Introduction to SDSC Comet





Comet "HPC for the long tail of science"



iPhone panorama photograph of 1 of 2 server rows

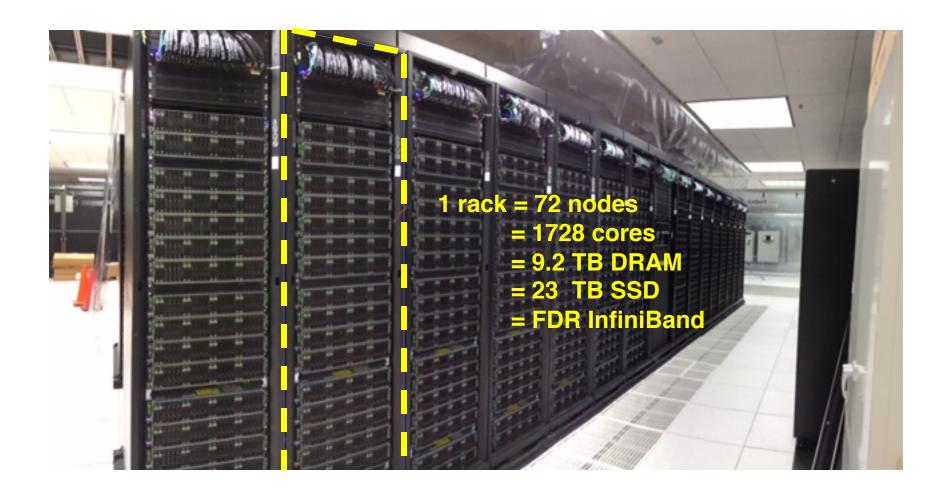


Comet: System Characteristics

- 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)
- 72 GPU nodes
 - 36 nodes same as standard nodes plus Two NVIDIA K80 cards, each with dual Kepler3 GPUs
 - 36 nodes, with 4 P100 GPUs per node
- 4 large-memory nodes
 - 1.5 TB DDR4 1866 MHz DRAM
 - Four Haswell processors/node
 - 64 cores/node

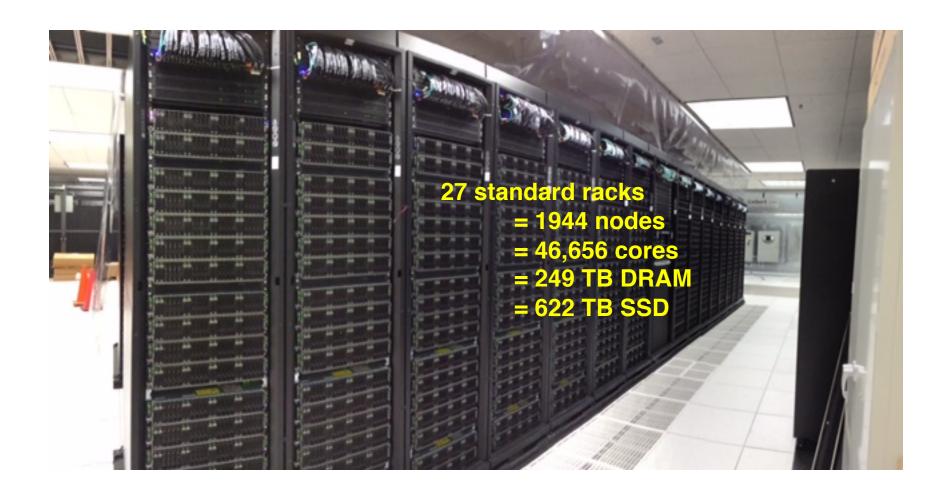
- Hybrid fat-tree topology
 - FDR (56 Gbps) InfiniBand
 - Rack-level (72 nodes, 1,728 cores) full bisection bandwidth
 - 4:1 oversubscription cross-rack
- Performance Storage (Aeon)
 - 7.6 PB, 200 GB/s; Lustre
 - Scratch & Persistent Storage segments
- Durable Storage (Aeon)
 - 6 PB, 100 GB/s; Lustre
 - · 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



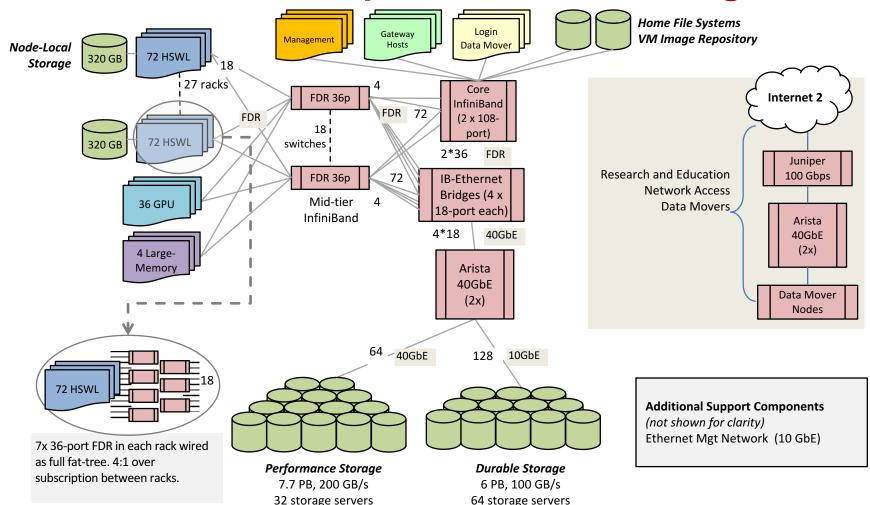


And 27 single-rack supercomputers





Comet Network Architecture InfiniBand compute, Ethernet Storage





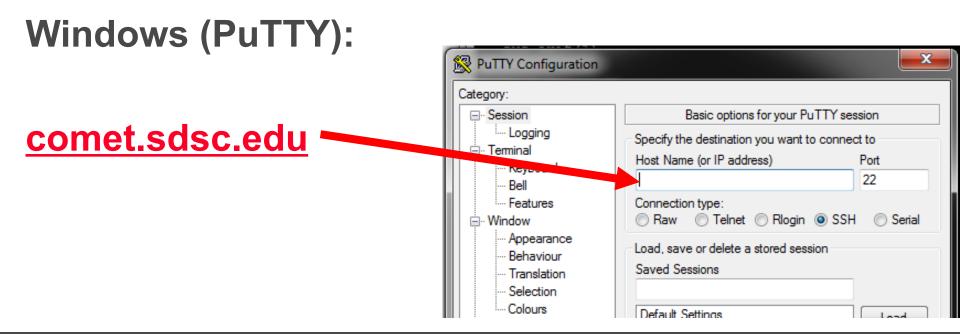
Getting Started

- 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

Logging into Comet

Mac/Linux:

ssh username@comet.sdsc.edu



Comet: Filesystems

Lustre filesystems – Good for scalable large block I/O

- Accessible from all compute and GPU nodes.
- /oasis/scratch/comet 2.5PB, peak performance: 100GB/s. Good location for storing large scale scratch data during a job.
- /oasis/projects/nsf 2.5PB, peak performance: 100 GB/s. Long term storage.
- Not good for lots of small files or small block I/O.

SSD filesystems

- /scratch local to each native compute node 210GB on regular compute nodes, 285GB on GPU, large memory nodes, 1.4TB on selected compute nodes.
- SSD location is good for writing small files and temporary scratch files. Purged at the end of a job.

Home directories (/home/\$USER)

- Source trees, binaries, and small input files.
- Not good for large scale I/O.



Comet: System Environment

- Modules used to manage environment for users.
- Default environment:

```
$ module liCurrently Loaded Modulefiles:1) intel/2013 sp1.2.144 2) mvapich2 ib/2.1 3) gnutools/2.69
```

Listing available modules:



Comet: System Environment

Loading modules:

```
$ module load fftw/3.3.4
```

\$ module li

Currently Loaded Modulefiles:

- 1) intel/2013_sp1.2.144 3) gnutools/2.69
- 2) mvapich2_ib/2.1 4) fftw/3.3.4

See what a module does:

\$ module show fftw/3.3.4

```
/opt/modulefiles/applications/.intel/fftw/3.3.4:
module-whatis fftw
module-whatis Version: 3.3.4
module-whatis Description: fftw
module-whatis Compiler: intel
module-whatis MPI Flavors: mvapich2_ib openmpi_ib
setenv FFTWHOME /opt/fftw/3.3.4/intel/mvapich2_ib
prepend-path PATH /opt/fftw/3.3.4/intel/mvapich2_ib/bin
prepend-path LD_LIBRARY_PATH /opt/fftw/3.3.4/intel/mvapich2_ib/lib
prepend-path LIBPATH /opt/fftw/3.3.4/intel/mvapich2_ib/lib
```



Comet: System Environment

\$ echo \$PATH

/opt/fftw/3.3.4/intel/mvapich2_ib/bin:/share/apps/compute/b bftp/bin:/home/mahidhar/pdsh/bin:/opt/gnu/gcc/bin:/opt/gn u/bin:/opt/mvapich2/intel/ib/bin:/opt/intel/composer_xe_201 3_sp1.2.144/bin/intel64:/opt/intel/composer_xe_2013_sp1.2.144/mpirt/bin/intel64:/opt/intel/composer_xe_2013_sp1.2.144/mpirt/bin/intel64:/opt/intel/composer_xe_2013_sp1.2.144/debugger/gdb/intel64_mic/bin:/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/sbin:/opt/ibutils/bin:/usr/java/latest/bin:/opt/pdsh/bin:/opt/rocks/bin:/opt/rocks/sbin:/opt/sdsc/sbin:/opt/sdsc/sbin:/home/mahidhar/bin

\$ echo \$FFTWHOME

/opt/fftw/3.3.4/intel/mvapich2_ib



Parallel Programming

- Comet supports MPI, OpenMP, and Pthreads for parallel programming. Hybrid modes are possible.
- GPU nodes support CUDA, OpenACC.
- MPI
 - Default: mvapich2_ib/2.1
 - Other options: openmpi_ib/1.8.4 (and 1.10.2), Intel MPI
 - mvapich2_gdr: GPU direct enabled version
- OpenMP: All compilers (GNU, Intel, PGI) have OpenMP flags.
- Default Intel Compiler: intel/2013_sp1.2.144;
 Versions 2015.2.164 and 2016.3.210 available.



Example Files for Class

Copy directory:

cp -r /share/apps/examples/UCSB2018 /home/\$USER

Make sure you have all the files:

\$ Is /home/\$USER/UCSB2018

CUDA HYBRID LOCALSCRATCH2 MPI pytorch TensorFlow HADOOP LOCALSCRATCH MKL OPENMP SPARK



Running Jobs on Comet

- Important note: Do not run on the login nodes even for simple tests.
- All runs must be via the Slurm scheduling infrastructure.
 - Interactive Jobs: Use **srun** command: srun --pty --nodes=1 --ntasks-per-node=24 -p debug -t 00:30:00 --wait 0 /bin/bash
 - Batch Jobs: Submit batch scripts from the login nodes.
 Can choose:
 - Partition (details on upcoming slide)
 - Time limit for the run (maximum of 48 hours)
 - Number of nodes, tasks per node
 - Memory requirements (if any)
 - Job name, output file location
 - Email info, configuration



Slurm Partitions

Queue Name	Max Walltime	Max Nodes	Comments
compute	48 hrs	72	Used for access to regular compute nodes
gpu	48 hrs	4	Used for access to the GPU nodes
gpu-shared	48 hrs	1	Used for shared access to a partial GPU node
shared	48 hrs	1	Single-node jobs using fewer than 24 cores
large-shared	48 hrs	1	Single-node jobs using large memory up to 1.45 TB
debug	30 mins	2	Used for access to debug nodes

Specified using -p option in batch script. For example:

#SBATCH-p gpu



Slurm Commands

Submit jobs using the sbatch command:

\$ sbatch Localscratch-slurm.sb Submitted batch job 8718049

Check job status using the squeue command:

```
$ squeue -u $USER
```

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON) 8718049 compute localscr mahidhar PD 0:00 1 (Priority)

Once the job is running:

```
$ squeue -u $USER
```

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON) 8718064 debug localscr mahidhar R 0:02 1 comet-14-01

Comet Compute Nodes

2-Socket (Total 24 cores) Intel Haswell Processors

Hands On Examples using:

- (1) MPI
- (2) OpenMP
- (3) HYBRID
- (4) Local scratch
- (5) MKL Example



Comet – Compiling/Running Jobs

 Copy and change to directory (assuming you already copied the PHYS244 directory):

cd /home/\$USER/UCSB2018/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:

```
Is -It hello_mpi
-rwxr-xr-x 1 mahidhar sdsc 721912 Mar 25 14:53 hello_mpi
```

Submit job from IBRUN directory:

```
cd /home/$USER/UCSB2018/MPI/IBRUN sbatch hellompi-slurm.sb
```



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 /s
hare/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/UCSB2018/OPENMP
- Compile using –openmp flag:
 ifort -o hello_openmp -openmp hello_openmp.f90
- Verify executable was created:

[mahidhar@comet-08-11 OPENMP]\$ Is -It 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 =
                                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 =
HELLO FROM THREAD NUMBER =
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-In3 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 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



Using SSD Scratch

```
#!/bin/bash
#SBATCH --job-name="localscratch"
#SBATCH --output="localscratch.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 01:30:00
#Copy binary to SSD
cp IOR.exe /scratch/$USER/$SLURM JOBID
#Change to local scratch (SSD) and run IOR benchmark
cd /scratch/$USER/$SLURM_JOBID
#Run IO benchmark
ibrun -np 4 $WKDIR/IOR.exe -F -t 1m -b 4g -v -v > IOR.out.$SLURM JOBID
#Copy out data you need
cp IOR.out.$SLURM_JOBID $SLURM_SUBMIT_DIR
```

Using SSD Scratch

Snapshot on the node during the run:

```
[mahidhar@comet-20-71 ~]$ squeue -u $USER
       JOBID PARTITION NAME
                                   USER ST
                                                TIME NODES NODELIST(REASON)
     15580587 compute localscr mahidhar R
                                               0:11
                                                      1 comet-20-71
[mahidhar@comet-20-71 ~]$ cd /scratch/mahidhar/15580587/
[mahidhar@comet-20-71 15580587]$ Is -It
total 9173887
-rw-r--r-- 1 mahidhar use300 1939865600 Apr 16 23:25 testFile.00000002
-rw-r--r-- 1 mahidhar use300 3865051136 Apr 16 23:25 testFile.00000000
-rw-r--r-- 1 mahidhar use300 2490368000 Apr 16 23:25 testFile.00000001
-rw-r--r-- 1 mahidhar use300 2777677824 Apr 16 23:25 testFile.00000003
-rw-r--r-- 1 mahidhar use300 1088 Apr 16 23:25 IOR.out.15580587
-rwxr-xr-x 1 mahidhar use300 346872 Apr 16 23:25 IOR.exe
```

- Performance from single node (in log file copied back):
 - Max Write: 606.49 MiB/sec (635.95 MB/sec)
 - Max Read: 19028.71 MiB/sec (19953.05 MB/sec)



Multi-node SSD example

\$HOME/UCSB2018/LOCALSCRATCH2

```
#!/bin/bash
                                                                #List files on both nodes
#SBATCH --job-name="localscratch2"
                                                                 for (( nn=1; nn<=$SLURM_NNODES; nn++ ))</pre>
#SBATCH --output="localscratch2.%j.%N.out"
                                                                 do
#SBATCH --partition=compute
                                                                    p="`sed -n ${nn}p nodes.unq.list`"
#SBATCH --nodes=2
                                                                    echo "Files on $p"
#SBATCH --ntasks-per-node=24
                                                                    ssh $p /bin/ls /coretch/fucco/fclurm JOBID
#SBATCH --export=ALL
                                                                 done
#SBATCH -t 00:10:00
#Get a list of hosts
                                                                 #Tar back the results from each node
export SLURM NODEFILE=`generate pbs nodefile`
                                                                 for (( nn=1; nn<=$SLURM_NNODES; nn++ ))</pre>
cat $SLURM_NODEFILE > nodes.list.$SLURM_JOBID
uniq nodes.list.$SLURM_JOBID > nodes.unq.list
                                                                    p="`sed -n ${nn}p nodes.ung.list`"
                                                                    echo "Tar files on $p"
#Change to local scratch (SSD) and run IOR benchmark
                                                                    ssh $p /bin/tar -cvf $SLURM_SUBMIT_DIR/node$nn.tar /scr/tch/$US
cd /scratch/$USER/$SLURM_JOBID
                                                                 ER/$SLURM_JOBID
#Run IO benchmark
                                                                 done
ibrun -np 48 $SLURM_SUBMIT_DIR/IOR.exe -F -t 1m -b 4m -v -v -w
                                                                 rm nodes.
#Change back to submit dir
                                                                 rm nodes.list.$SLURM_JUBIL
cd $SLURM_SUBMIT_DIR
```



Intel Math Kernel Libraries (MKL)

Installed on Comet as part of the Intel compiler distributions.

 Covers BLAS, LAPACK, FFT, BLACS, and SCALAPACK libraries.

Most useful link for MKL: The Intel link advisor:

https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

Intel MKL Example

- cd /share/apps/examples/UCSB2018/MKL
- The compile line is available in the compile.txt file:

mpicc -o pdpttr.exe pdpttr.c -I\$MKL_ROOT/include \${MKL_ROOT}/lib/intel64/libmkl _scalapack_lp64.a -WI,--start-group \${MKL_ROOT}/lib/intel64/libmkl_intel_lp64.a \${MKL_ROOT}/lib/intel64/libmkl_sequential. a -WI,--end-group \${MKL_ROOT}/lib/intel64/libmkl_blacs_intelmpi_lp64.a -lpthread -lm

Submit script: scalapack.sb



Comet GPU Nodes

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

- [1] CUDA code compile and run example
- [2] Hands On Examples using Singularity to enable Tensorflow



Compiling CUDA Example

Load the CUDA module:

module load cuda

Compile the code:

cd /home/\$USER/UCSB2018/CUDA

nvcc -o matmul -I. matrixMul.cu

Submit the job:

sbatch cuda.sb

CUDA Example: Batch Submission Script

```
#!/bin/bash
#SBATCH --job-name="CUDA"
#SBATCH --output="CUDA.%j.%N.out"
#SBATCH --partition=gpu-shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=6
#SBATCH --gres=gpu:1
#SBATCH -t 01:00:00
#Load the cuda module
module load cuda
#Run the job
./matmul
```



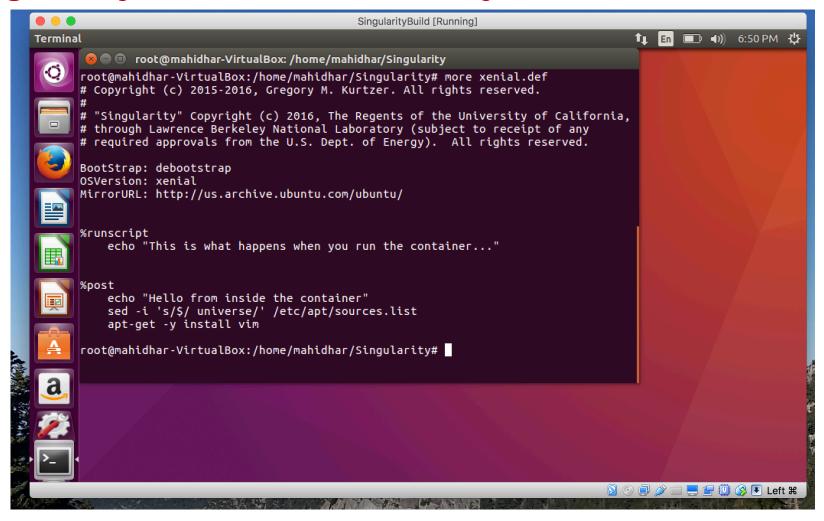
Singularity: Provides Flexibility for OS Environment

- 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, Torch, Fenics, and custom user applications.
- Docker images can be imported into Singularity.

36



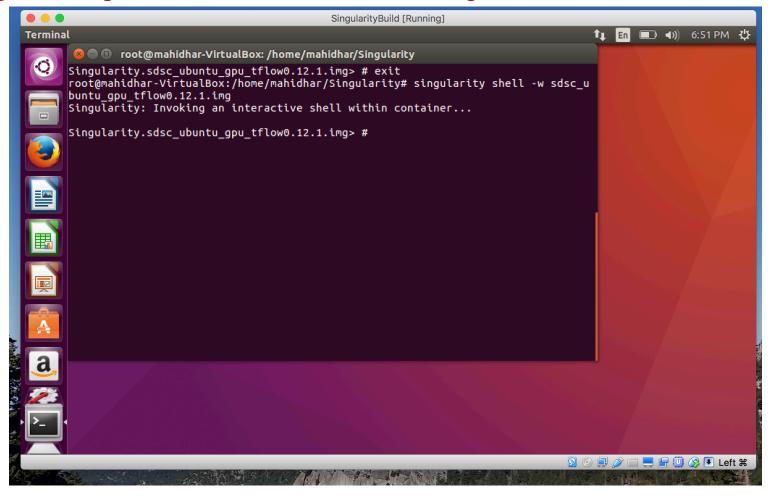
Singularity: Provides Flexibility for OS Environment



 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.



Singularity Image Sources

- SDSC staff have some useful images in:
 - /share/apps/compute/singularity
 - /share/apps/gpu/singularity
- Users can build their own images on their laptops/desktops/cloud - as long as you have singularity installed and have root access on your own machine (or VM or cloud instance)
- Pull an image from Singularity Hub
- Import a docker image
- Comet specific documentation available at:
 - http://www.sdsc.edu/support/user_guides/tutorials/about_comet_sing ularity_containers.html

39



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/UCSB2018/TensorFlow

Submit the job:

sbatch 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 can be directly accessed using a ssh client.
- Always run via the batch scheduler for both interactive and batch jobs. Do not run on the login nodes.
- Choose your filesystem wisely Lustre parallel filesystem for large block I/O. SSD based filesystems for small block I/O, lots of small files. Do not use home filesystem for intensive I/O of any kind.
- Comet can handle MPI, OpenMP, Pthreads, Hybrid, CUDA, and OpenACC jobs. See /share/apps/examples for details!