Application Readiness at NERSC

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NERSC: the Mission HPC Facility for DOE Office of Science Research

U.S. DEPARTMENT OF
ENERGY

Office of
Science

Largest funder of physical science research in U.S.

Bio Energy, Environment

Computing

Materials, Chemistry, Geophysics

Particle Physics, Astrophysics

Nuclear Physics

Fusion Energy, Plasma Physics

6,000 users, 48 states, 40 countries, universities & national labs
Current Production Systems

Edison
5,560 Ivy Bridge Nodes / 24 cores/node
133 K cores, 64 GB memory/node
Cray XC30 / Aries Dragonfly interconnect
6 PB Lustre Cray Sonexion scratch FS

Cori Phase 1
1,630 Haswell Nodes / 32 cores/node
52 K cores, 128 GB memory/node
Cray XC40 / Aries Dragonfly interconnect
24 PB Lustre Cray Sonexion scratch FS
1.5 PB Burst Buffer
Cori Phase 2 – Being installed now!

Cray XC40 system with 9,300 Intel Knights Landing compute nodes
68 cores / 96 GB DRAM / 16 GB HBM
Support the entire Office of Science research community
Begin to transition workload to energy efficient architectures

Data Intensive Science Support
10 Haswell processor cabinets (Phase 1)
NVRAM Burst Buffer 1.5 PB, 1.5 TB/sec
30 PB of disk, >700 GB/sec I/O bandwidth
Integrate with Cori Phase 1 on Aries network for data / simulation / analysis on one system
First American woman Nobel Prize winner, third ever, and first woman in Physiology & Medicine

... for the discovery of the mechanism by which glycogen—a derivative of glucose—is broken down in muscle tissue into lactic acid and then resynthesized in the body and stored as a source of energy.

Edison, Hopper, Franklin, Bassi, Carver, Seaborg, Mcurie, Pierre, Jacquard, Bhaskara, Euclid, DaVinci, JWatson, FCrick, Kileen
Cori Integration Status

July-August
9300 KNL nodes arrive, installed, tested

Monday
P1 shut down, P2 stress test

This week
Move I/O, network blades
Add Haswell to P1 to fill holes
Cabling/Re-cabling
Aries/LNET config
Cabinet reconfigs

Now to now+6 weeks
…continue, test, resolve issues
configure SLURM
NESAP code team access ASAP!
Goal: Prepare DOE Office of Science users for many core
Partner closely with ~20 application teams and apply lessons
learned to broad NERSC user community

NESAP activities include:

Close interactions with vendors
Developer Workshops
Early engagement with code teams
Postdoc Program
Leverage community efforts
Training and online modules
Early access to KNL
NESPAP Focus on 20 codes

10 codes make up 50% of the workload
25 codes make up 66% of the workload
Edison will be available until 2019
Training and lessons learned will be made available to all application teams
A few NERSC staff have been on Cori Phase 2 as stand-alone system, but with limited usability and access. Just trying to get things to run; had some success, some failures.

NESAP team will get access once the system is integrated and checks out OK. ~Late October ???

Preparation and optimization work continues with NERSC/LBNL application readiness team, IXPUG, Cray, Intel, DOE labs

Details in Jack Deslippe’s talk this afternoon!
NESAP Postdocs

Taylor Barnes  
Quantum ESPRESSO

Zahra Ronaghi

Andrey Ovsyannikov  
Chombo-Crunch

Mathieu Lobet  
WARP

Tuomas Koskela  
XGC1

Tareq Malas  
EMGeo

Target Application Team Concept

(1 FTE Postdoc +)  
0.2 FTE AR Staff

0.25 FTE COE  
1.0 FTE User Dev.

1 Dungeon Ses. +  
2 Week on site w/ Chip vendor staff
Waiting for KNL …

We just can’t wait to get staff and users on Cori Phase 2!!!!