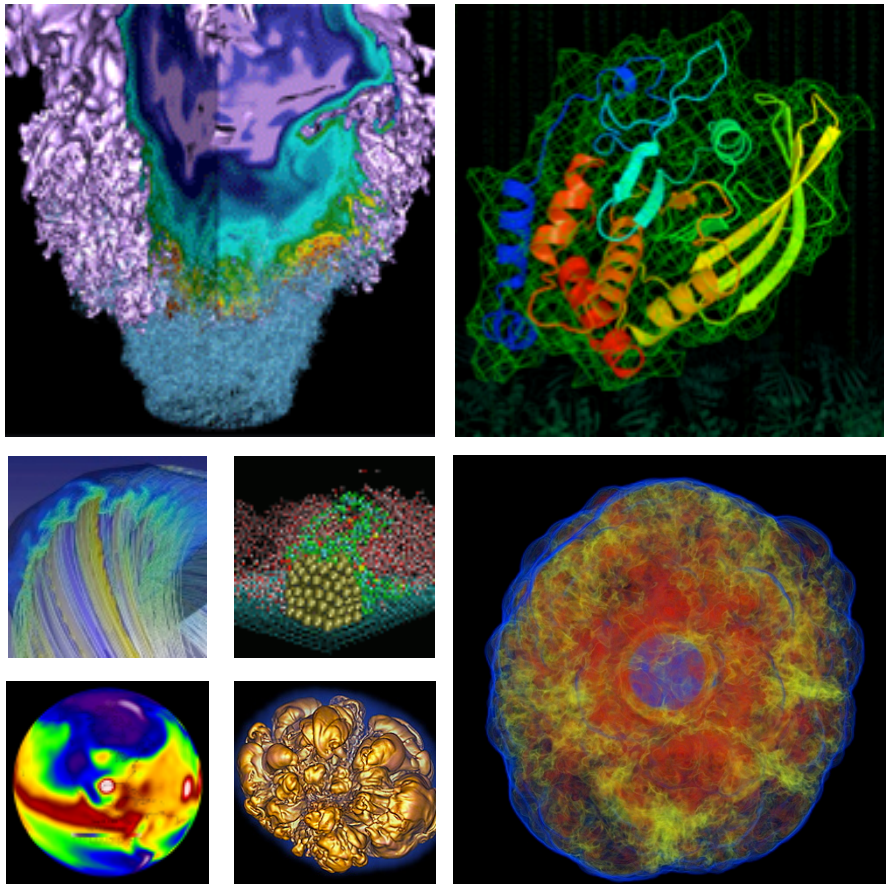
NUG Teleconference March 2013



Richard Gerber
Zhengji Zhao
NERSC User Services

March 8, 2013

Connection Info

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Topic: NUG Web Conference
Date and Time:
Thursday, March 7, 2013 11:00 am, Pacific Standard Time (San Francisco, GMT-08:00)
Event number: 661 898 953
Event password: edison

https://nersc-training.webex.com/ and chose from the list of events.

Teleconference information

1-866-740-1260
PIN: 4866820

Agenda

- **Early user experiences on Edison**
  - What issues are users reporting?; common solutions
  - Feedback from you
- **Email list for users to share experiences on Edison**
- **NUG 2013 Summary**
  - Update on action items from NUG 2013 Business Meeting
- **NUGEX/NERSC Committee for soliciting nominees & selecting 2014 NERSC achievement swards**
- **Scheduled outage email reminders**
- **Anything else that comes up**

Observations

- **System continues to be very stable; utilization close to 90%**
- **All users added March 2, 2013**
  - A few account issues at first, but all have been resolved
  - Fair share scheduling in place, DARPA mission partners get up to 25%
- **User reports are very positive**
  - Typical performance 2X+ Hopper
  - Report of python startup times up to 15X faster than Hopper
- **Please report problems & observations**
  - consult@nersc.gov or help.nersc.gov
- **Don't publish performance results until you get the OK from NERSC**
- **Common user issues to follow on next slide**

Issues with Intel MKL (Math Kernel Library)

- **How to link to MKL library with Intel compilers**
  - Use the –mkl option, available options are

    `-mkl=parallel` or **`-mkl`** links to threaded libraries

    `-mkl=sequential` links to non-threaded libraries

    `-mkl=cluster` links to "cluster MKL" (LAPACK, ScaLAPACK, BLAS, PBLAS, BLACS, VML, FFT libs) (non-threaded)
  - The position of the –mkl option in the link line matters, you need to put this option after all the object files that use the mkl libraries.
- **To link with all other library combination with the Intel and other compilers, please refer to the Intel's link advisor website**
  - http://software.intel.com/sites/products/mkl/

Issues with netcdf and hdf5

- Netcdf and HDF5 are available
- They are renamed and have a prefix `cray-` in the module names now

```
module load cray-netcdf
module load cray-hdf5
module load cray-hdf5-parallel
```

PETSc and Super_LU

- **Support for Intel compiler coming later this year**
- **Available now using Cray or GNU compilers**

  - `module swap PrgEnv-intel PrgEnv-cray`

  or

  - `module swap PrgEnv-intel PrgEnv-gnu`

Thread Core Affinity (Binding)

- **Threads are not bound to cores as you might expect with the Intel Compiler**
  - Currently binds all threads to first core if use aprun **`-cc cpu option`** (default)
  - Use **`-cc none or -cc numa_node`**
  - Don't use **`KMP_AFFINITY environment variable`** (unless you're an expert using this)
- **With Cray and GNU compilers, thread 0-15 can be bound to cores 0-15 as expected**
- **With hyperthreading, threads 0,1 -> physical core 0, etc.**

Home Directory Links

- /global/home/u/username are missing from compute nodes
- Use /global/u1/u/username or /global/u2/u/username
- /usr/common link is missing, too
- This will be fixed very soon!

Problems Now Fixed

- Slow login nodes (huge page memory setting)
- Queuing system (most issues resolved)
- Account management issues
- PrgEnv-gnu: `cc –version` was not working
- Cmake didn't work with Intel compiler

Edison-forum User Email List

- **Optional list**
  - Send email to edison-forum-admin@nersc.gov with Subject: Subscribe
- **For users to share tips and answer each other's questions**
- **Unmoderated**
  - But joining requires approval
- **Will be monitored informally by NERSC staff**
- **Archived**
  - https://mailman.nersc.gov/mailman/private/edison-forum/

NUG 2013 Summary

- **Four days March 12-15**
- **~225 total attendees over the 4 days**
- **Business Day**
  - 23 attendees (local & remote)
  - New NUGEX members announced
  - Action Items
- **Science Day (next slide)**
  - NERSC Achievement Awards announced
- **Training Day 1: Edison**
  - 31 attendees
  - Great presentations from Nathan Weichmann, Cray
- **Training Day 2: New User**
  - 41 attendees
  - Outstanding effort from NERSC staff

Trends, Discovery, & Innovation at NUG User Day 2013

UC Berkeley graduate student Edgar Solomonik receives the inaugural Early Career NERSC Award for Innovative use of HPC from Richard Gerber (right) and NERSC Director Sudip Dosanjh.

The day's attendance of 130 was split almost evenly between local and remote participants.

Total NUG 4-day attendance was ~ 225

The second day of the NERSC User Group (NUG) 2013 meeting was focused on community engagement and celebrating scientific achievement.

Featured Presentations

- *The Future of HPC*, Kathy Yelick, Berkeley Lab CS AD
- *The Future of NERSC*, Sudip Dosanjh, NERSC Director
- *Discovery of the Higgs and the role of Berkeley Lab HPC*, Ian Hinchliffe, head of Berkeley Lab ATLAS effort, former ATLAS physics coordinator
- *Discovery of the θ_{13} Weak Mixing Angle using ESnet & NERSC*, Craig Tull, U.S. Manager for Software and Computing for the Daya Bay Experiment
- Planck Satellite Data Analysis at NERSC, *Julian Borrill*, Berkeley Lab

Six contributed talks described novel uses of High Performance Computing and Data facilities.

NERSC Award for High Impact Scientific Achievement 2013

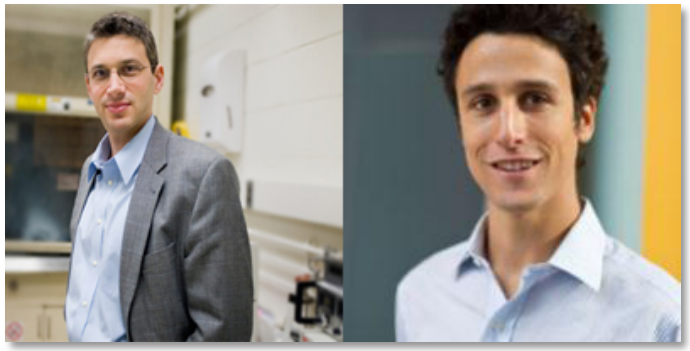
A New Approach to Water Desalination

Jeff Grossman and David Cohen-Tanugi, MIT

New material's water permeability is several orders of magnitude greater than conventional membranes.

Using supercomputers at NERSC, Grossman and Cohen-Tanugi came up with a new approach for desalinating seawater using sheets of graphene, a one-atom-thick form of the element carbon. This method holds the promise of being far more efficient and less expensive than existing desalination systems.

Grossman's project "Quantum Simulations of Nanoscale Energy Conversion" has used 5.6 Million hours at NERSC since 2010.



Jeff Grossman (left) and David Cohen-Tanugi are the recipients of the inaugural NERSC award.

One of Smithsonian Magazine's Top Ten "Surprising Scientific Milestones of 2012"

Early Career Award

Tanmoy Das, Las Alamos National Laboratory

Das completed groundbreaking computational work to understand fundamental properties of novel superconductors and spin-orbit ordering effects in two-dimensional electron gases. A postdoctoral researcher at LANL, Das was the first author on three 2012 articles published in the highly regarded journal Physical Review Letters.

NERSC Award for Innovative Use of High Performance Computing

Data Pipeline Transfers, Analyzes, Stores, & Disseminates Astronomical Observations

Peter Nugent and the PTF Team, Berkeley Lab & UC Berkeley, California Institute of Technology

Innovative workflow enables earliest supernova discovery, first direct observations of progenitor systems.

Every night observations from the Palomar Observatory in Southern California are sent to NERSC where computers running machine learning algorithms scour the data for transients. Once an interesting event is discovered, an automated system sends its coordinates to ground-based telescopes around the world for follow-up observations. NERSC also archives this data and allows collaborators to access it over the Internet through a web-based science gateway.

Peter Nugent, the PTF's Realtime Transient Detection Lead, is interviewed on the PBS News Hour following the discovery of supernova PTF 11kly within hours of its appearance.

Early Career Award

Edgar Solomonik, UC Berkeley

Solomonik, a graduate student at UC Berkeley, has developed novel algorithms for massively parallel tensor contractions and applied them to quantum chemistry problems. Solomonik's algorithmic developments are instantiated in the Cyclops Tensor Framework (CTF), which has been used on some of the largest supercomputers in the world, including the NERSC Hopper system, and the IBM Blue Gene/Q systems at the Lawrence Livermore National Laboratory and Argonne Leadership Computing Facility.

2014 NERSC Achievement Awards Committee

- **Propose: Awards Committee**
  - Made up of ~ 6 NERSC Staff and ~6 NUGEX members (one representing each office?)
  - Review and modify nomination procedures
  - Manage reviews and make recommendations to NERSC
  - NERSC Director will make final decision based on committee recommendations
  - NUGEX Chair and Co-Chair select NUGEX committee members

NUG 2013 Business Day Action Items

- **Facilitate NUGEX involvement with NUFO**
- **Ability to request permanent quota increases**
  - Yes, but NERSC will review yearly
- **Web queue display improvements**
  - Under active development
- **Mobile web site improvements ('ls' submit directory; 'tail' output files)**
  - Under active development
- **HPSS tools for efficient data retrieval from tape**
  - Script exists; training event ~June; more user-friendly idea being evaluated
- **Space for user-provided modules**
  - Being evaluated
- **User backup directories to HPSS tool**
  - Being evaluated

Notification Emails

- **NERSC announces planned outages at least 7 days in advance via email and places on MOTD**
- **Request for reminder email 1 day prior**
- **What other methods would you like?**
  - Twitter
  - Facebook
  - ????

Next NUG Teleconference

- Next scheduled: Thu. April 4, 2013
- Send suggested topics and comments to ragerber@lbl.gov
- Start planning for NUG 2014 and NERSC's 40th anniversary

National Energy Research Scientific Computing Center