Current Status of TSUBAME3.0 Operation (Mar 2019)

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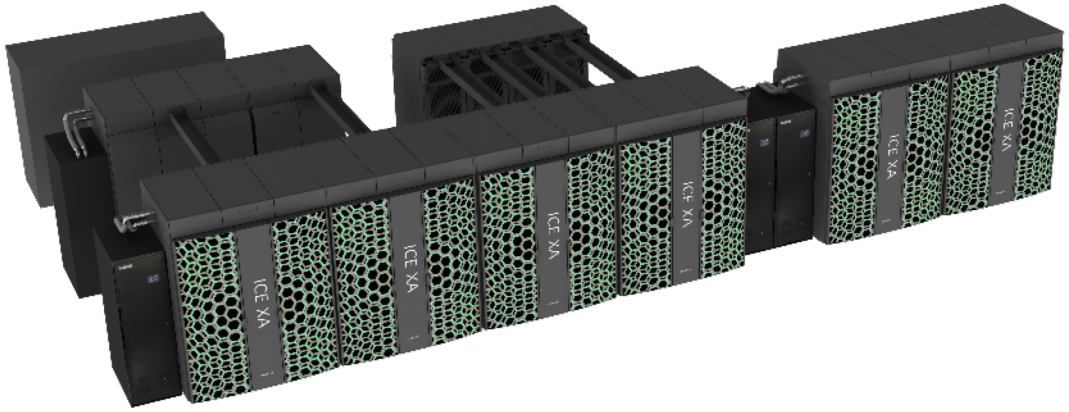
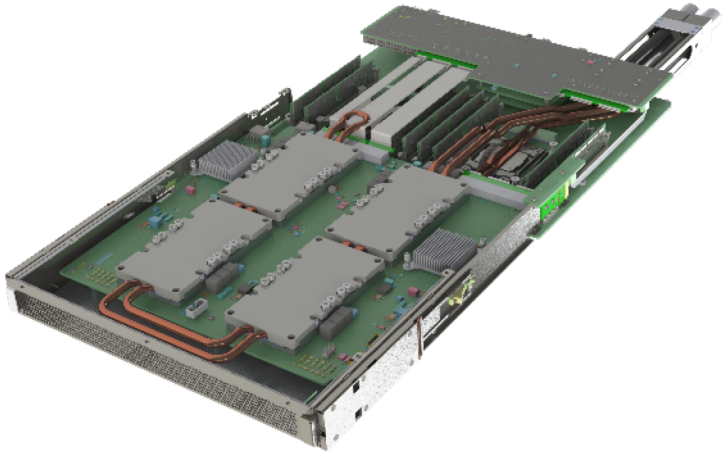




TSUBAME Series

2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019

TSUBAME1

TSUBAME1.0
Opteron+ClearSpeed, 85TF Peak

TSUBAME1.1
ClearSpeed/ Storage added

TSUBAME1.2
680 NVIDIA S1070 added

TSUBAME2.0
Westmere + 4224 M2050, 2.4PF Peak

TSUBAME2.5
Upgraded to K20X
5.7PF Peak

TSUBAME2

experiment

TSUBAME-KFC → KFC/DL

Testbed with oil-immersion cooling

TSUBAME3.0
Broadwell + 2160 P100, 12PF Peak

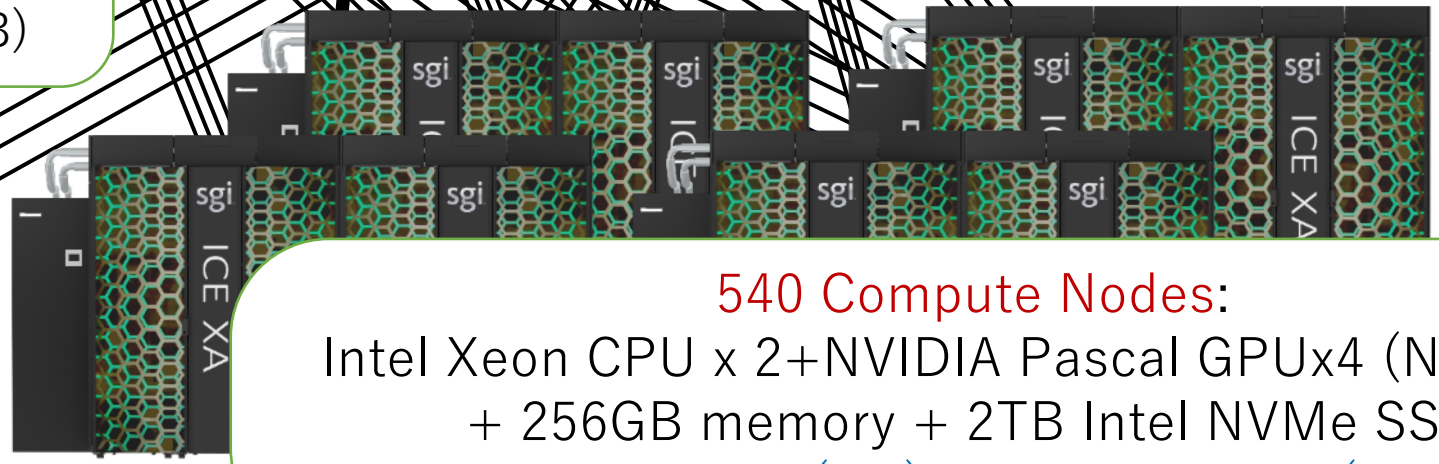
TSUBAME3

Overview of TSUBAME3.0
BYTES-centric Architecture, Scalability to all 2160 GPUs, all nodes, the entire memory hiearchy

Hewlett Packard Enterprise

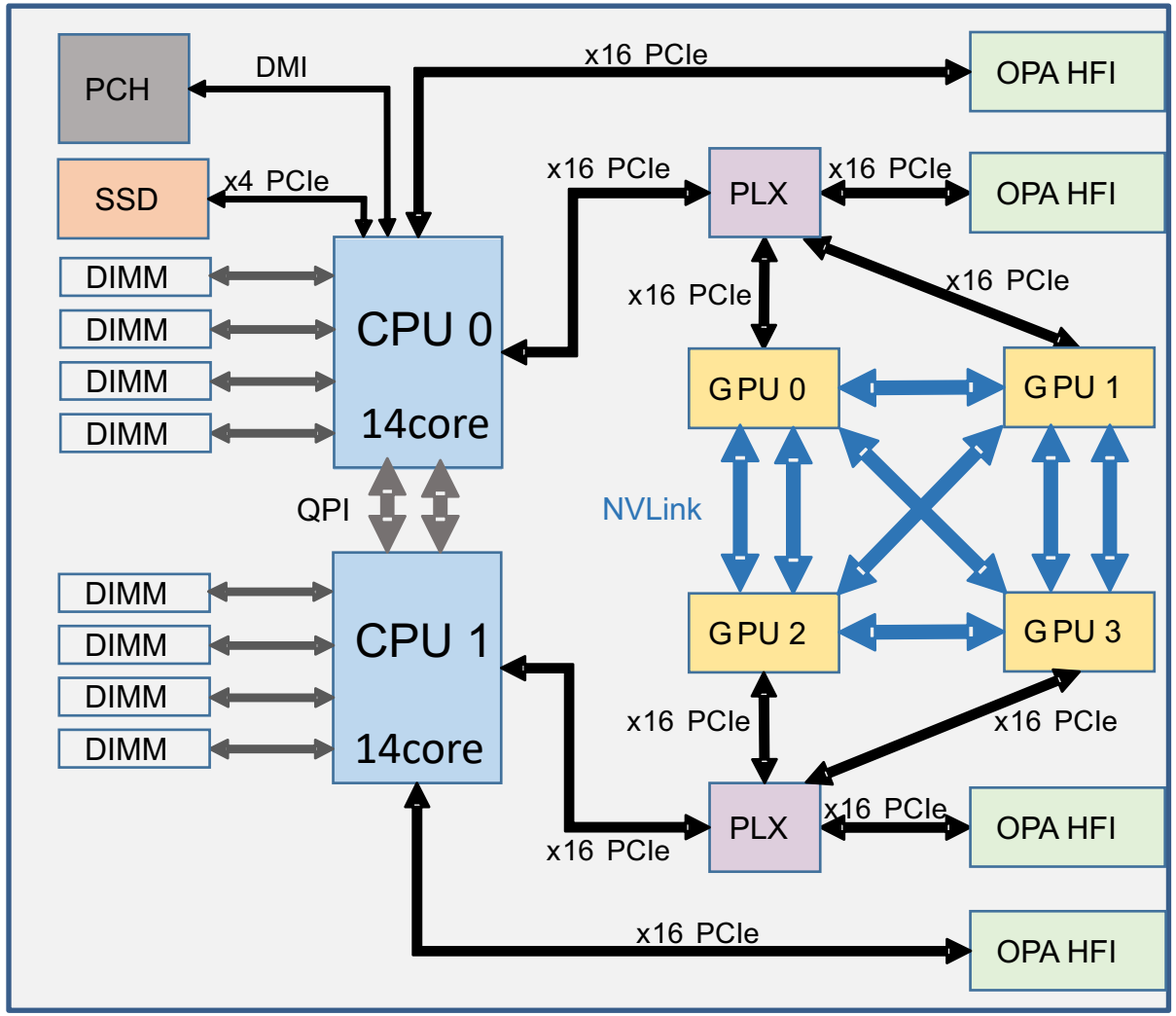
Full Bisection Bandwidth
Intel Omni-Path Interconnect. 4 ports/node
Full Bisection / 432 Terabits/s bidirectional
~x2 BW of entire Internet backbone traffic

DDN Storage
(Lustre FS 15.9PB+Home 45TB)



540 Compute Nodes:
Intel Xeon CPU x 2+NVIDIA Pascal GPUx4 (NV-Link)
+ 256GB memory + 2TB Intel NVMe SSD
12.1 Petaflops (DP) , 47.2 Petaflops (FP16)

TSUBAME3.0 Compute Node



x 540 nodes

Ultra high performance & bandwidth "Fat Node"

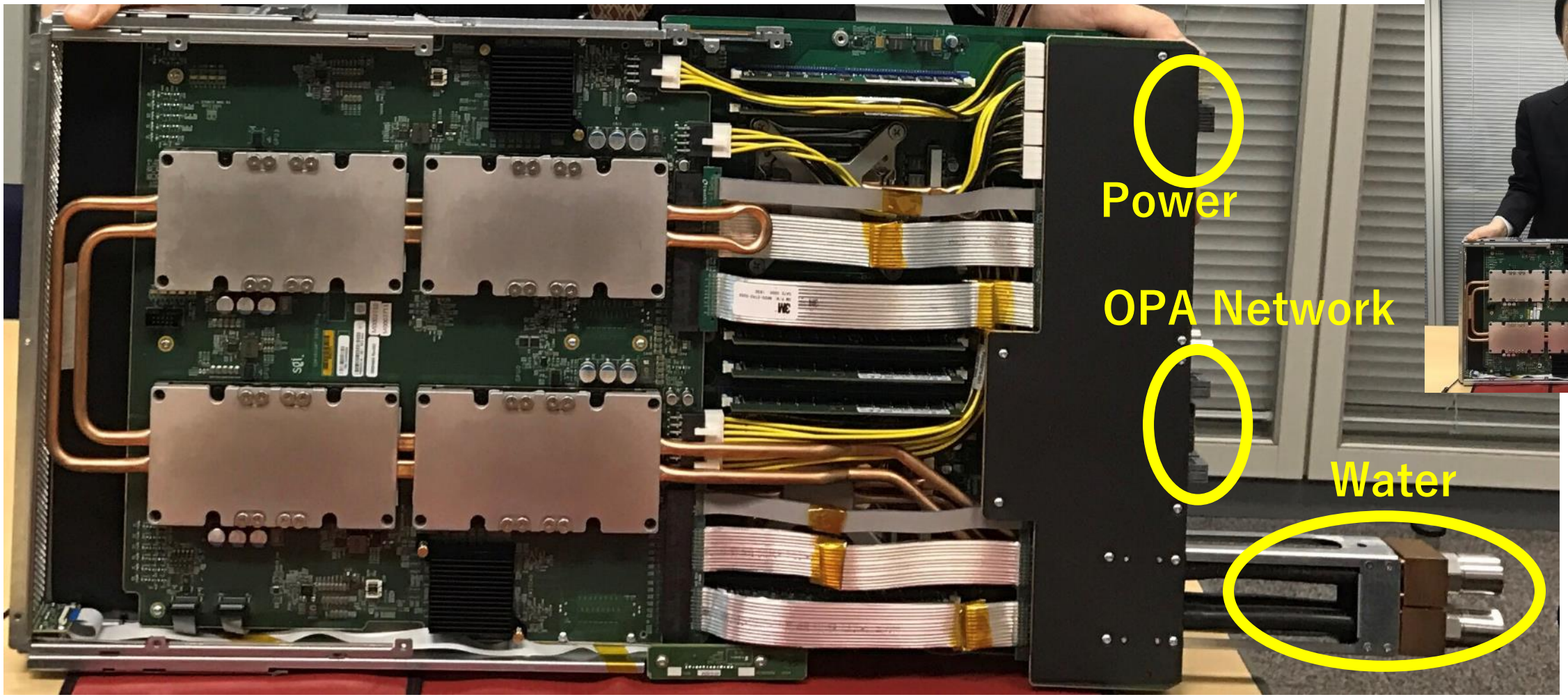
- High Performance:
  - 4 NVIDIA Pascal P100 (NVLink)
  - 2 Intel Broadwell 14-core Xeon
- High Network Bandwidth:
  - Intel Omnipath 100GBps x 4 = 400Gbps
- Memory Hierarchy for BD
  - 256GiB DDR4 memory
  - 2TB Intel NVMe SSD

  → > 1PB & 1.5~2TB/s system total
- Ultra High Density, Hot Water Cooled Blades:
  - 36 blades / rack = 144 GPU + 72 CPU

  → 50-60KW / rack

TSUBAME3.0 Node

- No exterior cable mess (power, NW, water)
- Plan to become a future HPE product



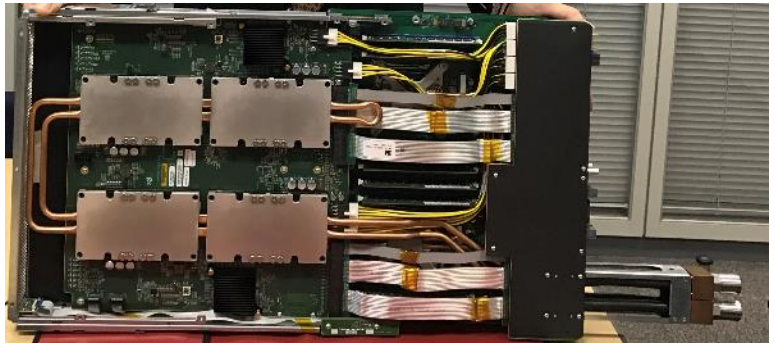
Main Topics

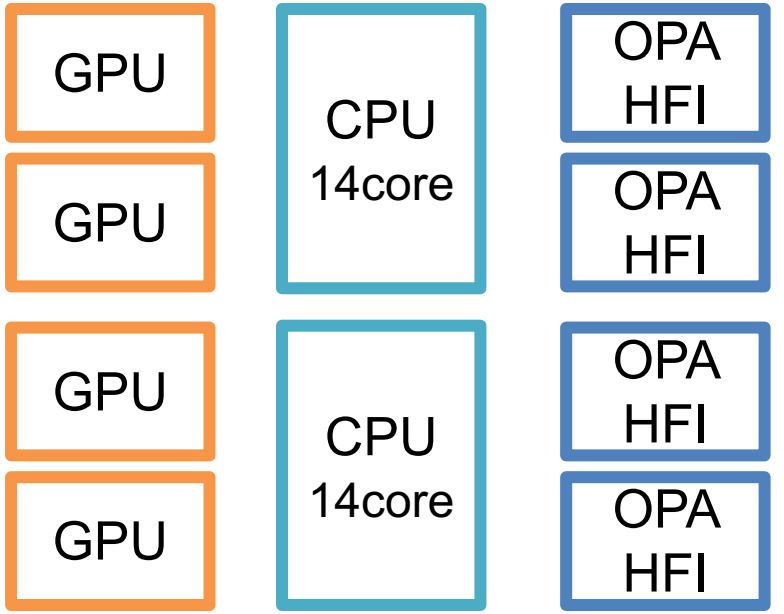
- *Efficient node usage*
  - TSUBAME3 nodes are rather “fat” → Node Partitioning
  - Usage statistics (New)
- *Software deployment for wider usage*
  - Statistics of users behavior
    - Collecting “module” command usage
  - Containers (New)
    - cf) “I want to use XYZ framework ver 123.4 instead of default version”
    - Now users can use Singularity
- *Hierarchical storage*
  - Lustre + temporal local file system on NVMe SSDs
  - BeeGFS for multi-node jobs

PART 1: NODE PARTITIONING

Node Partitioning: Motivation

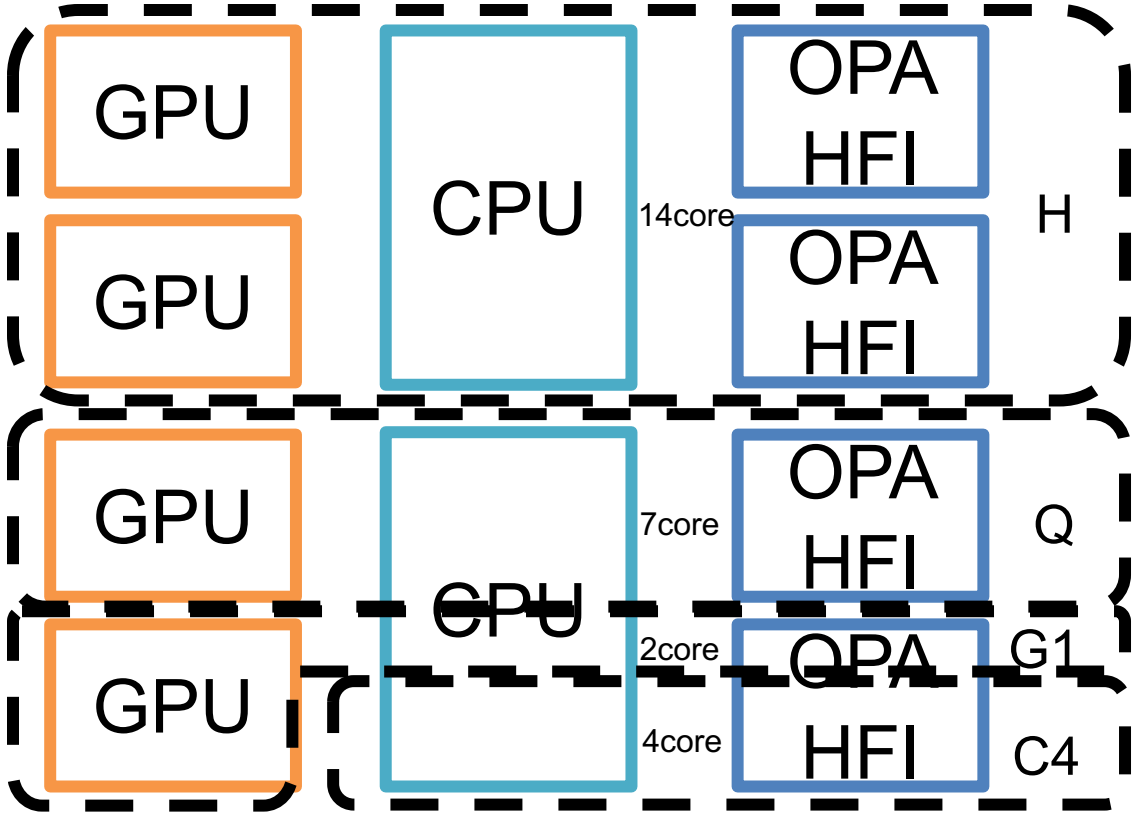
- We should support jobs with various resource requests
  - CPU centric jobs, GPU centric jobs…
  - Some users do “parameter survey” with plenty of 1-core jobs !
- Each TSUBAME3 node is “fat”, and partitioning is more important for efficient resource usage
  - 2 CPUs (28 cores) + 4 GPUs + 4 NICs
- On the other hand, “too flexible” partitions would introduce fragmentation of nodes





Node Partitioning: Overview

- We define several “resource types” on TSUBAME3
  - Like “instance types” on AWS



- F: A node without partitioning
- H: ½ node
- Q: ¼ node
- C1: 1 CPU Core
- C4: 4 CPU Core
- G1: 1 GPU + 2 CPU Core

Node Partitioning: Details

type	Resource type Name	Physical CPU cores	Memory (GB)	GPUs
F	f_node	28	240	4
H	h_node	14	120	2
Q	q_node	7	60	1
C1	s_core	1	7.5	0
C4	q_core	4	30	0
G1	s_gpu	2	15	1

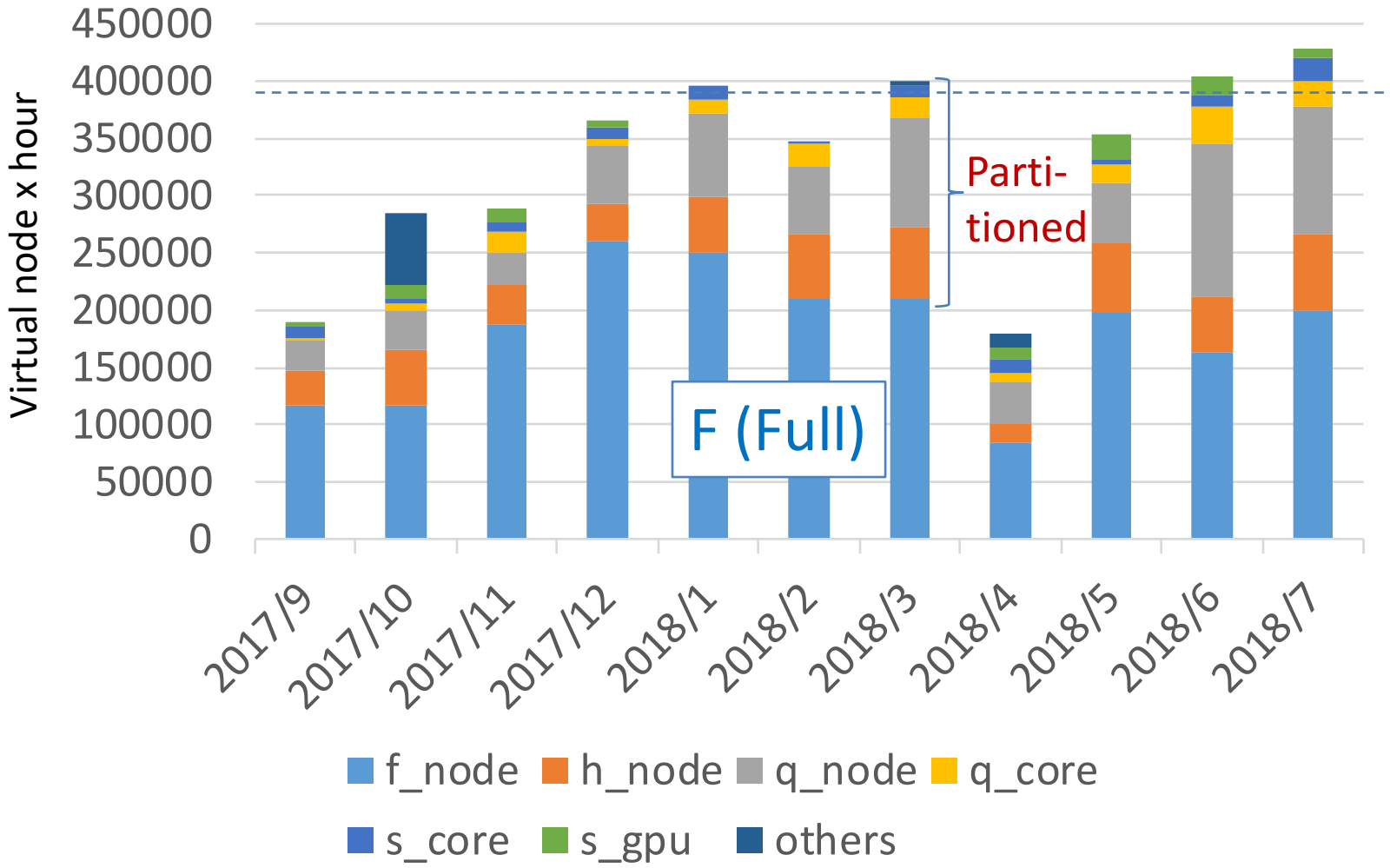
- Users choose “resource type” × “# of nodes” in job submissions
  - cf) 15 x Q, 10 x C4

- Implementation is done with cgroups in cooperation with UNIVA Grid Engine

  →CPU cores, GPU, memory, HCA are assigned to each resource correctly

  →Currently, a partition can see processes on other partitions ☹. Better isolation will be achieved with containers

Node Partitioning: Statistics



Accumulated (virtual nodes x hour) are shown
→It can exceed 388,800
= 540 nodes x 24h x 30d

In FY 2017, F (Full) occupied 60%
In FY 2018, F (Full) occupied 47%

Users tend to use node partition intensively after experiences

PART 2: USERS' APPLICATION DEPLOYMENT AND STATISTICS

How Users Deploy/Select Software Packages on TSUBAME3

1) The ‘module’ command for pre-installed packages

Programming tools

- Compilers: gcc, Intel, PGI
- MPI: OpenMPI, Intel, SGI MPT
- CUDA, JAVA, Python, R, MATLAB…

Pre-installed applications/libraries

- Caffe, Tensorflow, Chainer…
- HDF5, OpenFoam, cuDNN …
- Gromacs, ABAQUS, AMBER, ANSYS, Gaussian, LS-DYNA, NASTRAN…

2) Using Singularity containers (Since Aug 2018)

A simpler way to deploy non-supported packages

3) Manual installation by themselves

Issues to Capture Users Behavior on TSUBAME

- Capturing users behavior is important to improve the system operation
- However, especially for internal users, we have very limited information on their usage
  - Tokyo Tech members (staffs, students) can apply TSUBAME accounts easily from the web. No research reports currently
  - On the other hand, we collect research reports from non Tokyo Tech users

→ We started to count invocations of “module” command

“Modules” usage of TSUBAME3 (1)

- Stats on compute nodes Nov 10, 2018 – Mar 12, 2019
- Only modules pre-defined by system operators

Applications/DL frameworks

module name	# of unique users	# of loads
gromacs/2016.3	19	255008
amber/16_cuda	9	11859
chainer/4.3.0	7	10385
abaqus/2017	56	8787
imagemagick/7.0.6	4	7908
tensorflow/1.9.0	22	6902
gaussian16/B01	59	6641
gamess/apr202017r1	4	5035
amber/16up12_cuda	7	4888
namd/2.13	5	4171
amber/18up5	12	3892
gaussian16/A03	42	3143
amber/16up10_cuda	7	3005
amber/16	5	2494

⋮

- Currently, most popular package is “gromacs”
- Traditional HPC packages (MD/MO…) are always important
- DL workload is increasing

“Modules” usage of TSUBAME3 (2)

- Stats on compute nodes Nov 10, 2018 – Mar 12, 2019
- Only modules pre-defined by system operators

Compilers/system software/libs

module name	# of unique users	# of loads
cuda/8.0.61	373	1111742
intel/18.0.1.163	288	754674
openmpi/2.1.2	216	372239
intel-mpi/18.1.163	122	371581
python/3.6.5	59	250273
fftw/3.3.8	25	171597
cuda/9.1.85	60	125892
intel/17.0.5.239	23	98316
hdf5/1.10.1	69	98023
intel-mpi/17.4.239	6	93669
cudnn/6.0	57	76501
nccl/1.3.4	59	75541
vtk/6.1.0	42	72447
python-extension/2.7	41	72360
cudnn/7.0	27	57514
intel/17.0.4.196	63	55969
intel-mpi/17.3.196	49	55796

Note:

- The numbers may be larger than actual usage for module dependencies
  - Ex) “cuda” module is required to load “openmpi” module

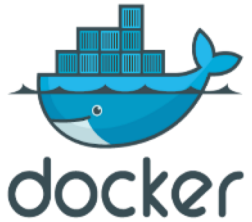
→ We should improve package configurations to reduce needless dependency

Motivation for Containers

- TSUBAME3 has many pre-installed software packages, but upgrading of DL frameworks is so rapid
- Some users may want to use the latest versions, while others use old versions
  - "pip --user install" everywhere?
  - It is troublesome for users; also there are package dependencies
  - It is not good for efficient storage usage

→We want to make such users use different images easier

Restriction: We CANNOT allow users to execute root on TSUBAME3



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Container Operation on TSUBAME3

We are providing “singularity” container for users

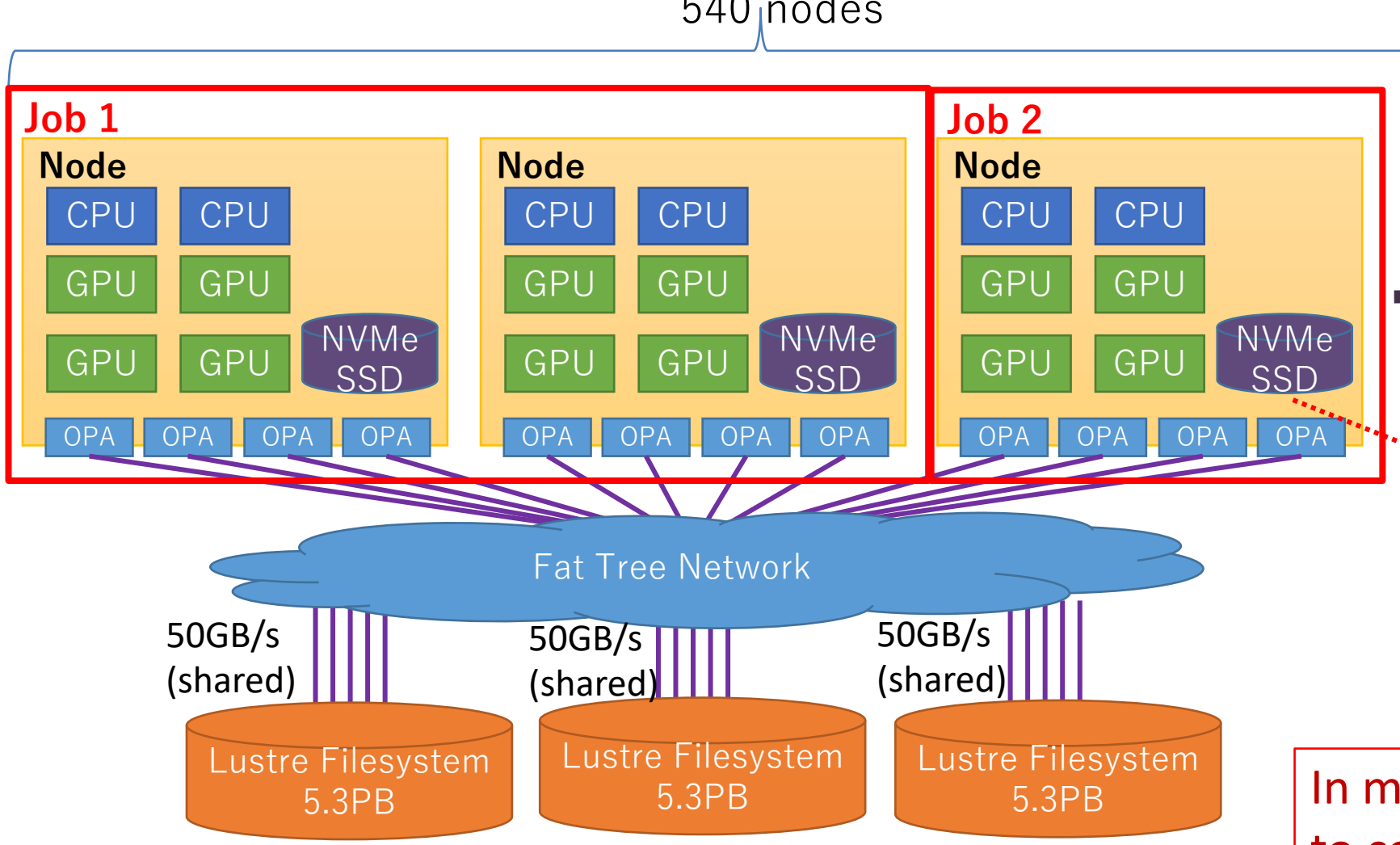
- It works with the UNIVA Grid Engine scheduler
  - It is realized in cooperation with HPE and UNIVA
- It works with node partitioning
- Currently users have to prepare their container images
  1) Download from web (ex: docker hub)
  2) Make own images on their local machines
  3) Several pre-defined images (planning)

A comment from a bio-informatics user:
“Software deployment by container technology is mandatory for us, since we daily use container images from BioContainers.pro. ☺”

A new issue for administrators:
We can capture the usage of “singularity” module, but we do NOT know what packages are used inside the containers ☹

PART 3: OPERATION OF HIERARCHICAL STORAGE WITH LUSTRE + SSDS

TSUBAME3 Hierarchical Storage



The largest storage is shared Lustre filesystems (5.3PB x 3)

Users can also use node local SSDs for temporary data

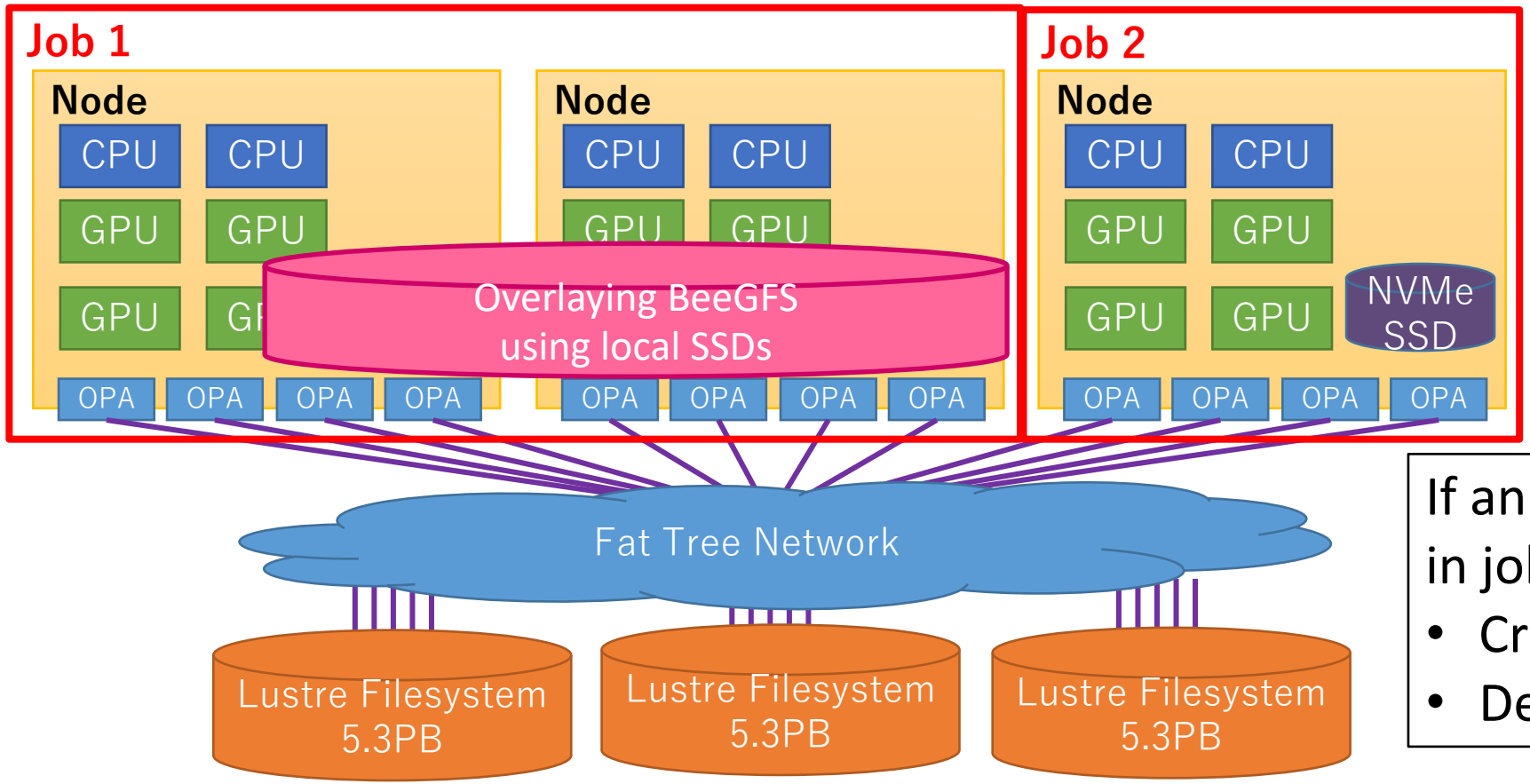
- Size 2TB
- Read 2.8GB/s
- Write 2.0GB/s

→ More stable performance

In multi-node jobs, users have to consider node affinity

BeeOND Service

- Users can use BeeOND (BeeGFS On Demand)
- Nodes in a single job can use a single temporary FS



If an user sets “BeeOND” flag in job submission, a BeeGFS is

- Created in job prologue
- Destroyed in job epilogue

Current BeeOND Operation

- Currently only jobs with F resource type (no partition) can use BeeOND

An example of job script

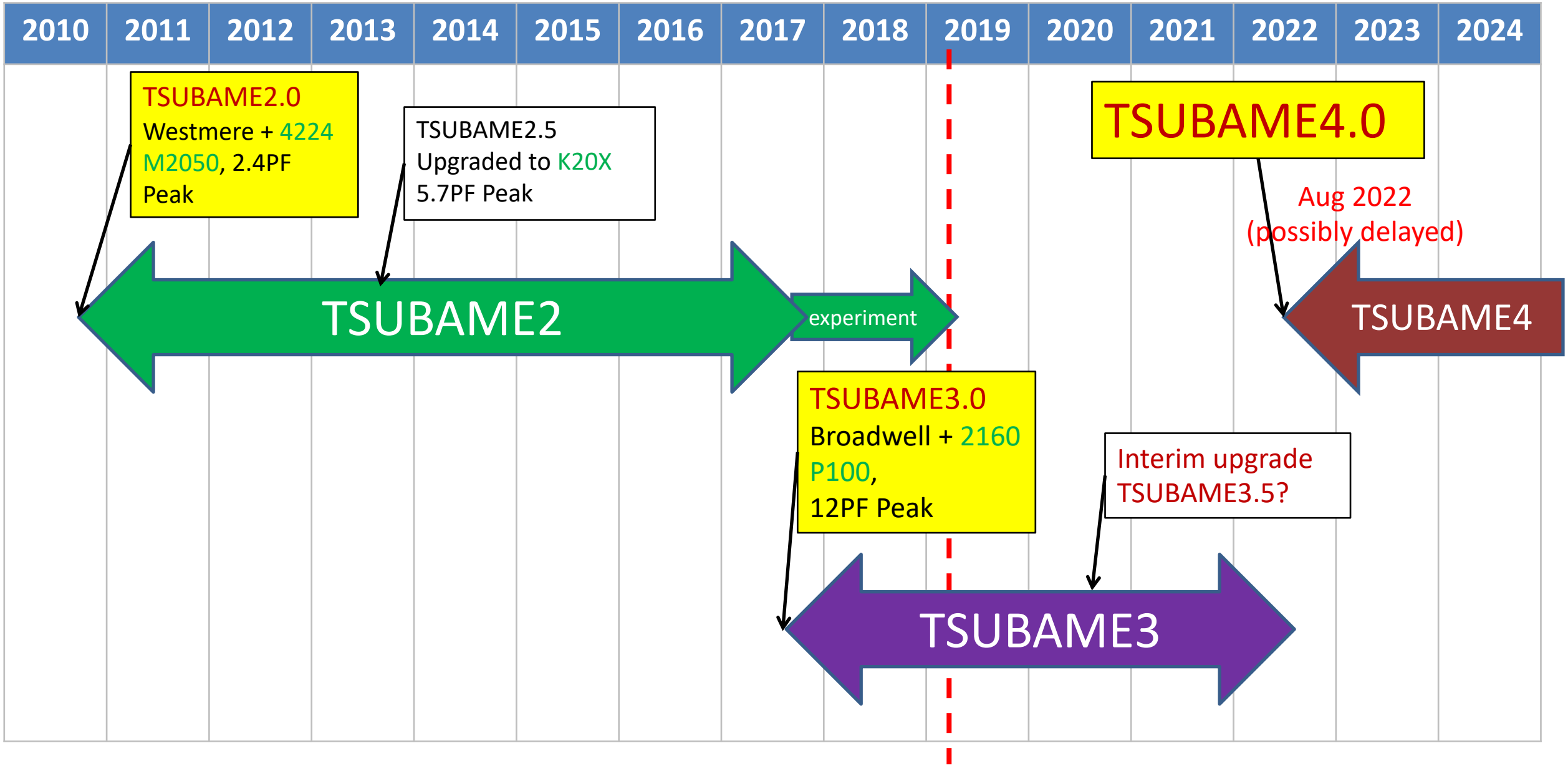
```
#!/bin/sh
#$ -cwd
#$ -l f_node=4
#$ -l h_rt=1:00:00
#$ -N flatmpi
#$ -v USE_BEEOND=1
. /etc/profile.d/modules.sh
module load cuda
module load intel
module load intel-mpi
mpiexec.hydra -ppn 8 -n 32 ./a.out
```

Usage: Dec 2018 -- Feb 2019

#nodes	# of jobs with BeeOND
1	560
2	388
3 -- 4	146
5 -- 8	59
9 -- 16	43
17 -- 32	3
33 -- 64	7
Total	1206

# of all F-type jobs (Dec 18-Feb19): 149,281

Schedule towards Next-Gen TSUBAME



Thank you for your attention

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