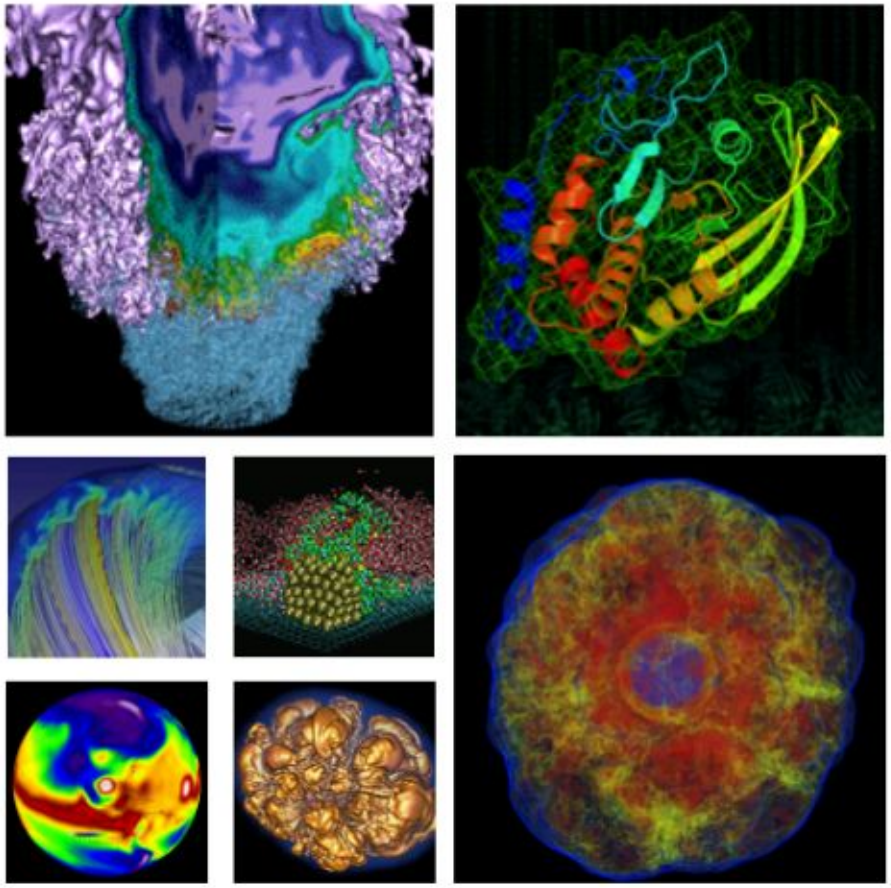
NERSC Users Group Monthly Meeting



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May 17, 2018

U.S. DEPARTMENT OF ENERGY

BERKELEY LAB
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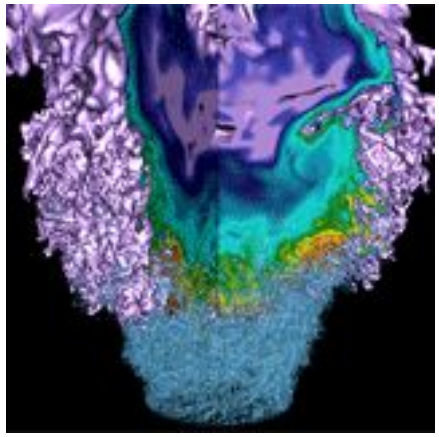
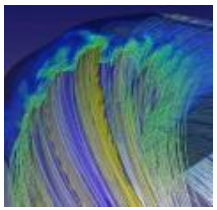
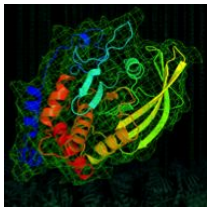
Agenda

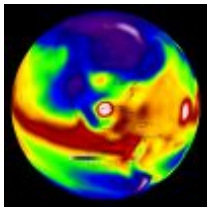
- Getting Optimal Throughput on Cori and Edison
- Variable-Time Jobs
- Upcoming Training Opportunities
- NERSC podcast

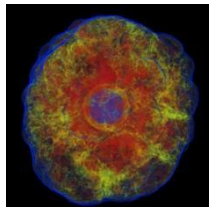
Getting Optimal Throughput on Edison & Cori

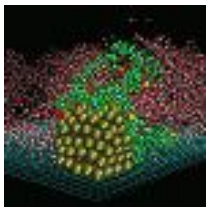












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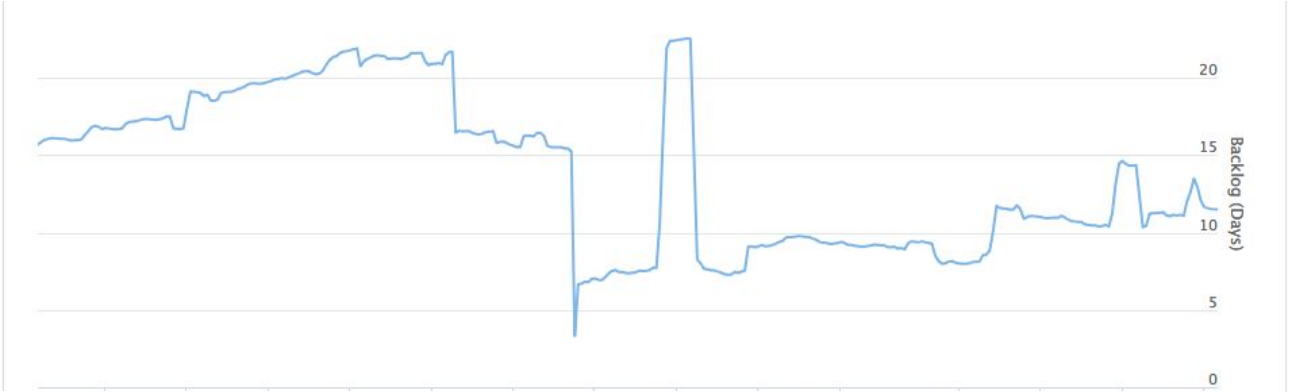
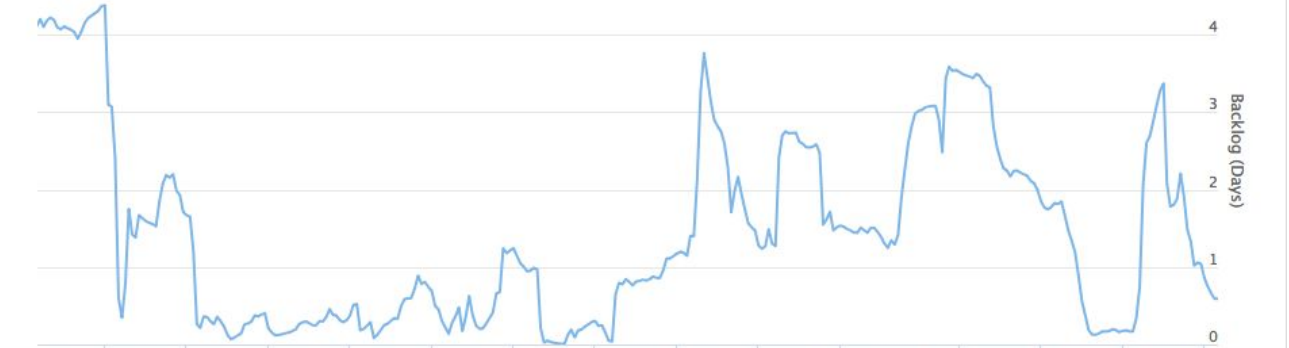
Queue Backlog Past 30 Days

Cori Haswell



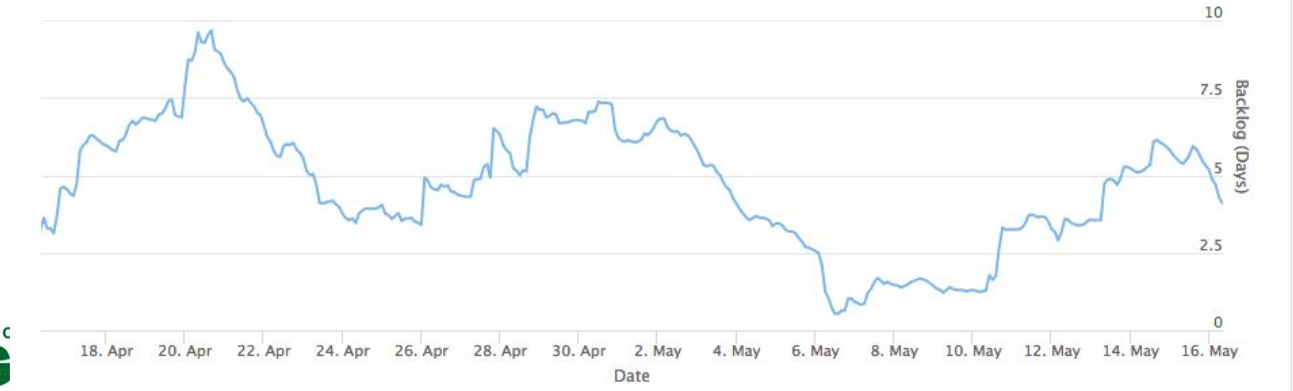
Scale: 20 days

Cori KNL



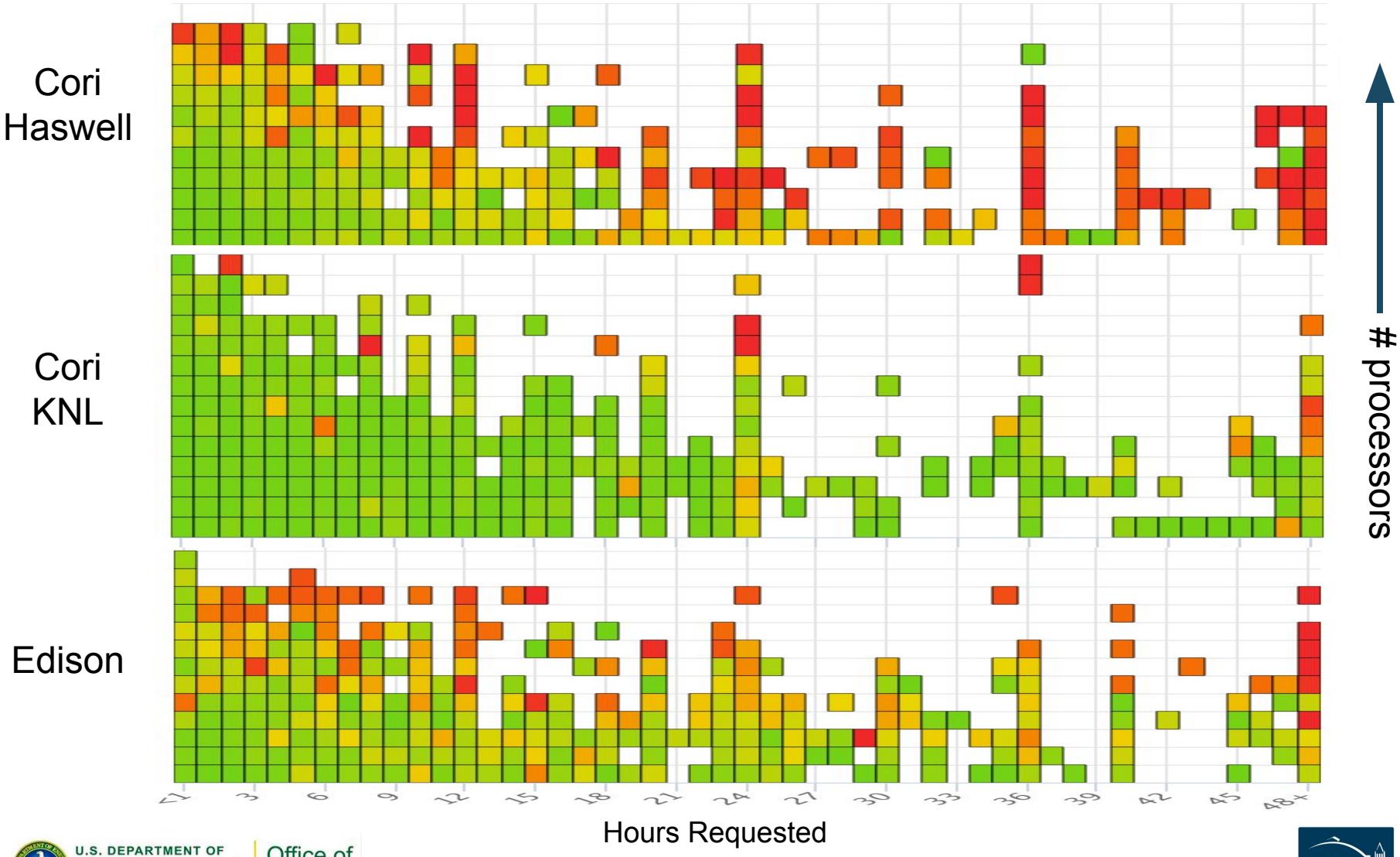
Scale: 4 days

Edison



Scale: 10 days

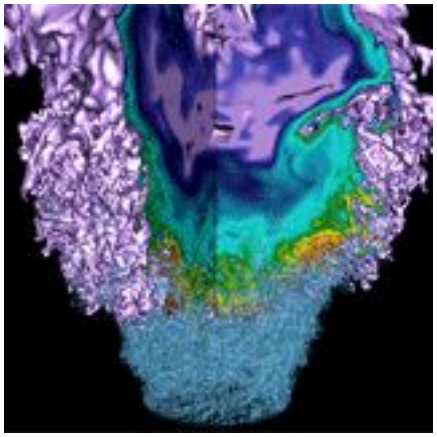
Avg Queue Wait Time Past 30 Days

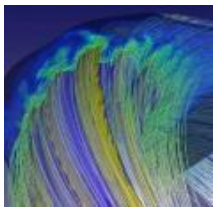


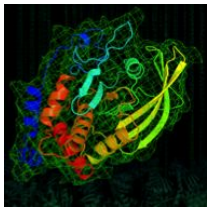
Strategies

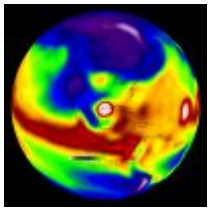
- **Use Cori KNL! (shortest backlog)**
  - What if my code won't run on KNL?
    - Ask NERSC for help! We can help you figure out what improvements need to be made in your code, & provide strategies for exploiting KNL architecture
- **Ask for less time (and more processors)**
  - What if the scalability of my code is not good?
    - If you're the developer, ask NERSC for help! We can help you figure out how to make your code better!
    - Implement checkpointing and use variable-time job options for better throughput (see next section)

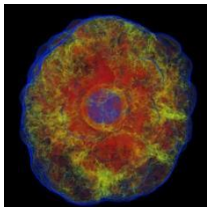
Variable-Time Jobs

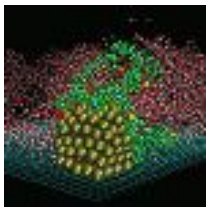












Acknowledgement:

The work was done by Tiffany Connors, a summer student at NERSC, under the supervision of Rebecca Hartman-Baker

Who should use variable-time jobs?

- Users who need to run long jobs, including jobs running for more than 48 hours - the max time allowed on Cori and Edison.
- Users who want improved queue turnaround time.

- Provided the code can do checkpointing by itself

Variable-Time jobs

- **Slurm allows jobs submitted with a minimum time limit in addition to the (max) time limit, e.g.,**

  #SBATCH --time=48:00:00

  #SBATCH --time-min=2:00:00

- **Jobs specifying --time-min can start execution earlier than otherwise with a time limit anywhere between the time-min and the requested time limit.**
  - This is performed by a backfill scheduling algorithm to allocate resources otherwise reserved for higher priority jobs.

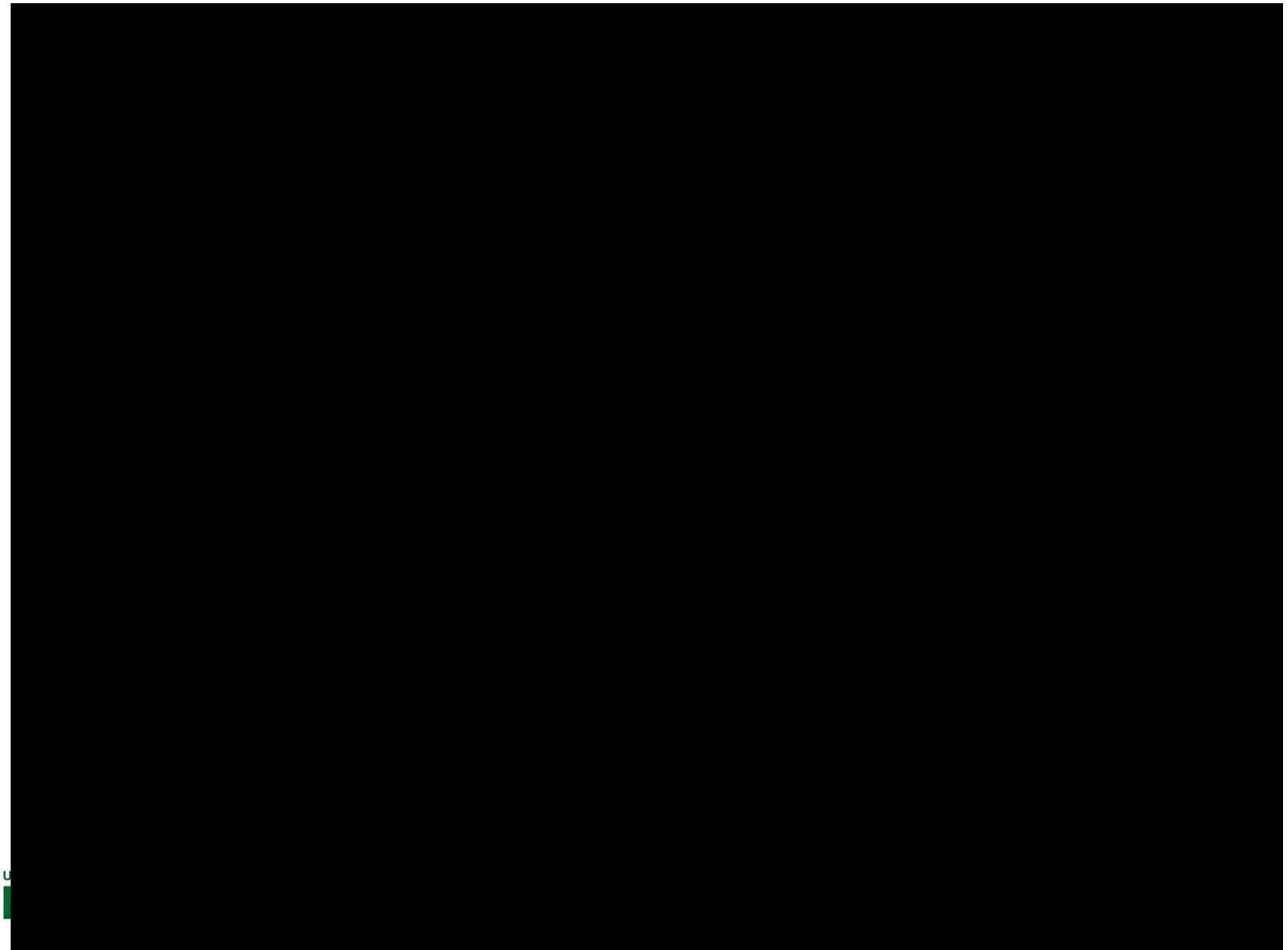
Variable-Time jobs - continued

- **The pre-terminated job can be requeued to resume from where the previous execution left off.**
  - #SBATCH --requeue
- **Requeuing the pre-terminated job can be done automatically until the cumulative execution time reaches the requested time limit or the job completes earlier before the requested time limit.**

Sample variable-time job script

```
#!/bin/bash
#SBATCH -J test
#SBATCH -q regular
#SBATCH -C haswell
#SBATCH -N 1
#SBATCH --comment=64:00:00
#SBATCH --time-min=00:30:00     #the minimum amount of time the job should run
#SBATCH --time=48:00:00
#SBATCH --error=test-%j.err
#SBATCH --output=test-%j.out
#
#SBATCH --signal=B:USR1@120
#SBATCH --requeue
#SBATCH --open-mode=append

#timelimit per job, the amount of time (in seconds) needed for checkpointing (same as in --signal)
#and the checkpont command if any
max_timelimit=48:00:00     #if not set default to 48:00:00
ckpt_overhead=120          #if not set, default to 60 seconds
ckpt_command=

#requeuing the job if remaining time >0
module load ata
. $ATA_DIR/etc/ATA_setup.sh

requeue_job func_trap USR1
#

#user setting
export OMP_PROC_BIND=true
export OMP_PLACES=threads
export OMP_NUM_THREADS=1

#srun must execute in background and catch signal on wait command
srun -n 1 -c 64 --cpu_bind=cores ./a.out &

wait
```

The variable-time job script generator - adaptive_launch.sh



How effective are variable-time jobs?

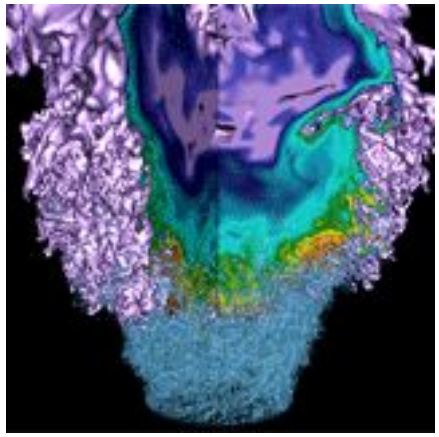
```
zz217@cori09:/global/cscratch1/sd/zz217/tests/queue_turnaround/haswell> sqs
JOBID     ST  USER   NAME  NODES REQUESTED USED     SUBMIT               QOS        SCHEDULED_START      FEATURES REASON
12537227  R   zz217  ata   1     4:35:00   3:30:13  2018-05-17T04:23:02  regular_1  2018-05-17T04:34:12  haswell  None
12537232  R   zz217  ata   1     3:55:00   3:30:13  2018-05-17T04:23:02  regular_1  2018-05-17T04:34:12  haswell  None
12537235  R   zz217  ata   1     3:55:00   3:30:13  2018-05-17T04:23:02  regular_1  2018-05-17T04:34:12  haswell  None
12537216  R   zz217  ata   1     4:49:00   3:34:01  2018-05-17T04:23:00  regular_1  2018-05-17T04:30:24  haswell  None
12537219  R   zz217  ata   1     4:49:00   3:34:01  2018-05-17T04:23:00  regular_1  2018-05-17T04:30:24  haswell  None
12537221  R   zz217  ata   1     4:49:00   3:34:01  2018-05-17T04:23:00  regular_1  2018-05-17T04:30:24  haswell  None
12537224  R   zz217  ata   1     4:49:00   3:34:01  2018-05-17T04:23:00  regular_1  2018-05-17T04:30:24  haswell  None
12537214  R   zz217  ata   1     4:35:00   3:30:09  2018-05-17T04:28:06  regular_1  2018-05-17T04:34:16  haswell  None
12537212  R   zz217  ata   1     4:36:00   1:40:55  2018-05-17T06:18:25  regular_1  2018-05-17T06:23:30  haswell  None
12537192  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:11  regular_1  avail_in_~2.8_days   haswell  Priority
12537194  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:12  regular_1  avail_in_~2.8_days   haswell  Priority
12537196  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:14  regular_1  avail_in_~2.8_days   haswell  Priority
12537198  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:15  regular_1  avail_in_~2.8_days   haswell  Priority
12537200  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:16  regular_1  avail_in_~2.8_days   haswell  Priority
12537202  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:18  regular_1  avail_in_~2.8_days   haswell  Priority
12537204  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:20  regular_1  avail_in_~2.8_days   haswell  Priority
12537206  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:21  regular_1  avail_in_~2.8_days   haswell  Priority
12537208  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:22  regular_1  avail_in_~2.8_days   haswell  Priority
12537210  PD  zz217  test  1     48:00:00  0:00     2018-05-17T03:27:23  regular_1  avail_in_~2.8_days   haswell  Priority

================================================================================================================
Note: The SCHEDULED_START column shows either the estimated start time provided by Slurm,
             or that an estimated start time will be "available in xxx hrs/days", meaning your job
             won't be scheduled by then (due to priority) unless via backfill, and the actual job
             start time could still be some period of time after then.
================================================================================================================

zz217@cori09:/global/cscratch1/sd/zz217/tests/queue_turnaround/haswell> squeue -u zz217 -o "%A %j %k" |grep -v null
JOBID NAME COMMENT
12537227 ata 42:57:00
12537232 ata 43:37:00
12537235 ata 43:37:00
12537216 ata 42:43:00
12537219 ata 42:43:00
12537221 ata 42:43:00
12537224 ata 42:43:00
12537214 ata 42:34:00
12537212 ata 40:48:00
```

Notes about variable jobs

- If you run into any issues please contact consult@nersc.gov for help. This feature is still experimental.
- For those applications that do not do checkpointing by themselves, DMTCP can be used to checkpointing externally. We are testing DMTCP + Variable-Time jobs now, and will make the job script available to users soon.

Questions?

Upcoming Training Opportunities



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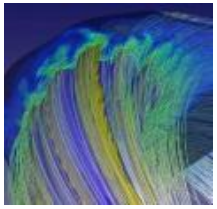
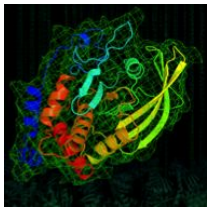
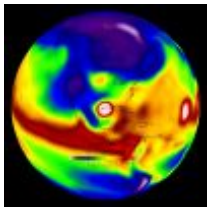
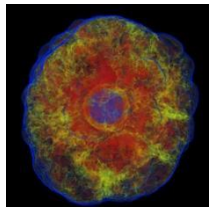
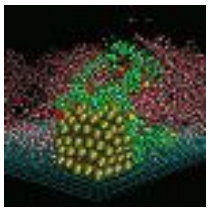

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Upcoming Training Opportunities

- **NERSC Training**
  - Cray PE Workshop, June 14
- **ECP Training**
  - Best Practices for HPC Software Developers, June 13
  - Kokkos Bootcamp, July 24-27

Cray PE Training, June 14

- **Topics covered in training:**
  - Applying the "Whack-A-Mole" Method Using Cray's Perftools to Identify the Moles
    - Tutorial, originally presented at Cray User Group meeting
    - Learn to use Cray's Perftools (performance tools) to identify bottlenecks and hotspots in your code
  - What's new in the Cray Programming environment?
  - Tips & Tricks for using & interpreting data from Perftools
  - Cray PE Deep Learning Scalability Plugin
    - Introduction to Deep Learning products available in the Cray programming environment
- **For more info and to register:** https://www.nersc.gov/users/training/events/cray-pe-workshop-june2018/

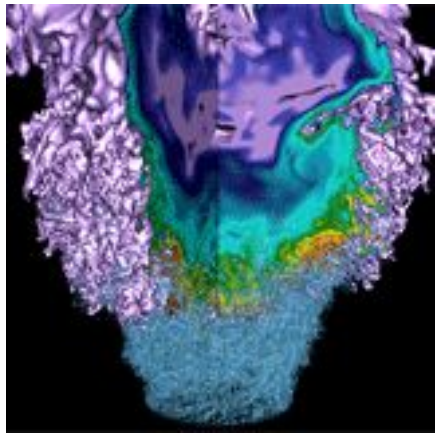
Best Practices for HPC SW Developers Webinar, June 13

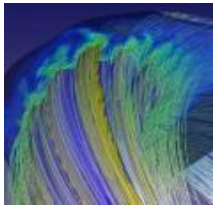
- **Topic: "Popper: Creating Reproducible Computational and Data Science Experimentation Pipelines"**
  - Presented by Ivo Jimenez, UC Santa Cruz
  - Trying to reproduce others' computational experiments is large time sink. Popper, a protocol and command language interpreter (CLI) tool for implementing scientific exploration pipelines, follows a DevOps approach of unifying software development and operation in order to handle complexity in large codebases.
- **For more info and to register: https://www.exascaleproject.org/event/popper/**

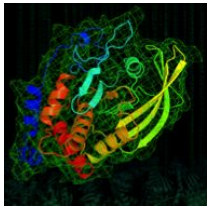
Kokkos Bootcamp, July 24-27

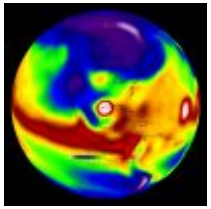
- **What is Kokkos?**
  - Programming model and library for writing performance portable code in C++
  - Includes abstractions for on-node parallel execution and data layout
- **What happens at Kokkos Bootcamp?**
  - New users learn about Kokkos in a tutorial
  - All users get hands-on experience with expert help to use Kokkos for their application
- **For more information and to register: https://www.exascaleproject.org/event/kokkosbc2/**

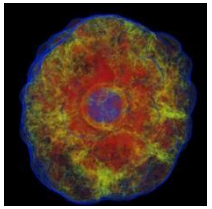
NERSC Podcast

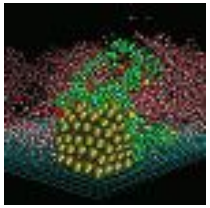












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NERSC Podcast

- New “NERSC News” Podcast
- Available at https://anchor.fm/nersc-news
- 10-15 minute segments about latest center news and interesting HPC topics
- 6-month experiment (discontinue if low uptake)
- Your feedback, suggestions for topics, etc., always welcome!


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