Introduction to Comet

SDSC's 2PF HPC Resource

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NSF

UC San Diego

NVIDIA

SDSC
SAN DIEGO SUPERCOMPUTER CENTER

DELL

intel

INDIANA UNIVERSITY

AEON COMPUTING

Mellanox
TECHNOLOGIES

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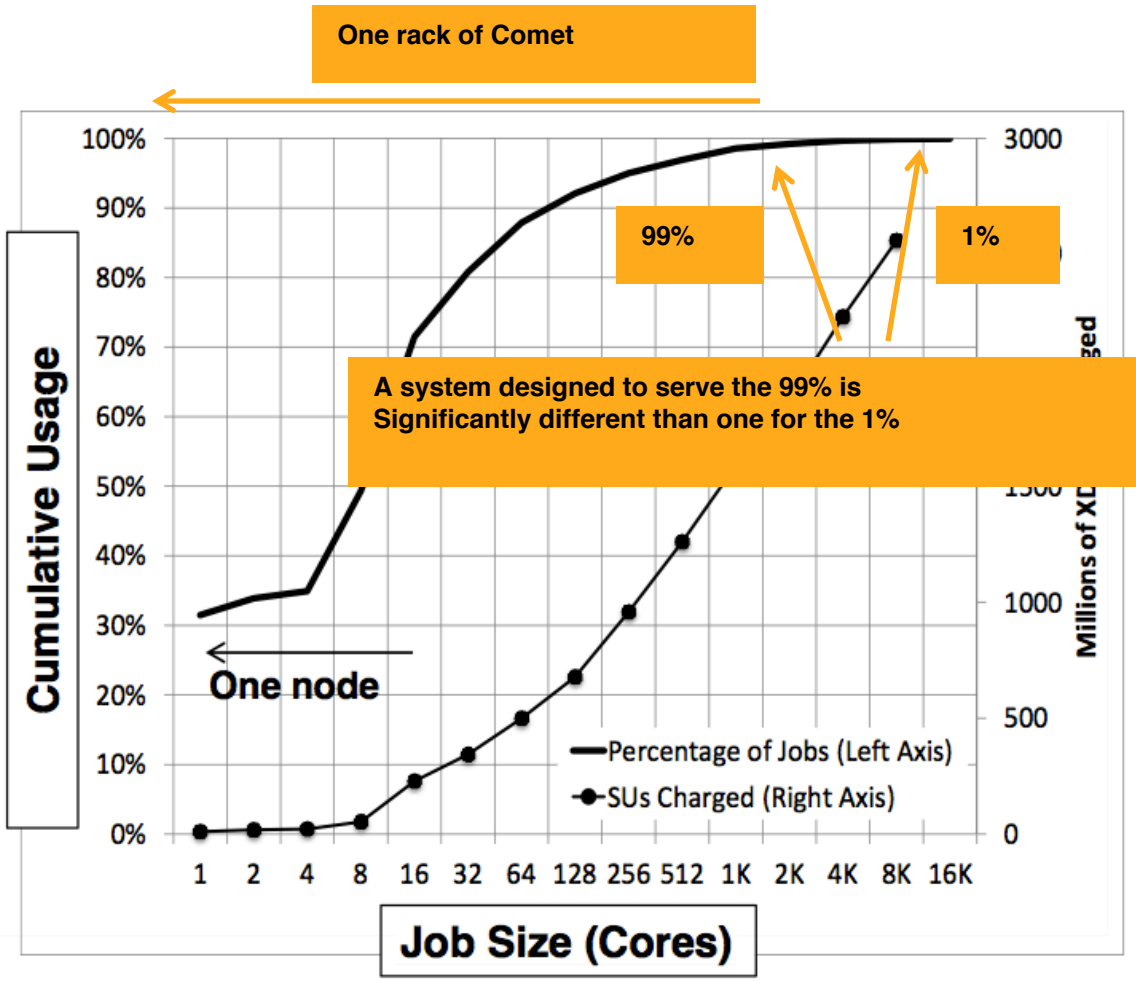
Comet
“HPC for the long tail of science”

iPhone panorama photograph of 1 of 2 server rows

Data extracted from NSF's XDMoD data base informed a design that reflects the way researchers actually use HPC systems

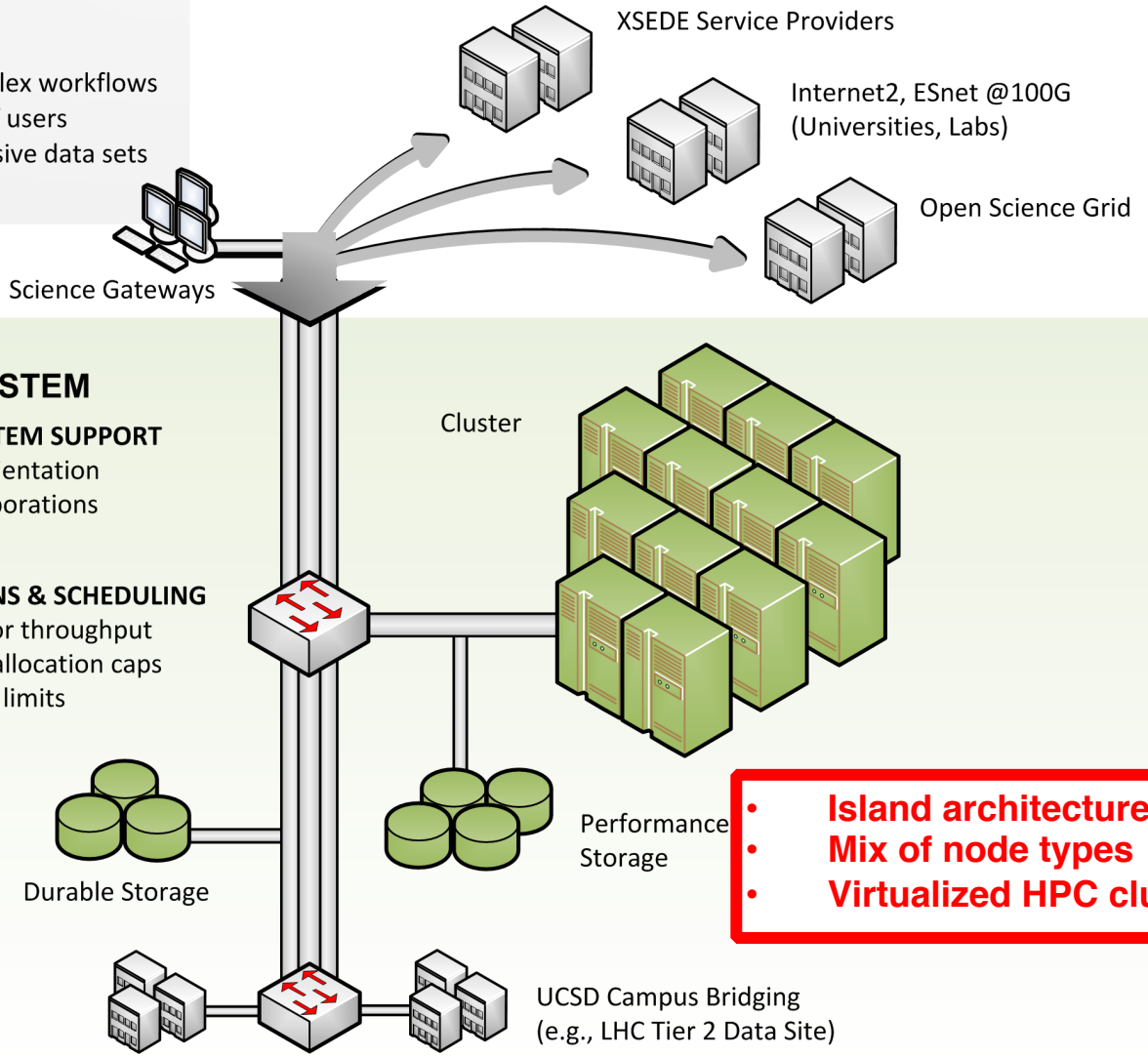
- **99% of jobs run on NSF's HPC resources in 2012 used <2,048 cores**
- **And consumed >50% of the total core-hours across all NSF resources**



Comet Built to Serve the 99%

CHALLENGES OUR PROPOSAL ADDRESSES

- ✓ Attract new users and communities
- ✓ Support diverse applications with complex workflows
- ✓ Ensure responsiveness for thousands of users
- ✓ Transfer, store, analyze, and share massive data sets
- ✓ Integrate with XSEDE



COMET COMPUTE SYSTEM

Cluster architecture
Fast standard nodes
Large-memory nodes
GPU-accelerated nodes
FDR InfiniBand

Storage architecture
Performance Storage
Durable Storage

Software
Science Gateways
Rich base of installed apps
Virtualization

USER & SYSTEM SUPPORT
New user orientation
XSEDE collaborations
FutureGrid

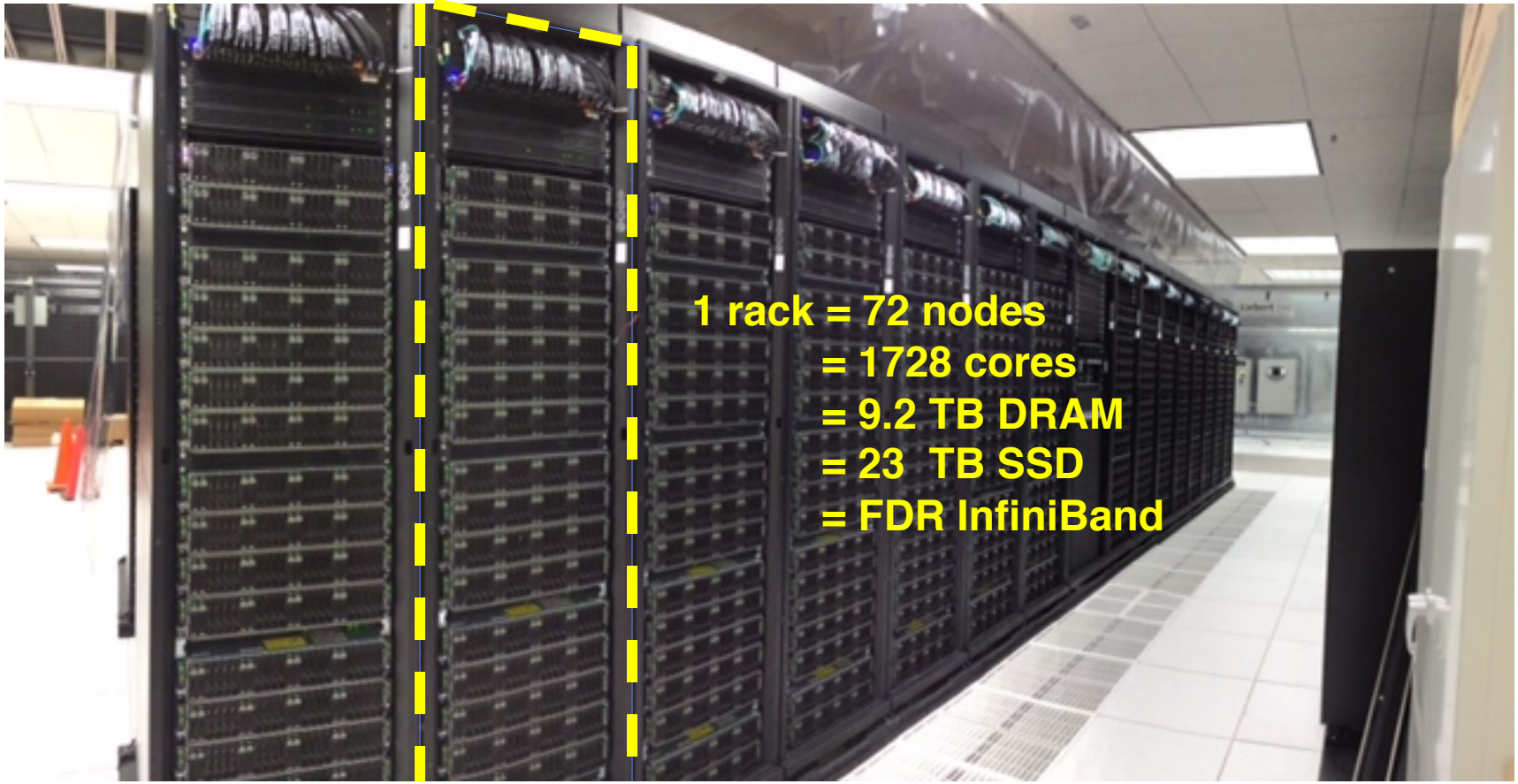
ALLOCATIONS & SCHEDULING
Optimized for throughput
Per-project allocation caps
Per-job core limits

- **Island architecture**
- **Mix of node types**
- **Virtualized HPC clusters**

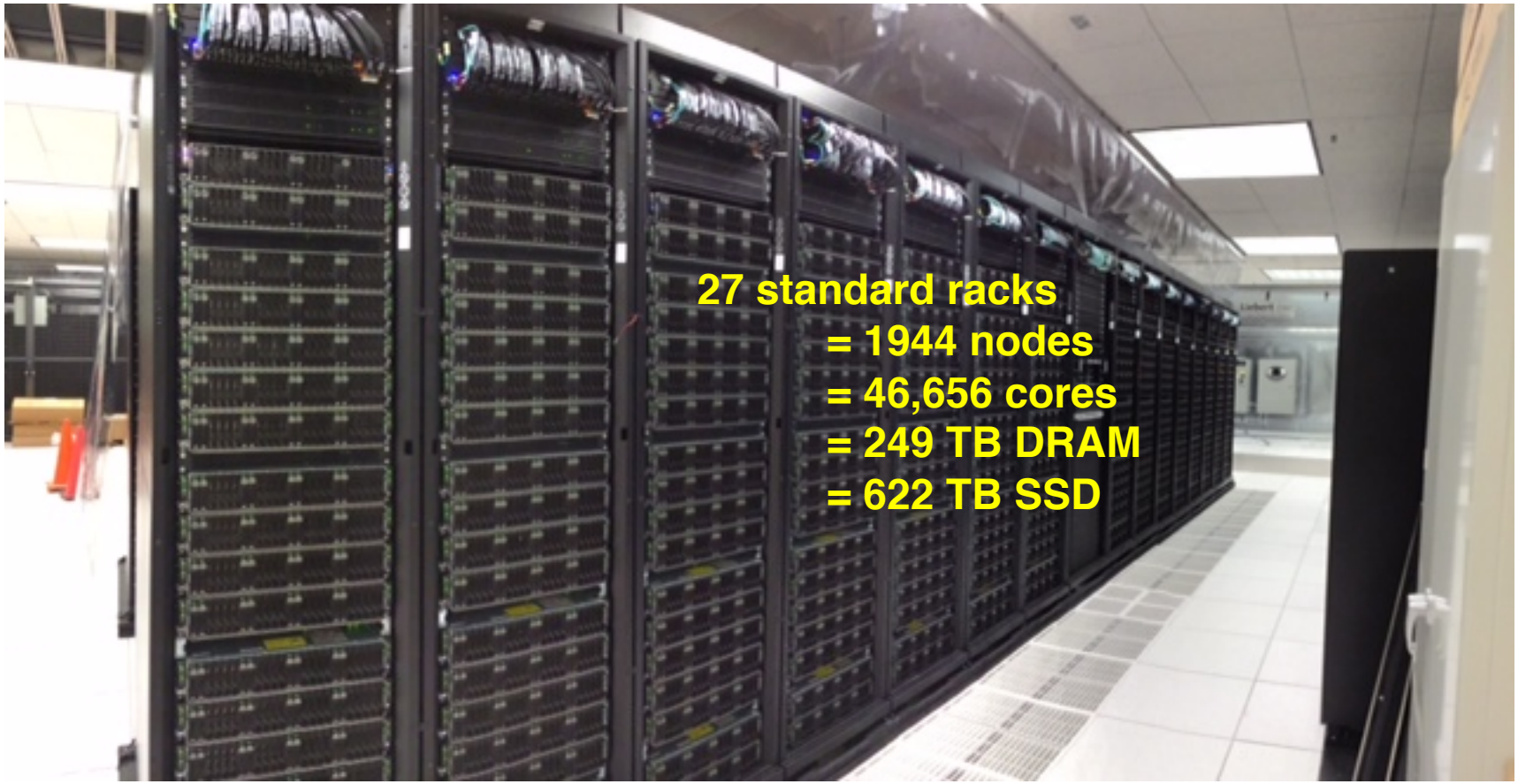
Comet: System Characteristics

- **Total peak flops ~2.1 PF**
- **Dell primary integrator**
  - Intel Haswell processors w/ AVX2
  - Mellanox FDR InfiniBand
- **1,944 standard compute nodes (46,656 cores)**
  - Dual CPUs, each 12-core, 2.5 GHz
  - 128 GB DDR4 2133 MHz DRAM
  - 2*160GB GB SSDs (local disk)
- **36 GPU nodes**
  - Same as standard nodes *plus*
  - Two NVIDIA K80 cards, each with dual Kepler3 GPUs
- **4 large-memory nodes**
  - 1.5 TB DDR4 1866 MHz DRAM
  - Four Haswell processors/node
  - 64 cores/node
- **Hybrid fat-tree topology**
  - FDR (56 Gbps) InfiniBand
  - Rack-level (72 nodes, 1,728 cores) full bisection bandwidth
  - 4:1 oversubscription cross-rack
- **Performance Storage (Aeon)**
  - 7.6 PB, 200 GB/s; Lustre
  - Scratch & Persistent Storage segments
- **Durable Storage (Aeon)**
  - 6 PB, 100 GB/s; Lustre
  - Automatic backups of critical data
- **Home directory storage**
- **Gateway hosting nodes**
- **Virtual image repository**
- **100 Gbps external connectivity to Internet2 & ESNet**

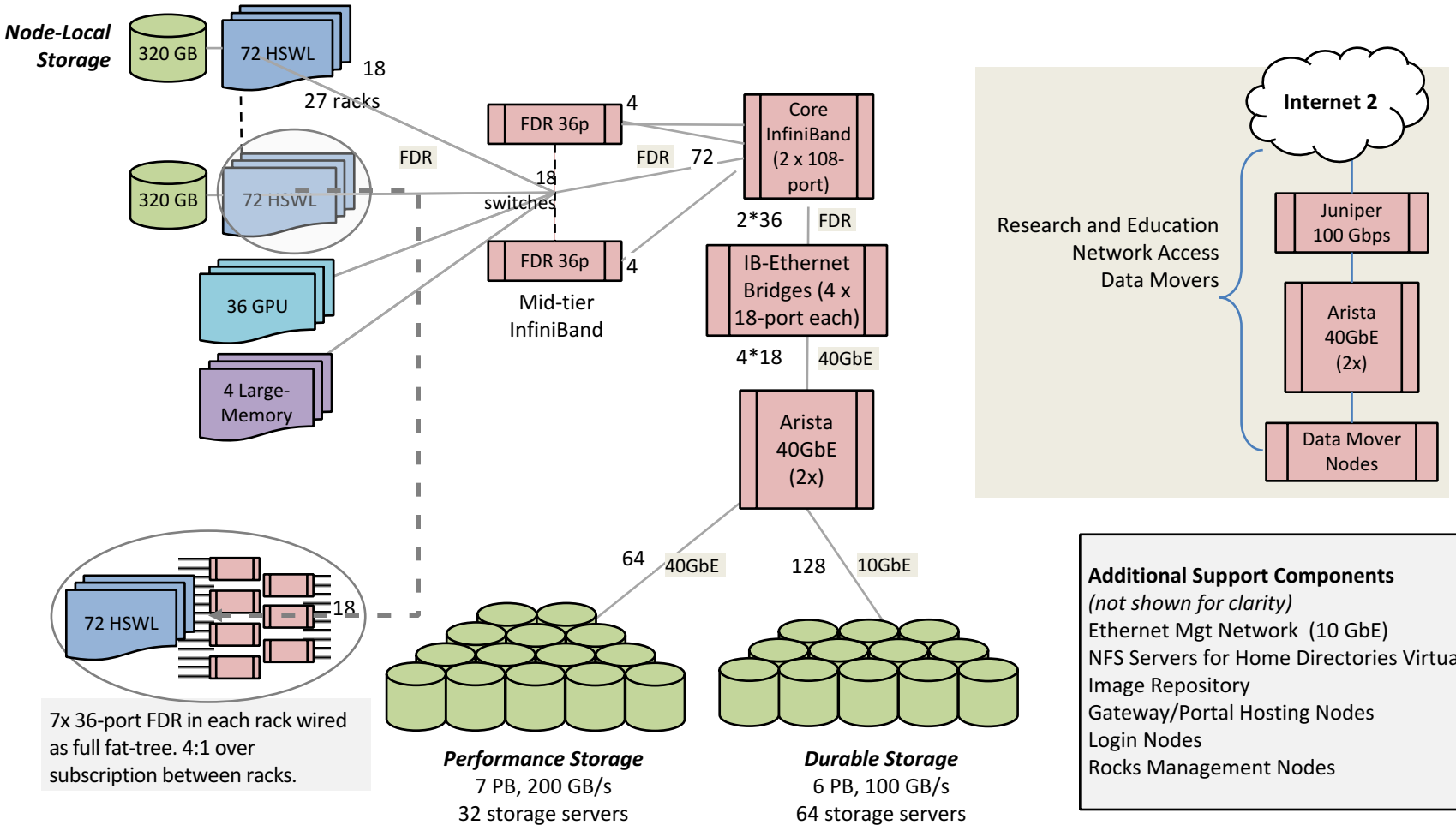
~67 TF supercomputer in a rack



And 27 single-rack supercomputers



Comet Network Architecture
InfiniBand compute, Ethernet Storage



Comet Flexibility Addresses Diverse Needs

- **Wide range of hardware options**
  - Large number of regular compute nodes (**1,944**) with **128GB** of memory and **210GB of local flash**.
  - Subset of compute nodes have **1.5TB of local flash**
  - 4 large memory (**1.5TB RAM**) nodes
  - **36 GPU nodes** with 4 GPUs each (in 2 K80s)
- **Flexible Software Environment**
  - **Rich set of applications** (>100) in regular compute environment
  - **Hadoop/Spark capability** can be enabled within regular scheduler environment.
  - Supports **Singularity based containerization** to enable other Linux based environments (for example Ubuntu). Users can upload their own images!
  - Virtual Clusters (VC) – see operational bullet below.
- **Flexible Operations**
  - **Flexible scheduler environment** – shared and exclusive queues, long running jobs, focus on quick turn around time
  - Research Groups/communities, who have people in their group with ***expert system administration skills***, can build their **own virtual clusters** with a custom OS and custom operational setup.

Extensive Software/Applications Stack

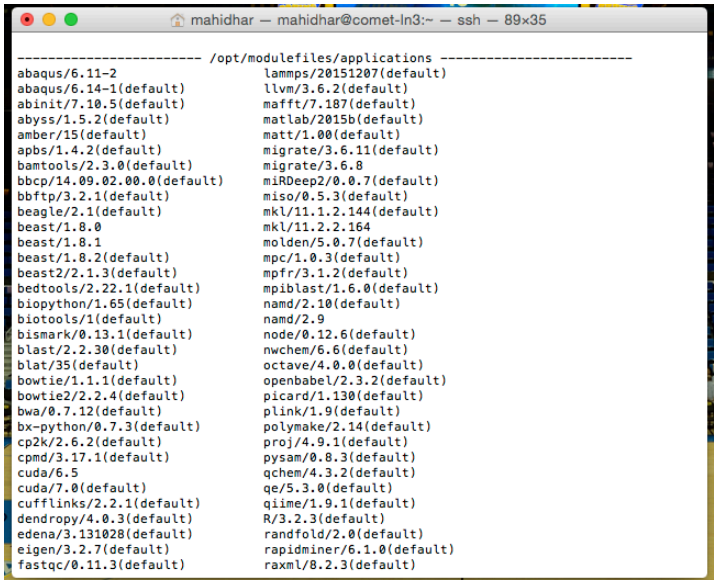
- ***Applications packaged into "Rocks Rolls"*** that are built and deployed on any of the SDSC systems. ***Benefits wider community deploying software*** on their Rocks clusters.

- Efficient system administration pooling software install/testing efforts from different projects/machines

- Users benefit from a familiar applications environment across SDSC systems.

- ***Rolls made available on Github**** **for all applications installed on Comet => easy replication of environment if users/groups wish to do so.**

*https://github.com/sdsc/?query=roll



Compilers, Applications, Libraries

Category	List of Software/Libraries
Compilers	**Intel, PGI, GNU, MVAPICH2,OPENMPI, IntelMPI**
Bioinformatics	**BamTools, BEAGLE, BEAST, BEAST 2, bedtools, Bismark, BLAST, BLAT, Bowtie, Bowtie 2, BWA, Cufflinks, DPPDiv, Edena, FastQC, FastTree, FASTX-Toolkit, FSA, GARLI, GATK, GMAP-GSNAP, IDBA-UD, MAFFT, MrBayes, PhyloBayes, Picard, PLINK, QIIME, RAxML, SAMtools, SOAPdenovo2, SOAPsnp, SPAdes, TopHat, Trimmomatic, Trinity, Velvet**
Chemistry	**CPMD, CP2K, GAMESS, Gaussian, MOPAC, NWChem, Q-Chem, VASP**
Molecular Dynamics	**AMBER, Gromacs, LAMMPS, NAMD**
Engineering	**ABAQUS**
Data Analysis/Analytics	**Hadoop 1, Hadoop 2 (with YARN), Spark, R, Weka, KNIME, Hadoop-RDMA, Spark-RDMA, ENVI; *Singularity Enabled Apps:* Torch, Keras, Tensorflow, Caffe, FEniCS**
Visualization	**VisIt, IDL; *Singularity Enabled*: Paraview**
Numerical libraries	**ATLAS, FFTW, GSL, LAPACK, MKL, ParMETIS, PETSc, ScaLAPACK, SPRNG, Sundials, SuperLU, Trilinios**
Debugging/Profiling	**DDT, PAPI, TAU, mpiP**
GPU enabled software	**AMBER, GROMACS, NAMD, LAMMPS, BEAST, HOOMD, mvapich2-gdr, RELION**

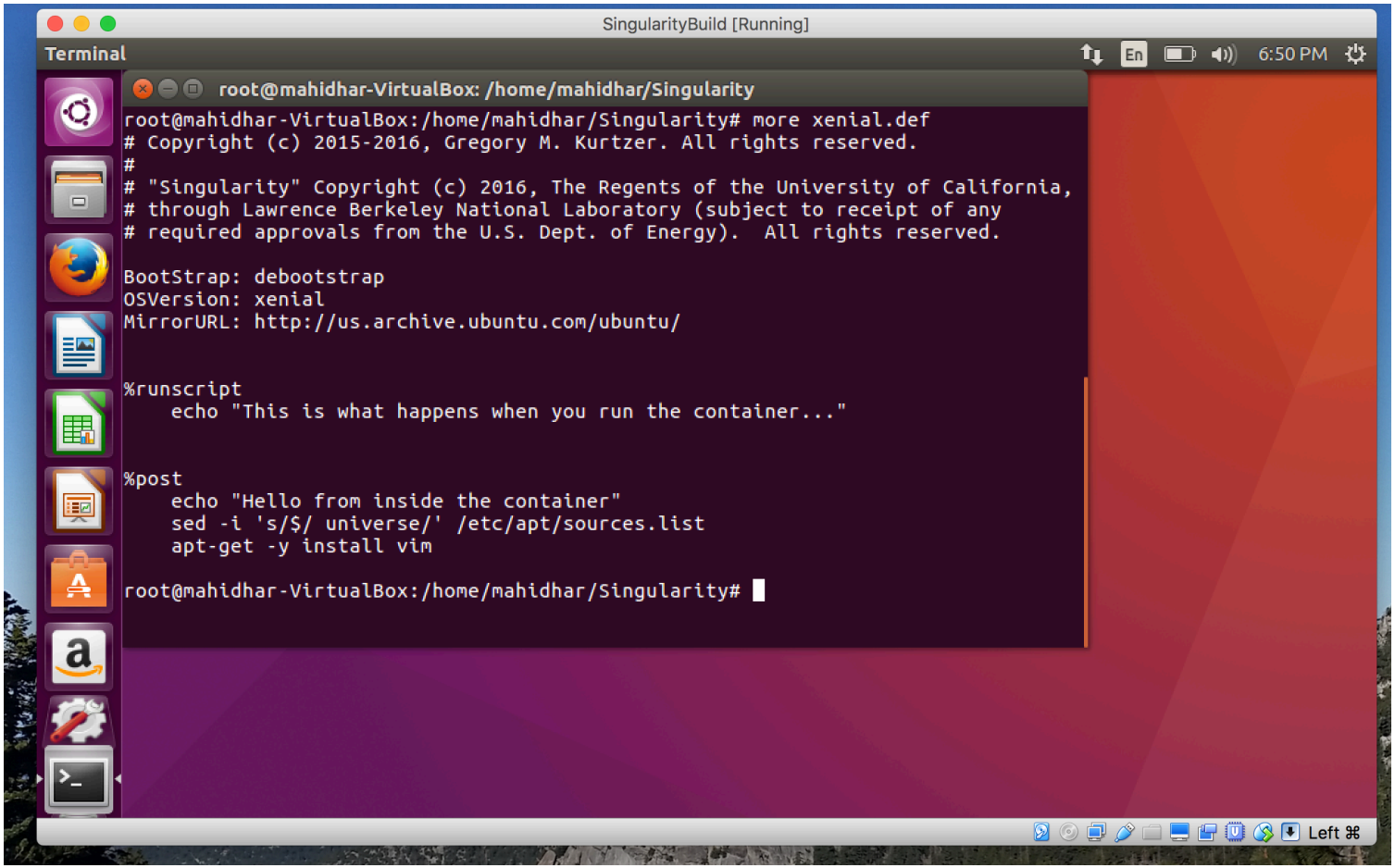
Data Intensive Computing & Visualization Stack

- **Comet's high performance computing and data components enable data intensive computing**
- **High speed Lustre filesystem with an aggregated peak measured data rate of 100 GB/s**
- **Several libraries and packages enable data intensive computing and visualization:**
  - **R** – Software environment for statistical computing and graphics
  - **Weka** – Tools for data analysis and predictive modeling
  - **RapidMiner** – Environment for machine learning, data mining, text mining, and predictive analytics
  - **Matlab, Octave, IDL**
  - **VisIt**
  - **Paraview *(via Singularity)***
- **The myHadoop infrastructure was developed to enable use Hadoop and Spark for distributed data intensive analysis *via the regular scheduler*.**
- **Several compute and GPU based data analytics tools enabled via Singularity (more details in Singularity slide).**

Singularity: Provides Flexibility for OS Environment

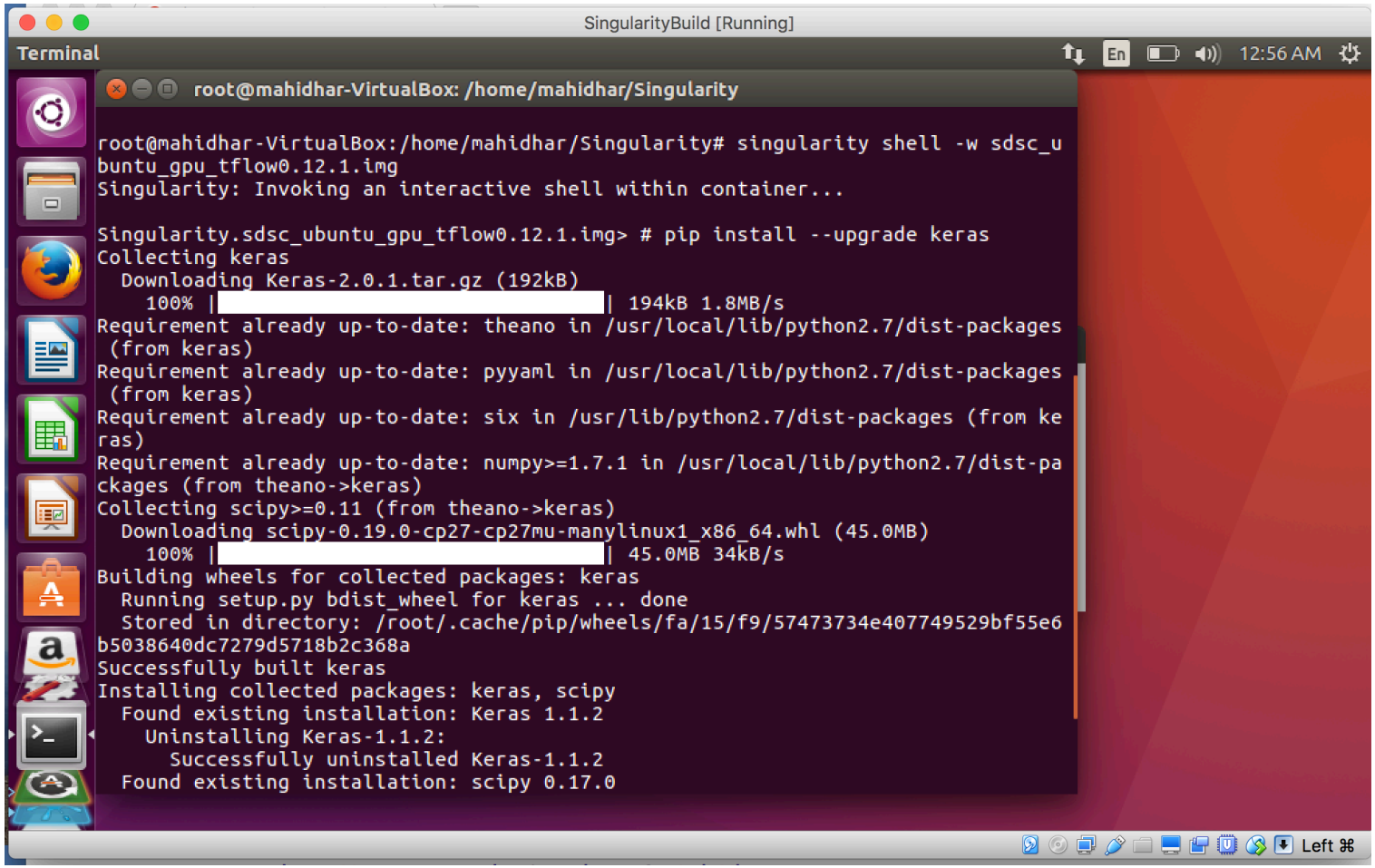
- Singularity (http://singularity.lbl.gov)is a relatively new development that has become very popular on Comet.
- Singularity allows groups to easily migrate complex software stacks from their campus to Comet.
- Singularity runs in user space, and requires very little special support – in fact it actually reduces it in some cases.
- We have roughly 15 groups running this on Comet.
- Applications include: Tensorflow, Paraview, Torch, Fenics, and custom user applications.
- Singularity was not available as an option during Comet's design. Adds another element of flexibility to Comet.
- Docker images can be imported into Singularity.
- Not possible to run services within Singularity environment -> *Virtual Clusters cover this class of applications.*

Singularity: Provides Flexibility for OS Environment



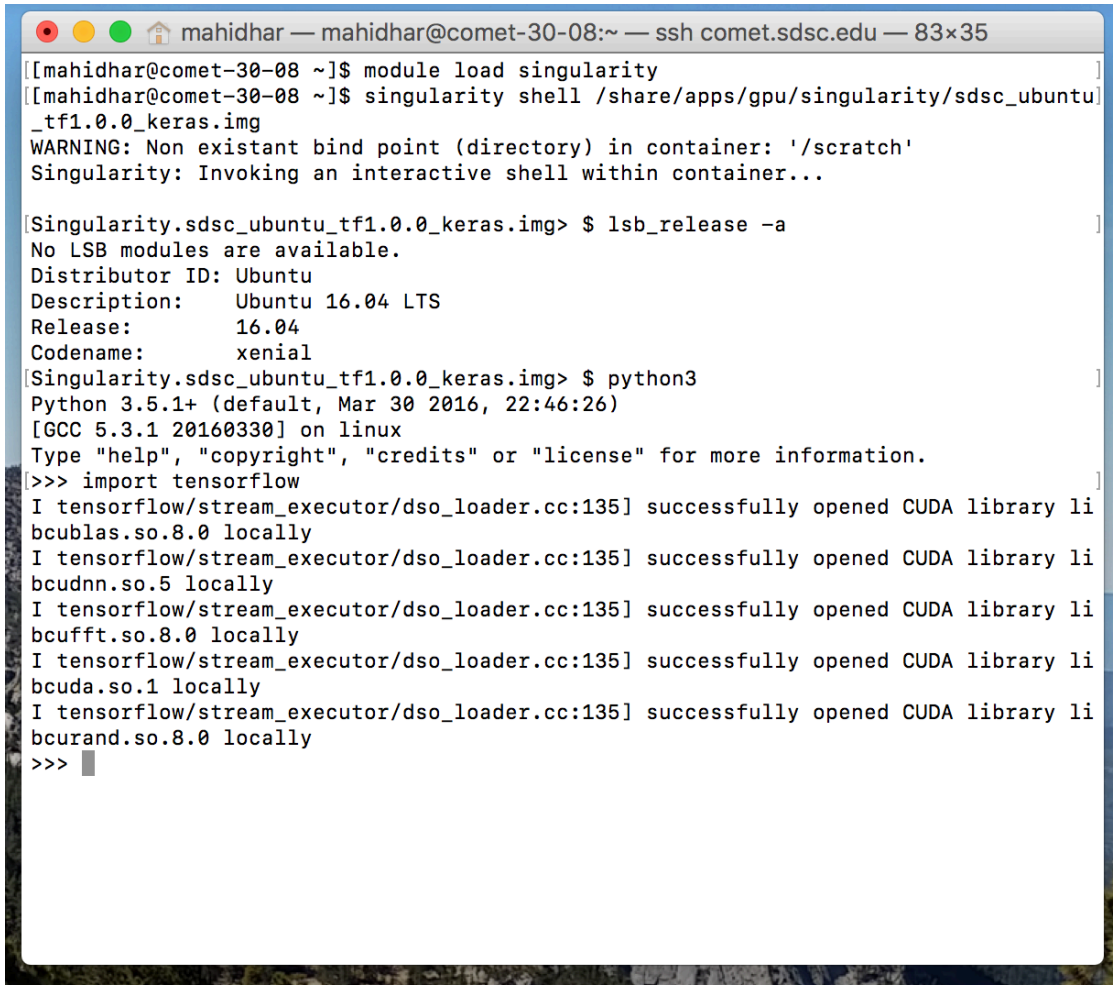
- **Above snapshot shows a definition file on a virtual box on personal laptop. The definition file lets you build a singularity image.**

Singularity: Provides Flexibility for OS Environment



- **Can open image in write mode on laptop via singularity and install packages (like Tensorflow). So an existing image on Comet can serve as a starting point. Here we are upgrading Keras!**

Singularity: Provides Flexibility for OS Environment



- **Copy image to Comet and we are running in an Ubuntu environment on a GPU node!**

Access Via Science Gateways (XSEDE)

- Community-developed set of tools, applications, and data that are integrated via a portal.
- Enables researchers of particular communities to use HPC resources through portals without the complication of getting familiar with the hardware and software details. Allows them to focus on the scientific goals.
- CIPRES gateway hosted by SDSC PIs enables large scale phylogenetic reconstructions using applications such as MrBayes, Raxml, and Garli. Enabled ~320 publications in 2013 and accounts for a significant fraction of the XSEDE users.
- NSG portal hosted by SDSC PIs enables HPC jobs for neuroscientists.

High performance virtualization (aka Virtual Clusters)

Motivation for Virtual Clusters

- OS and software requirements are diversifying. Growing number of user communities that can't work in traditional HPC software environment.
- Communities that have expertise and ability to utilize large clusters but need hardware.
- Institutions that have bursty or intermittent need for computational resources.

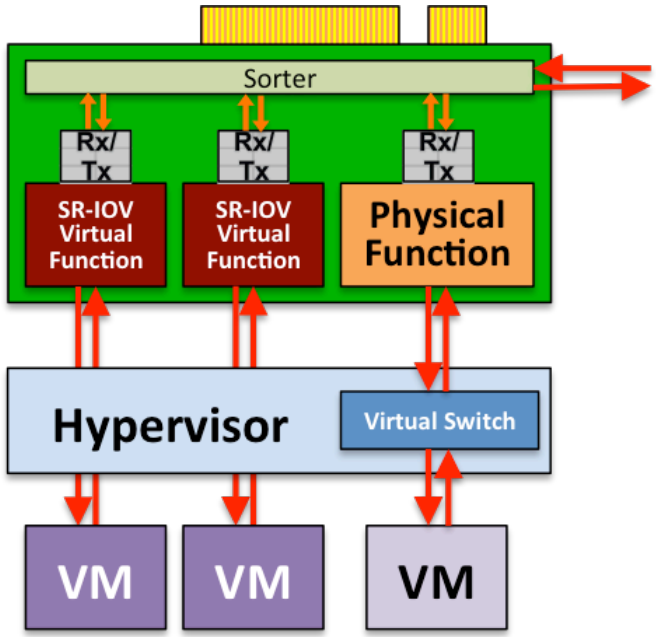
Goal: Provide near bare metal HPC performance and management experience for groups that can manage their own clusters.

Comet's virtual cluster (VC) technology bridges communities with software needs not typically well-supported by national cyberinfrastructure

- VC's use a single root I/O virtualization, KVM, and Rocks cluster management software to deliver bear metal resources at near-native IB performance.
- Through our partnership with Indiana University/Future Grid, we have developed an on-ramping process that carefully assesses the readiness of these communities to maintain their own VC.
- VC's are provisioned on the fly through an integration with the Slurm resource manager.

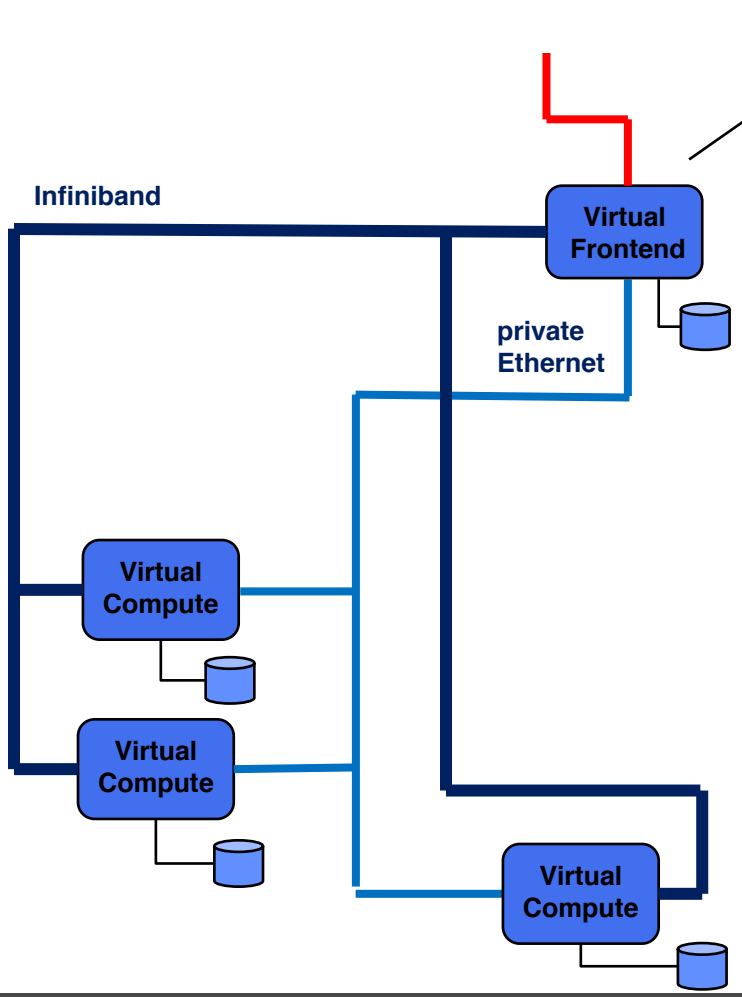
Key for Performance:
Single Root I/O Virtualization (SR-IOV)

- **Problem**: Virtualization generally has resulted in significant I/O performance degradation (e.g., excessive DMA interrupts)
- **Solution**: SR-IOV and Mellanox ConnectX-3 InfiniBand host channel adapters
  - One physical function → multiple virtual functions, each light weight but with its own DMA streams, memory space, interrupts
  - Allows DMA to bypass hypervisor to VMs
- ***SRIOV enables virtual HPC cluster w/ near-native InfiniBand latency/bandwidth and minimal overhead***



Mellanox TECHNOLOGIES

High Performance Virtual Cluster Characteristics



Comet: Providing Virtualized HPC for XSEDE

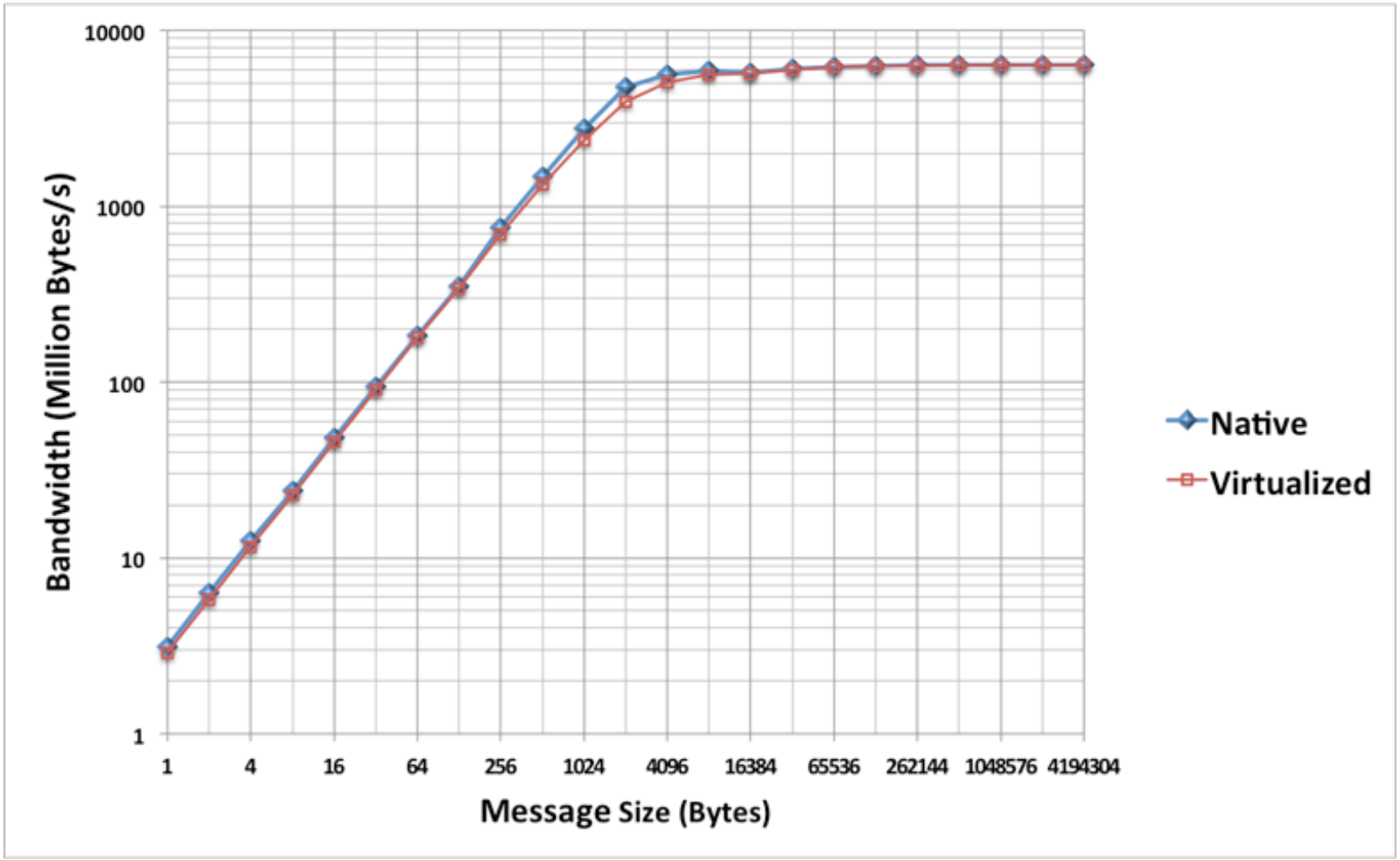
Infiniband Virtualization
- 8% latency overhead.
- Nominal bandwidth overhead

All nodes have
- Private Ethernet
- Infiniband
- Local Disk Storage

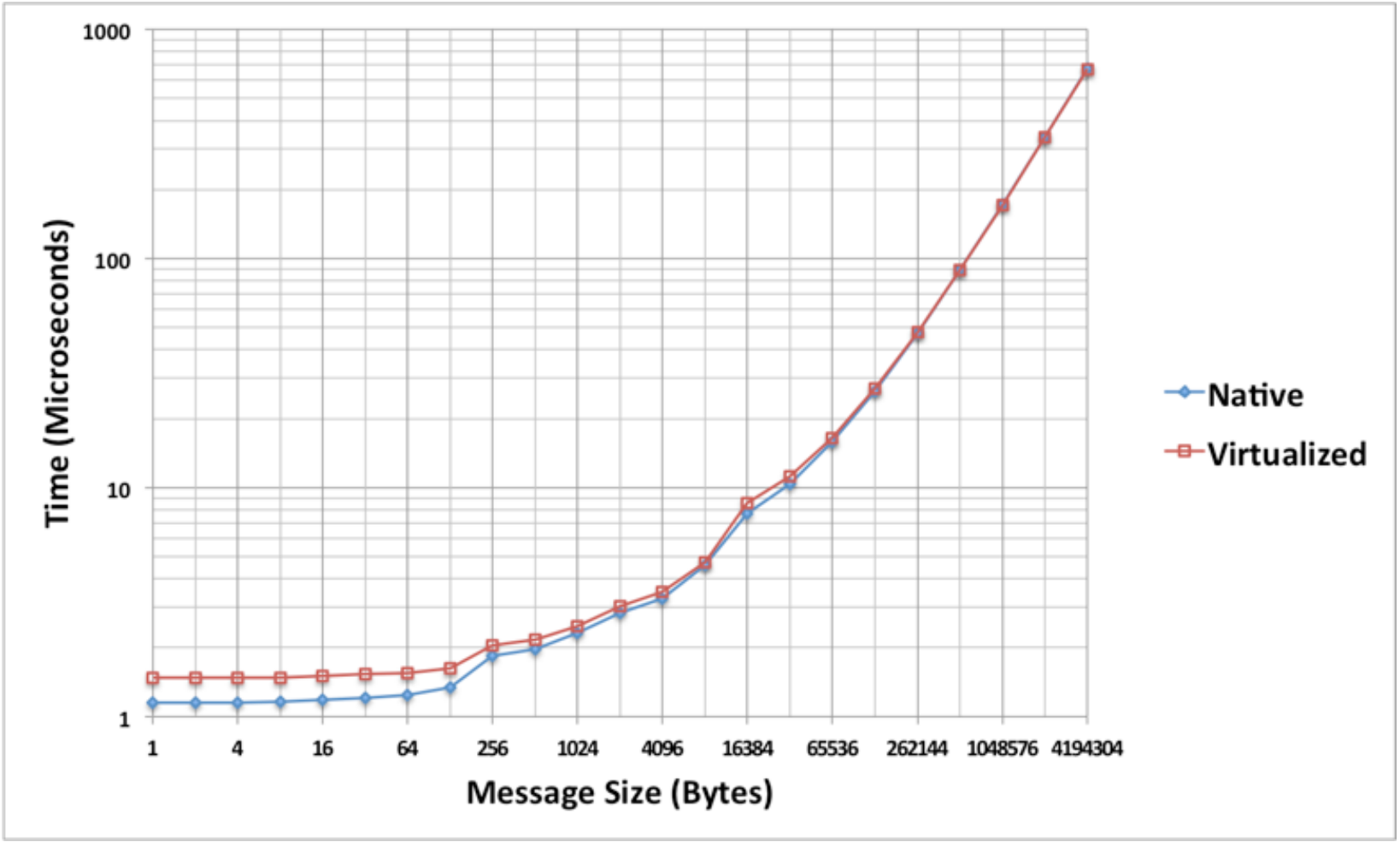
Virtual Compute Nodes can Network boot (PXE) from its virtual frontend

All Disks retain state
- keep user configuration between boots

Comet: MPI bandwidth slowdown from SR-IOV is at most 1.21 for medium-sized messages & negligible for small & large ones



Comet: MPI latency slowdown from SR-IOV is at most 1.32 for small messages & negligible for large ones



- Next: Hands On work with Comet

Getting Started

- **System Access – Logging in**
  - Linux/Mac – Use available ssh clients.
  - ssh clients for windows – Putty, Cygwin
    - http://www.chiark.greenend.org.uk/~sgtatham/putty/
  - Login hosts for the SDSC Comet:
    - comet.sdsc.edu
- **For NSF Resources – Users can login via the XSEDE user portal:**
  - https://portal.xsede.org/

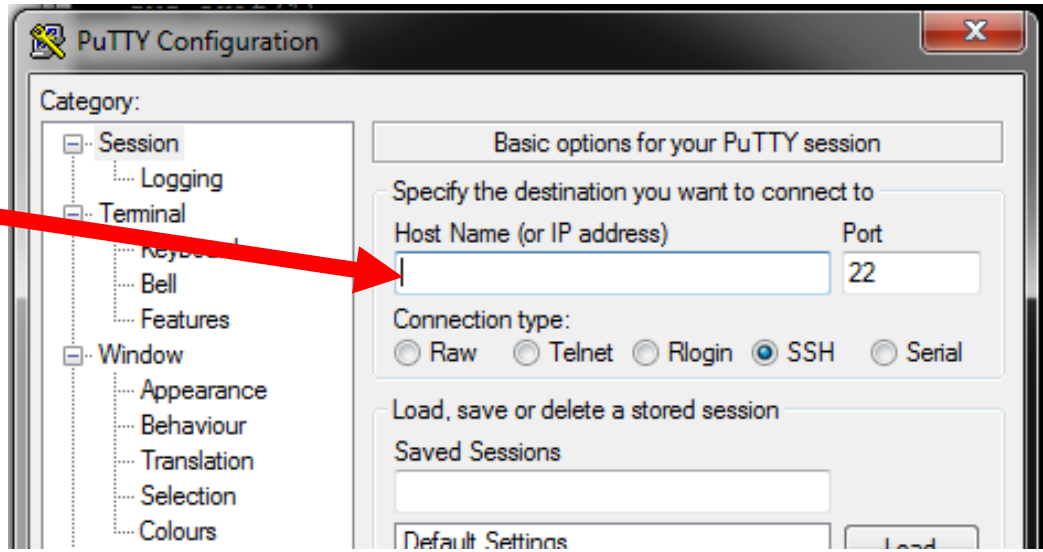
Logging into Comet

Mac/Linux:

```
ssh etrainXY@comet.sdsc.edu
```

Windows (PuTTY):

comet.sdsc.edu



Comet Compute Nodes

2-Socket (Total 24 cores) Intel Haswell Processors

Hands On Examples using:

(1) MPI

(2) OpenMP

(3) HYBRID

Comet – Compiling/Running Jobs

- **Copy and change to workshop directory:**

  cd /home/$USER/workshop/mpi-openmp/MPI

- **Verify modules loaded:**

  module list

  Currently Loaded Modulefiles:

  1) intel/2013_sp1.2.144 2) mvapich2_ib/2.1 3) gnutools/2.69

- **Compile the MPI hello world code:**

  mpif90 -o hello_mpi hello_mpi.f90

- **Verify executable has been created:**

  ls -lt hello_mpi

  -rwxr-xr-x 1 mahidhar sdsc 721912 Mar 25 14:53 **hello_mpi**

Comet: Hello World on compute nodes

The submit script is hellompi-slurm.sb:

```
#!/bin/bash
#SBATCH --job-name="hellompi"
#SBATCH --output="hellompi.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 01:30:00

#This job runs with 2 nodes, 24 cores per node for a total of 48 cores.
#ibrun in verbose mode will give binding detail

ibrun -v ./hello_mpi
```

Comet: Hello World on compute nodes

IBRUN: Command is ../hello_mpi
IBRUN: Command is /share/apps/examples/MPI/hello_mpi
…
…
IBRUN: MPI binding policy: compact/core for 1 threads per rank (12 cores per socket)
IBRUN: Adding MV2_CPU_BINDING_LEVEL=core to the environment
IBRUN: Adding MV2_ENABLE_AFFINITY=1 to the environment
IBRUN: Adding MV2_DEFAULT_TIME_OUT=23 to the environment
IBRUN: Adding MV2_CPU_BINDING_POLICY=bunch to the environment
…
…
IBRUN: Added 8 new environment variables to the execution environment
IBRUN: Command string is [mpirun_rsh -np 48 -hostfile /tmp/rssSvauaJA -export /share/apps/examples/MPI/hello_mpi]
node 18 : Hello world
node 13 : Hello world
node 2 : Hello world
node 10 : Hello world

Compiling OpenMP Example

- **Change to the examples directory:**
  cd /home/$USER/workshop/mpi-openmp/OPENMP

- **Compile using –openmp flag:**
  ifort -o hello_openmp -openmp hello_openmp.f90

- **Verify executable was created:**

[mahidhar@comet-08-11 OPENMP]$ **ls -lt hello_openmp**
-rwxr-xr-x 1 mahidhar sdsc 750648 Mar 25 15:00 **hello_openmp**

OpenMP job script

```
#!/bin/bash
#SBATCH --job-name="hell_openmp"
#SBATCH --output="hello_openmp.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 01:30:00

#SET the number of openmp threads
export OMP_NUM_THREADS=24

#Run the job using mpirun_rsh
./hello_openmp
```

Output from OpenMP Job

```
$ more hello_openmp.out
 HELLO FROM THREAD NUMBER =      7
 HELLO FROM THREAD NUMBER =      6
 HELLO FROM THREAD NUMBER =      9
 HELLO FROM THREAD NUMBER =      8
 HELLO FROM THREAD NUMBER =      5
 HELLO FROM THREAD NUMBER =      4
 HELLO FROM THREAD NUMBER =      0
 HELLO FROM THREAD NUMBER =     12
 HELLO FROM THREAD NUMBER =     14
 HELLO FROM THREAD NUMBER =      3
 HELLO FROM THREAD NUMBER =     13
 HELLO FROM THREAD NUMBER =     10
 HELLO FROM THREAD NUMBER =     11
 HELLO FROM THREAD NUMBER =      2
 HELLO FROM THREAD NUMBER =      1
 HELLO FROM THREAD NUMBER =     15
```

Running Hybrid (MPI + OpenMP) Jobs

- Several HPC codes use a hybrid MPI, OpenMP approach.
- "ibrun" wrapper developed to handle such hybrid use cases. Automatically senses the MPI build (mvapich2, openmpi) and binds tasks correctly.
- "ibrun –help" gives detailed usage info.
- hello_hybrid.c is a sample code, and hello_hybrid.cmd shows "ibrun" usage.

hello_hybrid.cmd

```
#!/bin/bash
#SBATCH --job-name="hellohybrid"
#SBATCH --output="hellohybrid.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 01:30:00

#This job runs with 2 nodes, 24 cores per node for a total of 48 cores.

# We use 8 MPI tasks and 6 OpenMP threads per MPI task
export OMP_NUM_THREADS=6
ibrun --npernode 4 ./hello_hybrid
```

Hybrid Code Output

```
[etrain61@comet-ln3 HYBRID]$ more hellohybrid.8557716.comet-14-01.out
Hello from thread 0 out of 6 from process 2 out of 8 on comet-14-01.local
Hello from thread 3 out of 6 from process 2 out of 8 on comet-14-01.local
Hello from thread 4 out of 6 from process 2 out of 8 on comet-14-01.local
Hello from thread 5 out of 6 from process 2 out of 8 on comet-14-01.local
Hello from thread 0 out of 6 from process 3 out of 8 on comet-14-01.local
Hello from thread 2 out of 6 from process 2 out of 8 on comet-14-01.local
Hello from thread 1 out of 6 from process 3 out of 8 on comet-14-01.local
Hello from thread 2 out of 6 from process 3 out of 8 on comet-14-01.local
…
…
Hello from thread 4 out of 6 from process 7 out of 8 on comet-14-02.local
Hello from thread 2 out of 6 from process 7 out of 8 on comet-14-02.local
Hello from thread 3 out of 6 from process 7 out of 8 on comet-14-02.local
Hello from thread 5 out of 6 from process 7 out of 8 on comet-14-02.local
Hello from thread 1 out of 6 from process 6 out of 8 on comet-14-02.local
```

Comet GPU Nodes

2 NVIDIA K-80 Cards (4 GPUs total) per node.

Hands On Examples using Singularity to enable Tensorflow

Tensorflow via Singularity

```
#!/bin/bash
#SBATCH --job-name="TensorFlow"
#SBATCH --output="TensorFlow.%j.%N.out"
#SBATCH --partition=gpu-shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=6
#SBATCH --gres=gpu:1
#SBATCH -t 01:00:00

#Run the job
#

module load singularity
singularity exec /share/apps/gpu/singularity/sdsc_ubuntu_gpu_tflow.img lsb_relea
se -a
singularity exec /share/apps/gpu/singularity/sdsc_ubuntu_gpu_tflow.img python -m
 tensorflow.models.image.mnist.convolutional
```

Tensorflow via Singularity

- **Change to the examples directory:**
  cd /home/$USER/workshop/tensorflow

- **Submit the job:**
  sbatch --res=UCSBRes TensorFlow.sb

Tensorflow Example: Output

```
Distributor ID: Ubuntu
Description: Ubuntu 16.04 LTS
Release: 16.04
Codename: xenial
I tensorflow/stream_executor/dso_loader.cc:108] successfully opened CUDA library libcublas.so locally
I tensorflow/stream_executor/dso_loader.cc:108] successfully opened CUDA library libcudnn.so locally
I tensorflow/stream_executor/dso_loader.cc:108] successfully opened CUDA library libcufft.so locally
I tensorflow/stream_executor/dso_loader.cc:108] successfully opened CUDA library libcuda.so.1 locally
I tensorflow/stream_executor/dso_loader.cc:108] successfully opened CUDA library libcurand.so locally
I tensorflow/core/common_runtime/gpu/gpu_init.cc:102] Found device 0 with properties:
name: Tesla K80
major: 3 minor: 7 memoryClockRate (GHz) 0.8235
pciBusID 0000:85:00.0
Total memory: 11.17GiB
Free memory: 11.11GiB
I tensorflow/core/common_runtime/gpu/gpu_init.cc:126] DMA: 0
I tensorflow/core/common_runtime/gpu/gpu_init.cc:136] 0:   Y
I tensorflow/core/common_runtime/gpu/gpu_device.cc:838] Creating TensorFlow device (/gpu:0) -> (device: 0, name:
Tesla K80, pci bus id: 0000:85:00.0)
Extracting data/train-images-idx3-ubyte.gz
…
Step 8500 (epoch 9.89), 11.6 ms
Minibatch loss: 1.601, learning rate: 0.006302
Minibatch error: 0.0%
Validation error: 0.9%
Test error: 0.9%
```

Summary

- **Comet's hardware options, both for compute and for storage, make it a very *flexible platform for research*.**
- **Baseline configuration supports a diverse HPC and data analytics workload with over *100 applications*. Will continue to add to existing software stack.**
- ***Singularity* provides a simple solution for users needing a *custom OS and software stack*.**
- ***Scheduling flexibility* to allow for quick turn around, shared jobs, long running jobs, and support of Science Gateways.**

Thanks!
Questions: Email mahidhar@sdsc.edu