MPAS on future Intel architectures
- Involves computer scientists, graduate students, Intel, and international partners
Data Workflows effort

- ASAP group working with CESM Software Engineering Group (CSEG) to accelerate post-processing of CESM results
  - Post-processing consumes a large fraction of simulation time for high-resolution runs

- Focusing on parallelizing the conversion of time-slice to time-series output
  - Single most expensive post-processing step for CMIP5 submission
Duration: Serial NCO

Convert 10 years of monthly time-slice files into time-slice files

Input dataset | GB
---|---
CAMFV-1.0 | 28.4
CAMSE-1.0 | 30.8
CICE-1.0 | 8.4
CAMSE-0.25 | 1077.1
CLM-1.0 | 9.0
CLM-0.25 | 84.0
CICE-0.1 | 569.6
POP-0.1 | 3183.8
POP-1.0 | 194.4
Duration:
NCO v. pyNIO + MPI w/compression

pyNIO = Python NCL I/O library

7.9x speedup (3 nodes)
35x speedup (13 nodes)
Google Apps update

- Transition schedule
  - Core IT: Already rolled out
  - Early adopters/coaches: Week of May 19
  - Global go-live: Targeting June 9

- Impacts on collaborators, end users
  - Should be no change to access via tokens to HPC systems, wiki, other services
  - Email forwarding will continue as it does now

- Bonus: UCAR email, other services will be available even through ML power downs and other incidents
Yellowstone Snapshot
Q1-2014

- 1M user jobs run & 140M core-hours provided
- 99% availability
- 91% utilization
- 400M files and directories currently on Glade
- 70 PB of data transferred to/from Glade
- 2.5 PB data added to the archive
Yellowstone allocations and usage
University projects and users

- **481 active projects**
  - 150 CHAP reviewed
  - 331 Small (≤ 200k)
- **303 have charged**
  Yellowstone use
  - 84% of Large projects
  - 53% of Small projects
- **43% of allocated core-hours have been used**

<table>
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<tr>
<th>Project lead</th>
<th>HPC charges</th>
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<tbody>
<tr>
<td>B. Arbic, U Mich</td>
<td>21,095,000</td>
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<tr>
<td>J. Marshall, MIT</td>
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<td>R. Stoll, U Minn</td>
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<td>N. Mahowald, Cornell</td>
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<tr>
<td>E. Bou-Zeid, Princeton</td>
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<td>C. Stan, COLA</td>
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<tr>
<td>W. Manchester, U Mich</td>
<td>1,700,000</td>
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<tr>
<td>T. Gombosi</td>
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University allocations and usage

Yellowstone University core-hours allocated and used

- Awarded
- Charges

FY12: 50,000,000
FY13: 90,000,000
FY14: 70,000,000
University FY14 use by institution
Potential new service to support CHAP process

- Early heads-up: We will be exploring a new service to support the CHAP process
  - If stars align, may be ready for fall submissions
  - More likely, spring 2015

- If ready, the tool will replace and automate aspects now handled manually and by disparate services (Drupal, Apache, email, Excel, tickets, and so on).

- Think: EasyChair for allocations
Climate Simulation Laboratory

• Two submissions to first call under revised eligibility rules
  – Previous CSL call had 10 submissions, only 5 had NSF support (including CESM)
  – Only 3 CSL awards (including (CESM) had NSF support

• Analysis/HPSS extensions offered to ending CSL awardees

• Thoughts, suggestions on promoting, emphasizing this opportunity in the future?
Discussion: Fall Review of CESM

- Focus on only the large CESM community allocation
- What review outcomes are desired? What should be emphasized?
- What input should be requested from CESM?
  - Length, format, detail of documentation
- What is appropriate format for the review?
- Balance need for review with effort to prepare
  - Same process every year? Alternate in-depth planning with progress review?