

National Energy Research Scientific Computing Center



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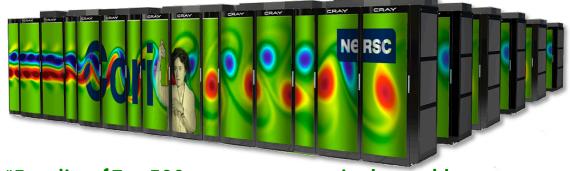
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Production High Performance Computing Systems



Cori

9,300 Intel Xeon Phi "KNL" manycore nodes 2,000 Intel Xeon "Haswell" nodes 700,000 processor cores, 1.2 PB memory Cray XC40 / Aries Dragonfly interconnect 30 PB Lustre Cray Sonexion scratch FS 1.5 PB Burst Buffer



#5 on list of Top 500 supercomputers in the world



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





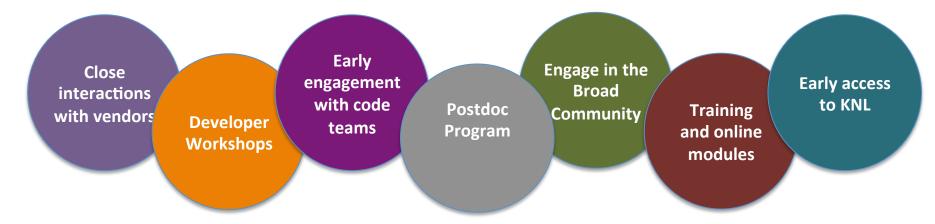
NERSC Exascale Scientific Application Program (NESAP)



Goal: Prepare DOE Office of Science users for Cori's manycore CPUs

Partner closely with ~20 application teams and apply lessons learned to broad NERSC user community

NESAP for Data is now underway as well

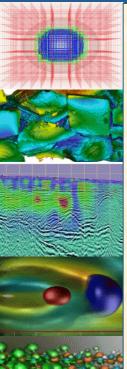






Application Readiness: NESAP





ASCR

Almgren (LBNL)
Trebotich (LBNL)

BoxLib

HACC

Chombo-crunch

HEP

Vay (LBNL)
Toussaint(Arizona)
Habib (ANL)

WARP & IMPACT MILC

NP

Maris (Iowa St.)
Joo (JLAB)
Christ (Columbia/BNL)

MFDn Chroma DWF/HISQ



B B S





BES

Kent (ORNL)
Deslippe (LBNL)
Chelikowsky (UT)
Bylaska (PNNL)
Newman (LBNL)

Quantum Espresso BerkeleyGW PARSEC NWChem EMGeo

BER

Smith (ORNL)
Yelick (LBNL)
Ringler (LANL)
Johansen (LBNL)
Dennis (NCAR)

Gromacs
Meraculous
MPAS-O
ACME
CESM

FES Jardin (PPPL) Chang (PPPL)

M3D XGC1

NESAP for Data Intensive Science on Cori KNL



Call for proposals in 2016 and six projects selected

- Dark Energy Spectroscopic Instrument Codes; Stephen Bailey, Berkeley Lab (HEP)
- Union of Intersections Framework; Kris Bouchard, Berkeley Lab (BER)
- Cosmic Microwave Background Codes (TOAST); Julian Borrill, Berkeley Lab (HEP)
- ATLAS Simulation/Analysis Code; Steve Farrell, Berkeley Lab (HEP)
- Tomographic Reconstruction; Doga Gursoy, Argonne (BES)
- CMS Offline Reconstruction Code; Dirk Hufnagel, FermiLab (HEP)





Cori KNL Status



NESAP teams are testing code and running science problems up to full scale on Cori KNL nodes with 24 hours time limit.

All NERSC users are enabled to run on up to 512 nodes for two hours at a time.

Users can gain access to the full system upon request and demonstration of code readiness for KNL.

Usage is not being charged through June 30, 2017.

System still has a few (software) bugs, which users are helping us discover and solve.



NERSC AY 2017 Allocations Forecast



System	"NERSC Hour" Charge per Node Hour	Nodes in System	~Hours in a Year	Overall System Availability Estimate	~Total NERSC Hours for AY2017 (M)	DOE Prod NERSC Hours (M) (80%)	ALCC NERSC Hours (M) (10%)	Directors Reserve NERSC Hours (M) (10%)
Edison	48	5576	8760	.85	2,000	1,600	200	200
Cori P1	80	2000	8760	.85	1,000	800	100	100
Cori P2 (6 months)	96*	9300	8760	.40 (6 months)	3,000†	2,400†	300 [‡]	300 [†]
2017					6,000	4,800	600	600
2016					3,000	2,400	300	300

Each Office/Reserve will have 2X the number of NERSC Hours in 2017 compared to 2016





^{* -} Estimate, may adjust once we measure application performance on system

^{†-}Supplemental allocation in Spring 2017

^{‡ -} Applies to 2017-18 ALCC allocation cycle

AY 2017 Augmentations for Cori KNL



Additional hours – equal again to initial allocation – placed in reserves on June 1, 2017 (Discuss)

~2.4 billion additional hours for use on Cori KNL

NERSC hours are fungible among Cori KNL, Cori Haswell, Edison, so codes must run on Cori KNL to use additional hours and therefore they must be ready to run on the architecture

NERSC will send pre-production Cori KNL usage report by repo to DOE managers on June 1, 2017 (Discuss)

Allocation managers transfer resources to selected repos after June 1, 2017 (annotate xfer with "KNL")



NERSC Hours Calculation



The currency for charging at NERSC is the the "NERSC Hour". 1 NERSC Hour ~ 1 core hour on Hopper (retired 2015)

Node Type	Cores per Node	Charge per Node per Hour
Cori KNL	68	96*
Cori Haswell	32	80
Edison	24	48
Hopper (retired)	24	24

^{* -} Production value TBD



Cori KNL Usage Nov. 2016 to Present



Office	KNL NERSC Hours (M)
ASCR	196 (includes app readiness repo)
BER	162
BES	101
FES	7
HEP	96
NP	517





NE Hrs

174 M

69 M

35 M

24 M

22 M

21 M

20 M

18 M

10 M

Office of

Science

KNL Nod	e Usage i	AY2017

KNL Node Usage AYZU17	

Domain Wall Fermions and Highly Improved Staggered Quarks for Lattice QCD (DWF)

Lattice QCD Monte Carlo Calculation of Hadronic Structure and Spectroscopy (Chroma)

Molecular Dynamics Simulations of Protein Dynamics and Lignocellulosic Biomass

Center for Computational Study of Excited-State Phenomena in Energy Materials

Theory of nanostructured materials (BerkeleyGW, Quantum Espresso)

Large Scale 3D Geophsycial Inversion & Imaging (EMGeo)

Quantum Chromodynamics with four flavors of dynamical quarks (MILC)

KNL Node Usage A12017	N

12

		1

PI

Christ (Columbia)

Liu (U Kentucky)

Leung (PNL)

Smith (ORNL)

Deslippe (LBNL)

Neaton (LBNL)

Newman (LBNL)

Toussaint (U Arizona)

Baron (U Oklahoma)

Synthetic Spectra of Astrophysical Objects

(GROMACS)

(BerkeleyGW)

Accelerated Climate Modeling for Energy (ACME)

Project



2016 Usage Summary



Program	Target (M)	NERSC Hours Used	Hours Charged
DOE Production	2,400	2,588	2,284
ALCC	300	291	226
DDR	300	69.7	66.9
TOTAL	3,000	2,949	2,576
Startup	-	3.5	1.7
Education	-	1.3	1.2



Office / Program Usage 2016



Office	Initial Allocation	Final Allocation*	Hours Used	Hours Charged	Scavenger Hours*	Balance
ASCR	142	151	135	131	4	20
BER	455	493	431	459	7.4	35
BES	712	758	715	662	67.7	97
FES	429	449	489	401	2.2	49
HEP	366	371	468	353	2.5	17
NP	264	278	372	265	21.6	13
SBIR	20.4	21.1	11	12.6	0	8.5
TOTAL	2,400	2,528	2,588	2,284	100	224

*Refunds ** Includes ALCC and DDR





AY 2017 begins

reserves

Allocation reduction

Allocation reduction

Allocation reduction

Cori KNL time transferred to

Cori KNL charging begins; New ALCC year begins

ERCAP application deadline

Award decision announcement

January 9, 2017

June 1, 2017 (discuss)

September 18, 2017

October 11, 2017

December 6, 2017

December 8, 2017

April 12, 2017

July 1, 2017



Office of

Science

If usage <10%, return 25% of balance to reserve

<40%, return 25%; <20%, return 75%, <10%, return

If no usage, close and return balance to reserve

Allocation Schedule	Nersc

Allocation Still		MONSC
Date	Item	

90%

16

2016 Queue Wait Times



Large job discount created extra allocation: ~500 M hours equivalent

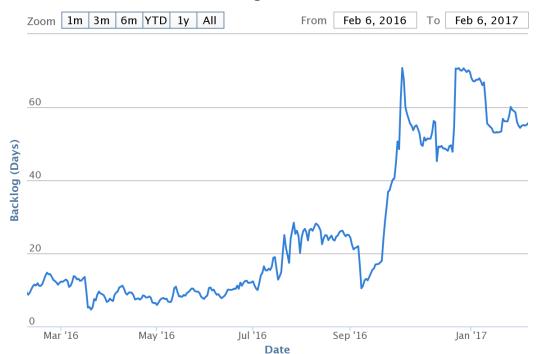
Cori downtime in September for KNL node integration

Placed huge pressure on Edison, resulting in long wait times

Payoff will be 2X hours in 2017 and 3X in 2018.

Edison Queue Backlog

Queue Backlog Over Time







Take Away Summary



- Cori KNL nodes are free through July 1, 2017
- Charging on Cori KNL nodes starts July 1, 2017
- Allocation augmentations placed in reserves on June 1
- Program managers will distribute additional time
- Codes need to be ready to use the Xeon Phi and program managers need to consider readiness in allocation decisions
- NERSC will send KNL usage report and other advice

Requirements Reviews



Cross cut meeting March 9-10 in Tyson's Corner http://www.orau.gov/crosscut2017/

Goal: integrated summary report of six requirements reviews

- Identify common cross-cutting needs
- Find areas of singular importance to each office
- Discuss a collaboratory path forward





Random Topics



Rename startup to "prototype"?

NERSC 9 procurement is underway for 2020 system

Edison will remain through sometime in 2019

DOE Production allocations will not decrease in 2019

Working with ECP in various areas