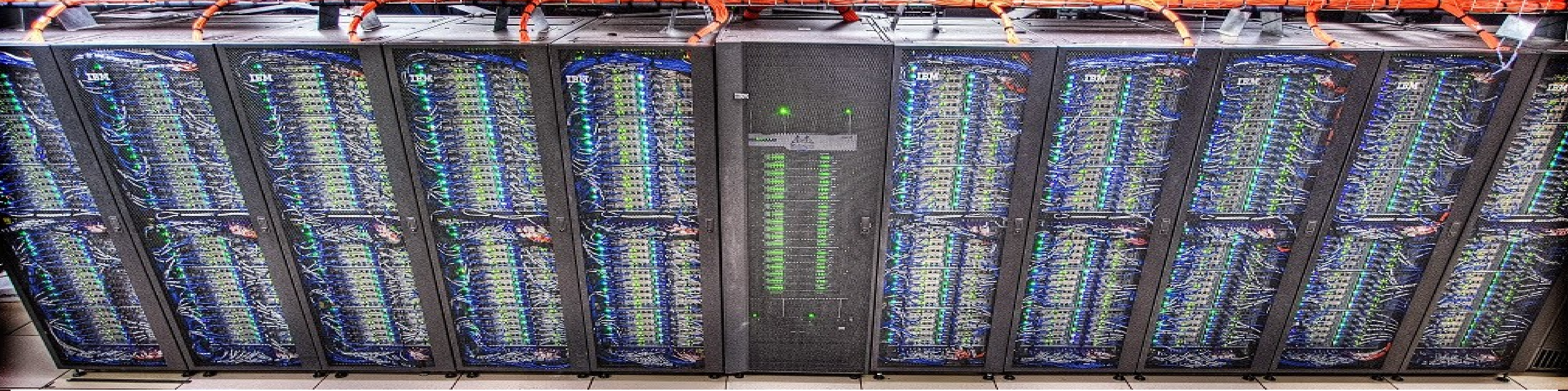

Introduction to Using the Ada Cluster

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HIGH PERFORMANCE RESEARCH COMPUTING
TEXAS A&M UNIVERSITY

HPRC Short Course – Spring 2017

Outline

- Usage Policies
- Hardware Overview of Ada
- Accessing Ada
- File Transfers
- File systems and User Directories
- Computing Environment
- Development Environment
- Batch Processing
- Common Problems
- Need Help?

If we have time, (in backup slides)

- Brief Introduction to Parallel Computing
- Compiling Programs on Ada
- Remote Visualization

Introduction

- Prerequisites:
  - Basic knowledge of UNIX/Linux
  - Slides from our UNIX/Linux short course are at:

    https://hprc.tamu.edu/wiki/index.php/HPRC:SC:Unix
- Examples:
  - Available in /scratch/training/Intro-to-ada directory
  - Copy these files to your scratch directory!!!

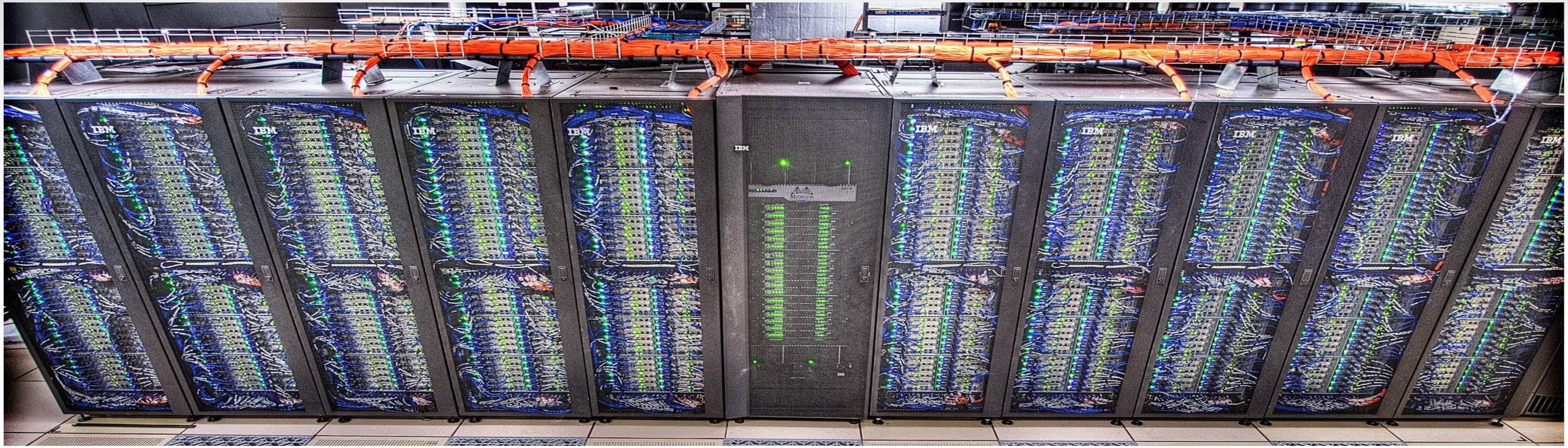
```
cp -r /scratch/training/Intro-to-ada $SCRATCH/
```

Usage Policies
(Be a good compute citizen)

- It is illegal to share computer passwords and accounts by state law and university regulation
- It is prohibited to use Ada in any manner that violates the United States export control laws and regulations, EAR & ITAR
- Abide by the expressed or implied restrictions in using commercial software

https://hprc.tamu.edu/wiki/index.php/Ada:Policies

Ada – an x86 Cluster

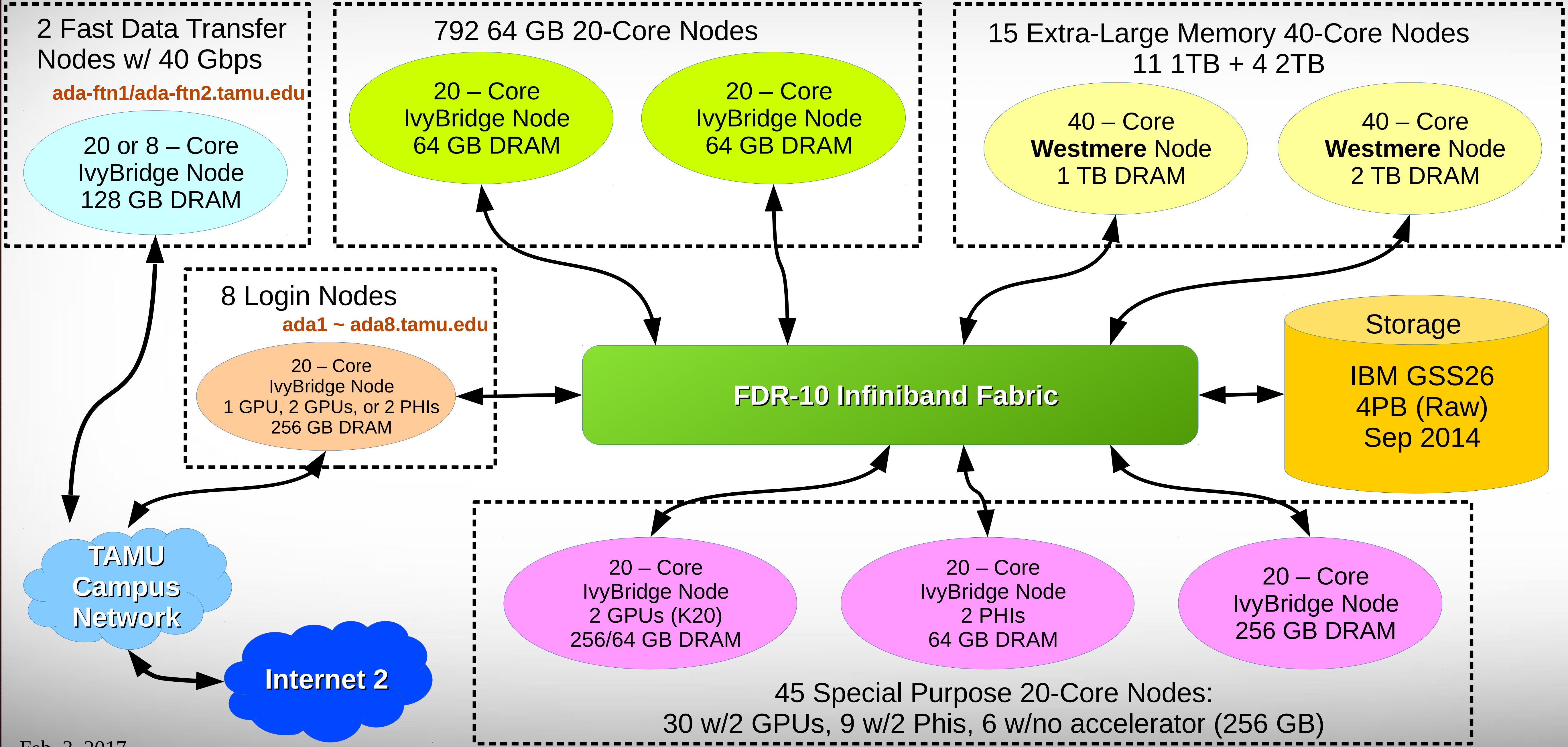


A 17,500-core, 860-node cluster with:

- **837** 20-core compute nodes with two Intel 10-core 2.5GHz *IvyBridge* processors.
  - Among these nodes, 30 nodes have 2 GPUs (*K20*) each and 9 nodes have 2 *Phi* coprocessors.
- **15** compute nodes are 1TB and 2TB memory, 4-processor SMPs with the Intel 10-core 2.26GHz Westmere processor.
- **8** 20-core login nodes with two Intel 10-core 2.5GHz *IvyBridge* processors and 1 GPU, 2 GPUs, or 2 *Phi* coprocessors
- Nodes are interconnected with FDR-10 InfiniBand fabric in a two-level (core switch shown above in middle rack and leaf switches in each compute rack) fat-tree topology.

https://hprc.tamu.edu/wiki/index.php/Ada:Intro

Ada Schematic: 17,500-core 860-node Cluster


2 Fast Data Transfer Nodes w/ 40 Gbps
ada-ftn1/ada-ftn2.tamu.edu
20 or 8 – Core IvyBridge Node 128 GB DRAM
792 64 GB 20-Core Nodes
20 – Core IvyBridge Node 64 GB DRAM
20 – Core IvyBridge Node 64 GB DRAM
15 Extra-Large Memory 40-Core Nodes 11 1TB + 4 2TB
40 – Core Westmere Node 1 TB DRAM
40 – Core Westmere Node 2 TB DRAM
8 Login Nodes
ada1 ~ ada8.tamu.edu
20 – Core IvyBridge Node 1 GPU, 2 GPUs, or 2 PHIs 256 GB DRAM
FDR-10 Infiniband Fabric
Storage
IBM GSS26 4PB (Raw) Sep 2014
TAMU Campus Network
Internet 2
20 – Core IvyBridge Node 2 GPUs (K20) 256/64 GB DRAM
20 – Core IvyBridge Node 2 PHIs 64 GB DRAM
20 – Core IvyBridge Node 256 GB DRAM
45 Special Purpose 20-Core Nodes:
30 w/2 GPUs, 9 w/2 Phis, 6 w/no accelerator (256 GB)

Accessing Ada

- SSH is required for accessing Ada:
  - On campus: ***`ssh NetID@ada.tamu.edu`***
  - Off campus:
    - Set up VPN: u.tamu.edu/VPnetwork
    - Then: ***`ssh NetID@ada.tamu.edu`***
- SSH programs for Windows:
  - MobaXTerm (preferred, includes SSH and X11)
  - PuTTY SSH
- Ada has 8 login nodes. Check the bash prompt.

```
NetID@ada1 ~]$
```

- Login sessions that are idle for *60* minutes will be closed automatically
- Processes run longer than *60* minutes on login nodes will be killed automatically.
- **Do not use more than 8 cores on the login nodes!**
- **Do not use the sudo command**. Contact us if you need assistance installing software.

https://hprc.tamu.edu/wiki/index.php/HPRC:Access

File Transfers with Ada

- Simple File Transfers:
  - scp: command line   (Linux, MacOS)
  - rsync: command line (Linux, MacOS)
  - MobaXterm: GUI (Windows)
  - WinSCP: GUI (Windows)
  - FileZilla: GUI (Windows, MacOS, Linux)
- Bulk data transfers:
  - Use fast transfer nodes (FTN; ada-ftn1/ada-ftn2) with:
    - Globus Connect (https://hprc.tamu.edu/wiki/index.php/SW:GlobusConnect)
    - GridFTP

https://hprc.tamu.edu/wiki/index.php/Ada:Filesystems_and_Files#Transfering_Files

File Systems and User Directories

Directory	Environment Variable	Space Limit	File Limit	Intended Use
/home/$USER	$HOME	10 GB	10,000	Small to modest amounts of processing.
/scratch/user/$USER	$SCRATCH	1 TB	50,000	Temporary storage of large files for on-going computations. Not intended to be a long-term storage area.
/tiered/user/$USER	$ARCHIVE	10 TB	50,000	Intended to hold valuable data files that are not frequently used

- View usage and quota limits: the ***`showquota`*** command
- Also, only home directories are backed up daily.
- Quota and file limit increases will only be considered for scratch and tiered directories
- Do not share your home/scratch/tiered directories. Request a group directory for sharing files.

https://hprc.tamu.edu/wiki/index.php/Ada:Filesystems_and_Files

Computing Environment

Try "`echo $PATH`"

- Paths:
  - $PATH: for commands (eg. /bin:/usr/bin:/usr/local/sbin:/usr/sbin:/home/netid/bin)
  - $LD_LIBRARY_PATH: for libraries
- Many applications, many versions, and many paths
  .... How do you manage all these software?!
- The solution: ***module*** (lmod)
  - Each version of an application, library, etc. is available as a module.
  - Module names have the format of package_name/version.

https://hprc.tamu.edu/wiki/index.php/Ada:Computing_Environment#Modules

Application Modules

- Installed applications are available as modules which are available to all users *(except for restricted modules)*
- **`module`** commands

```
– module avail                            #show all available modules
– module spider tool_name                 #search all modules
– module key genomics                     #search with keyword
– module load tool_name                   #load a specific module
– module list                             #list loaded modules
– module purge                            #unload all loaded modules
– module load Stacks                      #load the default version of a tool
– module load Stacks/1.37-intel-2015B     #load a specific version (recommended way)
```

- It's a good habit to purge unused modules before loading new modules.
- **Avoid loading modules in *.bashrc***

Software

- Search module first:
  - ***module avail***
  - ***module spider software_name***
- Check Software wiki page (https://hprc.tamu.edu/wiki/index.php/SW) for instructions and examples
- License-restricted software: contact license owner for approval
- Contact us for software installation help/request

Development Environment - Toolchains

- Intel toolchain (eg. software stack) is recommended, which includes:
  - Intel C/C++/Fortran compilers
  - Intel Math Kernel Library
  - Intel MPI library
- Intel toolchain modules are named intel/version
- To load/use the current recommended Intel toolchain module (as Jan 2017):

```
module load intel/2015B
```

- For applications which must use gcc/g++, run `module spider GCC` to find available versions.

Modules and Toolchains

- Use the same toolchains in your job scripts
  - The **`intel-2015B`** is the recommended toolchain

```
module load Bowtie2/2.2.6-intel-2015B
module load TopHat/2.1.0-intel-2015B
module load Cufflinks/2.2.1-intel-2015B
```

- Avoid mixing tool chains if loading multiple modules in the same job script:

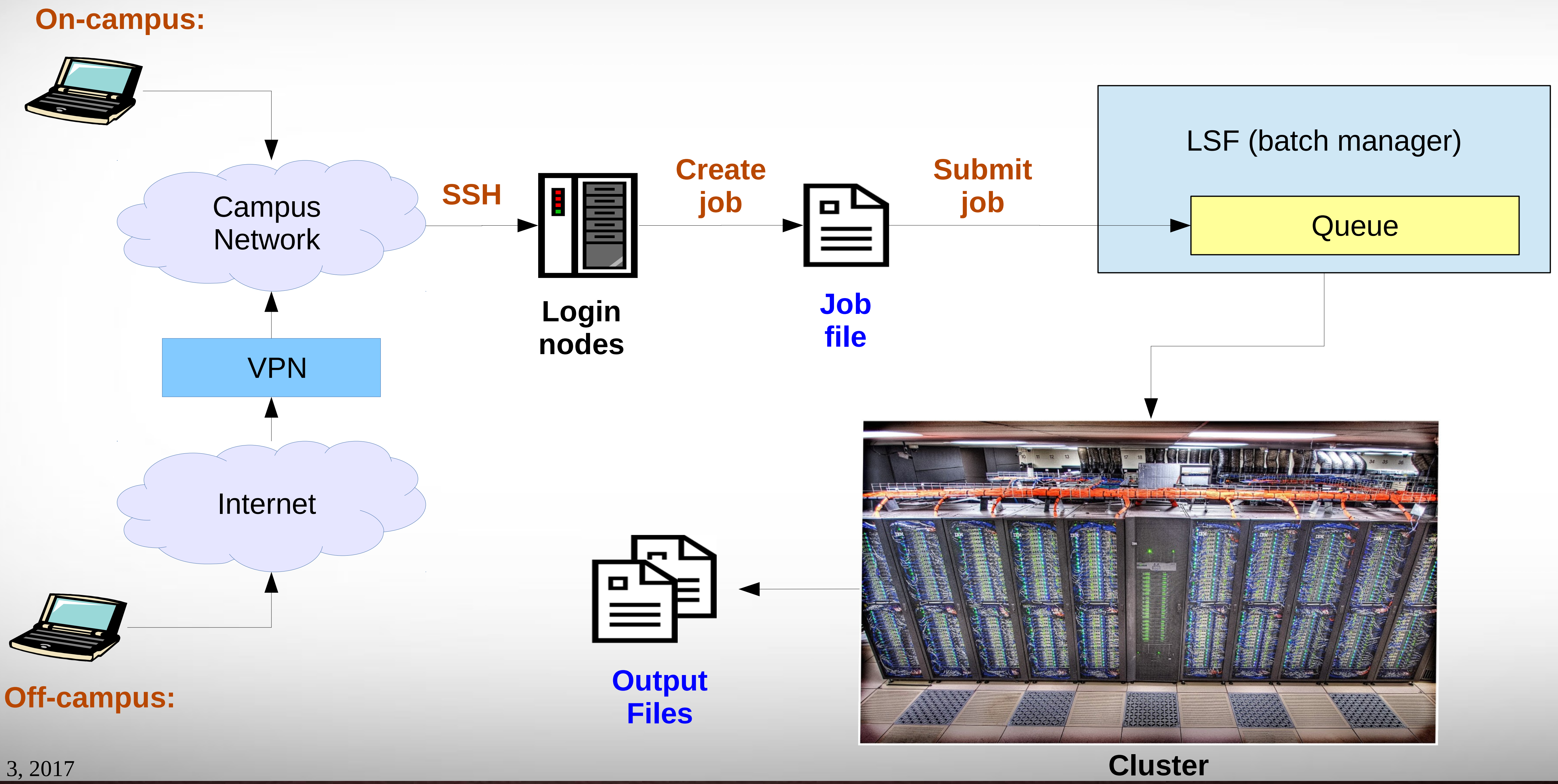
```
module load Bowtie2/2.2.2-ictce-6.3.5
module load TopHat/2.0.14-goolf-1.7.20
module load Cufflinks/2.2.1-intel-2015B
```

- Same rule applies to compilers and libraries.

Development Environment: Compilers

- The commands to invoke each compiler are:
  - ***`icc`*** for C
  - ***`icpc`*** for C++
  - ***`ifort`*** for Fortran
- Man pages (documentation) are available for each compiler:
  - ***`man icc`***
- Help for compiler options also available with *-help* option.
  - Also organized by categories (see ***`icc -help help`*** for more information).

Batch Computing on Ada



Batch Queues

- Job submissions are assigned to batch queues based on the resources requested (number of cores/nodes and wall-clock limit)
- Some jobs can be directly submitted to a queue:
  - If the 1TB or 2TB nodes are needed, use the xlarge queue (via ***`#BSUB -q xlarge`***)
  - Jobs that have special resource requirements are scheduled in the special queue (must request access to use this queue)
- Batch queue policies are used to manage the workload and may be adjusted periodically.

Current Queues

$ bqueues

```
QUEUE_NAME      PRIO STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN  SUSP
staff           450  Open:Active       -    -    -    -     0     0     0     0
special         400  Open:Active       -    -    -    -  2124     0  2124     0
xlarge          100  Open:Active       -    -    -    -   240   160    80     0
vnc              90  Open:Active       -    -    -    -     4     0     4     0
sn_short         80  Open:Active       -    -    -    -    20     0    20     0
mn_short         80  Open:Active    2000    -    -    -     0     0     0     0
mn_large         80  Open:Active    5000    -    -    -     0     0     0     0
general          50  Closed:Inact      0    -    -    -     0     0     0     0
sn_regular       50  Open:Active       -    -    -    -  1224   108  1116     0
sn_long          50  Open:Active       -    -    -    -  3599   290  3309     0
sn_xlong         50  Open:Active       -    -    -    -    56    10    46     0
mn_small         50  Open:Active    6000    -    -    -  5369  1320  4049     0
mn_medium        50  Open:Active    6000    -    -    -  6160  1240  4920     0
curie_devel      40  Open:Active      32   32    -    -     0     0     0     0
curie_medium     35  Open:Active     512  192    -    -  1328  1136   192     0
curie_long       30  Open:Active     192   64    -    -  2448  2256   192     0
curie_general    25  Closed:Inact      0    -    -    -     0     0     0     0
preempt_medium   10  Open:Active       -    -    -    -     0     0     0     0
low_priority      1  Open:Active    2500  500    -    -     0     0     0     0
preempt_low       1  Open:Active      40    -    -    -     0     0     0     0
```

https://hprc.tamu.edu/wiki/index.php/Ada:Batch_Queues

Queue Limits

Queue	Min/Default/ Max Cores	Default/Max Walltime	Compute Node Types	Pre-Queue Limits	Aggregate Limits Across Queues	Per-User Limits Across Queues	Notes
sn_short	1 / 1 / 20	10 min / **1 hr**	64 GB nodes (811) 256 GB nodes (26)		Maximum of **6000** cores for all running jobs in the single-node (sn_*) queues.	Maximum of **1000 cores and 50 jobs per user** for all running jobs in the single node (sn_*) queues.	For jobs needing **only one compute node**.
sn_regular		1 hr / **1 day**					
sn_long		24 hr / **4 days**					
sn_xlong		4 days / **7 days**					
mn_short	2 / 2 / 200	10 min / **1 hr**		Maximum of **2000** cores for all running jobs in this queue.	Maximum of **12000** cores for all running jobs in the multi-node (mn_*) queues.	Maximum of **3000 cores and 150 jobs per user** for all running jobs in the multi-node (mn_*) queues.	For jobs needing **more than one compute node**.
mn_small	2 / 2 / 120	1 hr / **7 days**		Maximum of **6000** cores for all running jobs in this queue.			
mn_medium	121 / 121 / 600	1 hr / **7 days**		Maximum of **6000** cores for all running jobs in this queue.			
mn_large	600 / 601 / 2000	1 hr / **5 days**		Maximum of **5000** cores for all running jobs in this queue.			
xlarge	1 / 1 / 280	1 hr / **10 days**	1 TB nodes (11) 2 TB nodes (4)				For jobs needing **more than 256GB of memory per compute node**.
vnc	1 / 1 / 20	1 hr / **6 hr**	GPU nodes (30)				For remote visualization jobs.
special	None	1 hr / **7 days**	64 GB nodes (811) 256 GB nodes (26)				Requires permission to access this queue.

Run ***"blimits -w"*** to show how policies are applied to users and queues.

https://hprc.tamu.edu/wiki/index.php/Ada:Batch_Queues

Consumable Computing Resources

- Resources specified in a job file:
  - Processor cores
  - Memory
  - Wall time
  - GPU
- Service Unit (SU) - Billing Account
- Other resources:
  - Software license/token
    - Use "**`license_status`**" to query

      https://hprc.tamu.edu/wiki/index.php/SW:License_Checker

Find available license for "ansys":

```
$ license_status -s ansys
```

```
License status for ANSYS:
-------------------------------------------------------------------
|License Name                    |  # Issued|  # In Use|# Available|
-------------------------------------------------------------------
|aa_mcad                         |        50|         0|         50|
|aa_r                            |        50|        32|         18|
|aim_mp1                         |        50|         0|         50|
|    ......                                                       |
-------------------------------------------------------------------
```

Find detail options:

```
$ license_status -h
```

Sample Job Script (structure)

```
#BSUB -L /bin/bash
#BSUB -J blastx
#BSUB -n 2
#BSUB -R "span[ptile=2]"
#BSUB -R "rusage[mem=1000]"
#BSUB -M 1000
#BSUB -W 2:00
#BSUB -o stdout.%J
#BSUB -e stderr.%J
```

These parameters are read by the job scheduler

Load the required module(s) first

```
module load BLAST+/2.2.31-intel-2015B-Python-3.4.3
```

Add a comment to the output

```
echo "BLAST manual: http://www.ncbi.nlm.nih.gov/books/NBK279690/"
```

This is a single line comment and not run as part of the script

```
#blastx: search protein databases using a translated nucleotide query

blastx -query mrna_seqs_nt.fasta -db /scratch/datasets/blast/nr \
-outfmt 10 -out mrna_seqs_nt_blastout.csv
```

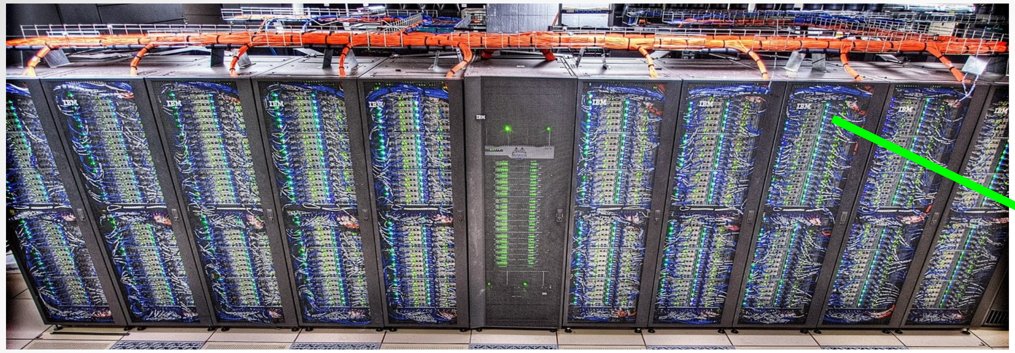
This is the command to run the application

This means the command is continued on the next line;
The space before the \ is required. Do not put a space after the \

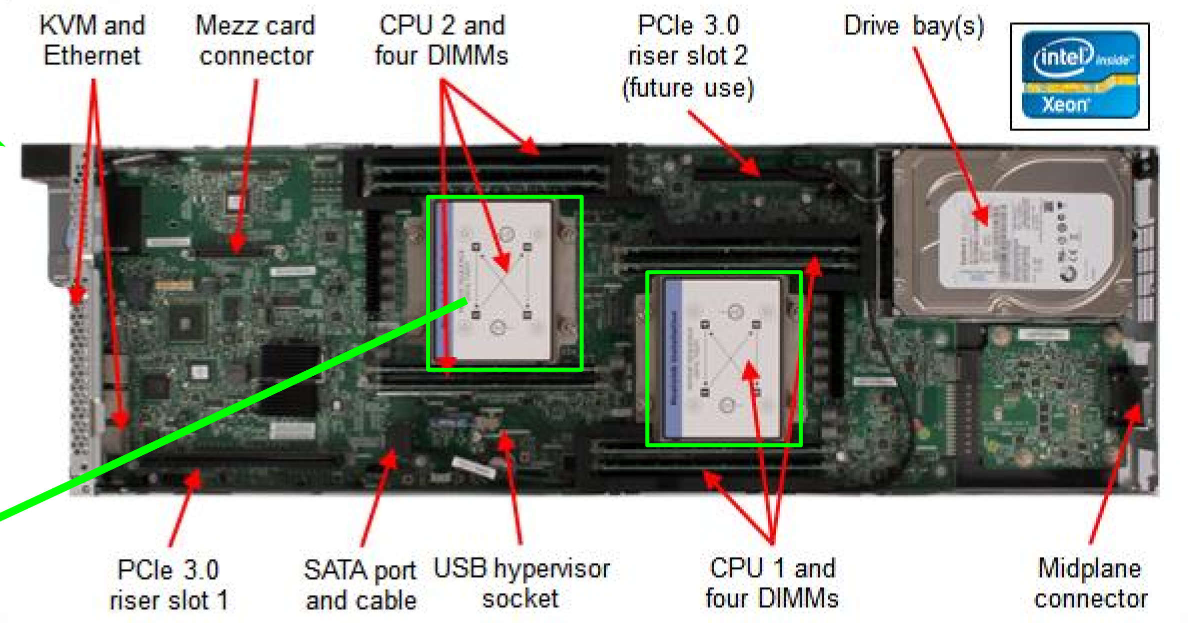
Important Job Parameters

```
#BSUB -n NNN

      # NNN: total number of cores or job slots to allocate for the job

#BSUB -R "span[ptile=XX]"

      # XX:  number of cores or job slots per node to use

#BSUB -R "rusage[mem=nnn]"

      # reserves nnn MBs per core or job slot for the job

#BSUB -M nnn

      # enforces (XX cores * nnn MB) as memory limit

      # per node for the job

#BSUB -W hh:mm or mm

      # sets job's runtime wall-clock limit in hours:minutes or just minutes
```

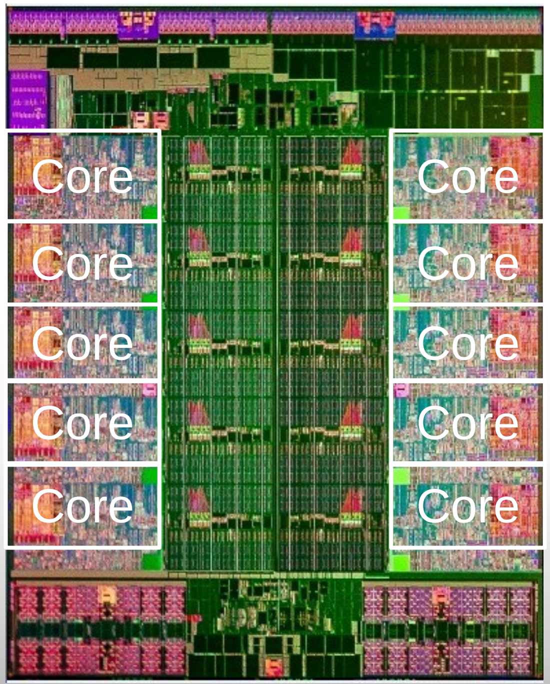
Node / Socket / Core



Part of Ada cluster.
Each blue light is a node.

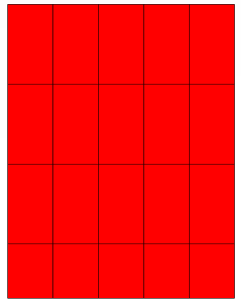


Each node has 2 sockets.



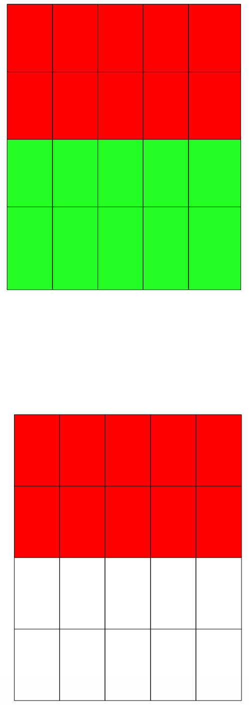
Each socket/CPU has 10 processor cores.
So, each node has 20 processor cores.

Processor Cores Mapping



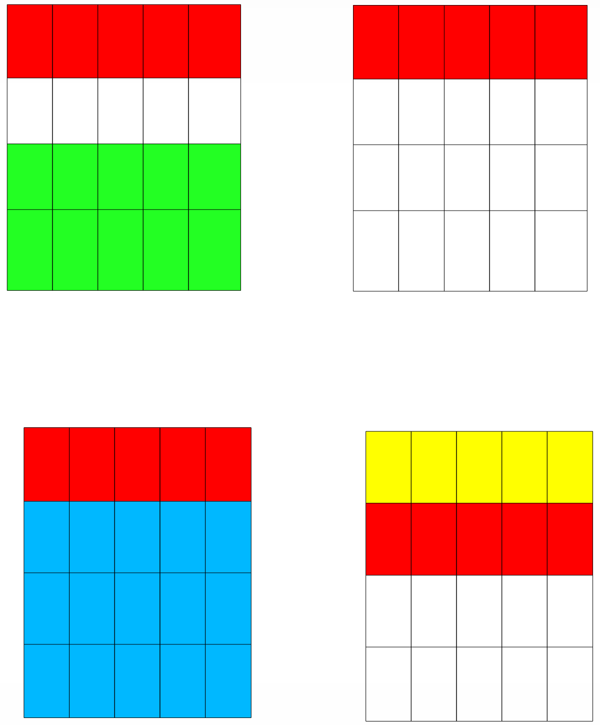
20 cores
on 1 node

#BSUB -n 20
#BSUB -R “span[ptile=20]



20 cores on 2 nodes

#BSUB -n 20
#BSUB -R “span[ptile=10]



20 cores on 4 nodes

#BSUB -n 20
#BSUB -R “span[ptile=5]

Job Resource Examples (node vs memory)

#BSUB -n 10 -R “span[ptile=2]”

#BSUB -R “rusage[mem=500]” -M 500 ...

Requests 10 job slots (2 per node). The job will span 5 nodes. The job can use up to 1000 MB per node.

#BSUB -n 80 -R “span[ptile=20]”

#BSUB -R “rusage[mem=2500]” -M 2500

Request 4 whole nodes (80/20), not including the xlarge memory nodes. The job can use up to 50GB per node.

Job Memory Requests

- Must specify both parameters for requesting memory:

  *#BSUB **-R** "rusage[mem=process_alloc_size]"*

  *#BSUB **-M** process_size_limit*

- Default value of 2.5 GB per job slot if -R/-M not specified, but it might cause memory contention when sharing a node with other jobs.
- On 64GB nodes, usable memory is at most **54 GB** (where 10 GB is used by the system). The per-process memory limit should not exceed **2700 MB** for a 20-core job.
- If more memory is needed, request the large memory nodes:
  - If under 256 GB and up to 20 cores per node: use -R "rusage[mem=12300]" or -R “select[mem256gb]”
  - If need up to 1 or 2 TB of memory or up to 40 cores:
    - use -R “select[mem1tb]” (40 cores) or -R “select[mem2tb]” with the -q xlarge option
    - The mem1tb and mem2tb nodes are accessible only via the *xlarge* queue.

Job Parameters Example
For Job Scripts on xlarge queue

```
#BSUB -L /bin/bash                   # use the bash login shell
#BSUB -J stacks_S2                   # job name
#BSUB -n 40                          # assigns 40 cores for execution
#BSUB -R "span[ptile=40]"            # assigns 40 cores per node
#BSUB -q xlarge                      # required if using mem1tb or mem2tb
#BSUB -R "rusage[mem=25000]"         # reserves 25GB memory per core
#BSUB -M 25000                       # sets to 25GB process limit
#BSUB -W 48:00                       # sets to 48 hours the job's limit
#BSUB -o stdout.%J                   # job standard output to stdout.jobid
#BSUB -e stderr.%J                   # job standard error to stderr.jobid
```

Specified xlarge queue to use 1TB or 2TB memory nodes

Job File (Serial Example)

```
##NECESSARY JOB SPECIFICATIONS
#BSUB -J ExampleJob1              #Set the job name to "ExampleJob1"
#BSUB -L /bin/bash                #Uses the bash login shell to initialize the job's execution environment.
#BSUB -W 2:00                     #Set the wall clock limit to 2hr
#BSUB -n 1                        #Request 1 core
#BSUB -R "span[ptile=1]"          #Request 1 core per node.
#BSUB -R "rusage[mem=5000]"       #Request 5000MB per process (CPU) for the job
#BSUB -M 5000                     #Set the per process enforceable memory limit to 5000MB.
#BSUB -o Example1Out.%J           #Send stdout and stderr to "Example1Out.[jobID]"
##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                   #Set billing account to 123456
#BSUB -u email_address            #Send all emails to email_address
#BSUB -B -N                       #Send email on job begin (-B) and end (-N)
#First Executable Line
module load intel/2015B           # loads the Intel software tool chain
prog.exe < input1 >& data_out1    # both input1 and data_out1 reside in the job submission dir
```

https://hprc.tamu.edu/wiki/index.php/Ada:Batch#Job_File_Examples

Job File (multi core, single node)

```
##NECESSARY JOB SPECIFICATIONS
#BSUB -J ExampleJob2              #Set the job name to "ExampleJob2"
#BSUB -L /bin/bash                #Uses the bash login shell to initialize the job's execution environment.
#BSUB -W 6:30                     #Set the wall clock limit to 6hr and 30min
#BSUB -n 10                       #Request 10 cores
#BSUB -R "span[ptile=10]"         #Request 10 cores per node.
#BSUB -R "rusage[mem=2560]"       #Request 2560MB per process (CPU) for the job
#BSUB -M 2560                     #Set the per process enforceable memory limit to 2560MB.
#BSUB -o Example2Out.%J           #Send stdout and stderr to "Example2Out.[jobID]"
##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                   #Set billing account to 123456
#BSUB -u email_address            #Send all emails to email_address
#BSUB -B -N                       #Send email on job begin (-B) and end (-N)
#First Executable Line
module load intel/2015B           # load intel module
./my_multicore_prog.exe           # run your program
```

https://hprc.tamu.edu/wiki/index.php/Ada:Batch#Job_File_Examples

Job File (multi core, multi node)

```
##NECESSARY JOB SPECIFICATIONS
#BSUB -J ExampleJob3                 #Set the job name to "ExampleJob3"
#BSUB -L /bin/bash                   #Uses the bash login shell to initialize the job's execution environment.
#BSUB -W 24:00                       #Set the wall clock limit to 24hr
#BSUB -n 40                          #Request 40 cores
#BSUB -R "span[ptile=20]"            #Request 20 cores per node.
#BSUB -R "rusage[mem=2560]"          #Request 2560MB per process (CPU) for the job
#BSUB -M 2560                        #Set the per process enforceable memory limit to 2560MB.
#BSUB -o Example3Out.%J              #Send stdout and stderr to "Example3Out.[jobID]"
##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                      #Set billing account to 123456
#BSUB -u email_address               #Send all emails to email_address
#BSUB -B -N                          #Send email on job begin (-B) and end (-N)
#First Executable Line
module load intel/2015B              # load intel module
./my_multicore_multinode_prog.exe    # run your program
```

https://hprc.tamu.edu/wiki/index.php/Ada:Batch#Job_File_Examples

Job File (serial GPU)

```
##NECESSARY JOB SPECIFICATIONS
#BSUB -J ExampleJob4                 #Set the job name to "ExampleJob4"
#BSUB -L /bin/bash                   #Uses the bash login shell to initialize the job's execution environment.
#BSUB -W 2:00                        #Set the wall clock limit to 2hr
#BSUB -n 1                           #Request 1 cores
#BSUB -R "span[ptile=1]"             #Request 1 core per node.
#BSUB -R "rusage[mem=2560]"          #Request 2560MB per process (CPU) for the job
#BSUB -M 2560                        #Set the per process enforceable memory limit to 2560MB.
#BSUB -o Example4Out.%J              #Send stdout and stderr to "Example4Out.[jobID]"
#BSUB -R "select[gpu]"               #Request a node with a GPU
##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                      #Set billing account to 123456
#BSUB -u email_address               #Send all emails to email_address
#BSUB -B -N                          #Send email on job begin (-B) and end (-N)
#First Executable Line
module load CUDA                     # load CUDA module
./my_CUDA_prog.exe                   # run your program
```

https://hprc.tamu.edu/wiki/index.php/Ada:Batch#Job_File_Examples

OpenMP Jobs

- Must set ***OMP_NUM_THREADS*** to take advantage of the requested cores
- All processes run on the same node.
  - Submit to the xlarge queue if you need up to 40 cores per node
- Example job:

```
#BSUB -n 20 -R 'rusage[mem=300] span[ptile=20]' -M 300
#BSUB -J omp_helloWorld
#BSUB -o omp_helloWorld.%J -L /bin/bash -W 1:00
module load intel/2015B
ifort -openmp -o omp_helloWorld.exe omp_helloWorld.f90
export OMP_NUM_THREADS=20
./omp_helloWorld.exe
```

MPI Jobs

- MPI programs may be run in batch jobs on multiple nodes
- Note, the mpiexec -np option must match the number of cores requested by the job (#BSUB -n option).

```
#BSUB -n 12 -R 'rusage[mem=150] span[ptile=4]' -M 150
#BSUB -J mpi_helloWorld -o mpi_helloWorld.%J
#BSUB -L /bin/bash -W 1:00
#
module load intel/2015B
mpiifort -o mpi_helloWorld.exe mpi_helloWorld.f90
mpiexec.hydra -np 12 ./mpi_helloWorld.exe
```

Pop Quiz #1

```
#BSUB -L /bin/bash
#BSUB -J stacks_S2
#BSUB -n 10
#BSUB -R "span[ptile=10]"
#BSUB -R "rusage[mem=2000]"
#BSUB -M 2000
#BSUB -W 36:00
#BSUB -o stdout.%J
#BSUB -e stderr.%J
```

- How much total memory is requested for this job?

- What is the maximum time this job is allowed to run?

Pop Quiz #2

```
#BSUB -L /bin/bash
#BSUB -J stacks_S2
#BSUB -n 80
#BSUB -R "span[ptile=80]"
#BSUB -R "rusage[mem=50000]"
#BSUB -M 50000
#BSUB -W 48:00
#BSUB -o stdout.%J
#BSUB -e stderr.%J
```

- Find two parameters that are either missing or not configured correctly.

Submit the Job and Check Status

- Submit your job to the job scheduler

```
bsub < sample01.job
```

```
Verifying job submission parameters...
Verifying project account...
     Account to charge:   082792010838
         Balance (SUs):      4871.5983
         SUs to charge:         0.0333
Job <2470599> is submitted to default queue <sn_short>.
```

- Summary of the status of your running/pending jobs

```
bjobs
```

```
JOBID   STAT USER       QUEUE    JOB_NAME  NEXEC_HOST SLOTS RUN_TIME     TIME_LEFT
2470599 RUN  tmarkhuang sn_short sample01  1          1     0 second(s)  0:5 L
```

- A more detailed summary of a running job

```
bjobs -l 2470599
```

Try yourself; copy examples: *cp -r /scratch/training/Intro-to-ada $SCRATCH/*

Debug job failures

- Debug job failures using the stdout and stderr files
  - `cat output.ex03.python_mem.2447336`

This job id was created by the parameter in your job script file

`#BSUB -o output.ex03.python_mem.%J`

```
TERM_MEMLIMIT: job killed after reaching LSF memory usage limit.
Exited with signal termination: Killed.

Resource usage summary:

    CPU time :                                     1.42 sec.
    Max Memory :                                   10 MB
    Average Memory :                               6.50 MB
    Total Requested Memory :                       10.00 MB
    Delta Memory :                                 0.00 MB
    Max Processes :                                5
    Max Threads :                                  6
```

Make the necessary adjustments to BSUB parameters in your job script and resubmit the job

Check your Service Unit (SU) Balance

- Show the SU Balance of your Account(s)

```
myproject -l
```

```
================================================================================
                    List of tmarkhuang's Project Accounts
--------------------------------------------------------------------------------
|   Account     | Default | Allocation |Used & Pending SUs|    Balance    |
--------------------------------------------------------------------------------
|082792010838|          N|     50000.00|             -10.38|     49989.62|
--------------------------------------------------------------------------------
```

- Use "**#BSUB -P project_id**" to charge SU to a specific project
- Run "**myproject -d accountNo**" to change default project account
- Run "**myproject -h**" to see more options

https://hprc.tamu.edu/wiki/index.php/HPRC:AMS:Service_Unit
https://hprc.tamu.edu/wiki/index.php/HPRC:AMS:UI

Job submission issue (SU)

```
$ bsub < myjob
Verifying job submission parameters...
Verifying project account...
     Account to charge:   082792010838
         Balance (SUs):       342.5322
         SUs to charge:       480.0000
         -------------------------------------------------------------
         |ERROR! Your project account does not have sufficient balance to submit your job!|
         ----------------------------------------------------------------
Request aborted by esub. Job not submitted.
```

- Insufficient SU
  - Ask PI to transfer SU to you
  - Apply for more SU (if you are eligible, as a PI or permanent researcher)

https://hprc.tamu.edu/wiki/index.php/HPRC:AMS:Service_Unit
https://hprc.tamu.edu/wiki/index.php/HPRC:AMS:UI

Job Submission and Tracking

Command	Description
`bsub < jobfile1`	Submit jobfile1 to batch system
`bjobs [-u all or user_name] [[-l] job_id]`	List jobs
`bpeek [-f] job_id`	View job's output and error files
`bkill job_id`	Kill a job
`bhist [-l] job_id`	Show historical information about a job
`lnu [-l] -j job_id`	Show resource usage for a job
`blimits -w`	Show how policies are applied to users and queues

https://hprc.tamu.edu/wiki/index.php/Ada:Batch#Job_tracking_and_control_commands

Node Utilization: *lnu*

lnu [-h] [-l] -j jobid # lists on stdout the utilization across all nodes for an executing job.

Run "*lnu -h*" to see more options

Examples:

```
$ lnu -l -j 795375
Job            User                      Queue           Status Node  Cpus
795375         jomber23                  medium               R    4    80
   HOST_NAME    status  r15s   r1m  r15m    ut    pg  ls    it   tmp   swp   mem  Assigned Cores
   nxt1417          ok  20.0  21.0  21.0   97%   0.0   0 94976  366M  3.7G 41.6G    20
   nxt1764 (L)      ok  19.7  20.0  20.0   95%   0.0   0 95040  366M  3.7G 41.5G    20
   nxt2111          ok  20.0  20.0  20.0   98%   0.0   0 91712  370M  4.2G 41.5G    20
   nxt2112          ok  20.0  21.1  21.0   97%   0.0   0 91712  370M  4.2G 41.6G    20
==============================================================================================
$ lnu -l -j 753454
Job            User                      Queue           Status Node  Cpus
753454         ajochoa                   long                 R    1    20
   HOST_NAME    status  r15s   r1m  r15m    ut    pg  ls    it   tmp   swp   mem  Assigned Cores
   nxt1222 (L)      ok   4.3   4.5   6.2   20%   0.0   0 54464  422M  4.7G 52.9G    20
==============================================================================================
```

The utilization (**ut**) and memory paging (**pg**), overall, are probably the most significant. Note that the **tmp**, **swp**, and **mem** refer to available amounts respectively. See "*man lsload*" for explanations on labels.

https://hprc.tamu.edu/wiki/index.php/Ada:Batch#Job_tracking_and_control_commands

Job Environment Variables

- ***$LSB_JOBID*** = job id
- ***$LS_SUBCWD*** = directory where job was submitted from
- ***$SCRATCH*** = /scratch/user/NetID
- ***$TMPDIR*** = /work/$LSB_JOBID.tmpdir
  - $TMPDIR is local to each assigned compute node for the job

Concurrent Program Execution in Jobs via Tamulauncher

- Useful for running many programs concurrently across multiple nodes within a job
- Can be used with serial or multi-threaded programs
- Distributes a set of commands from an input file to run on the cores assigned to a job
- Can only be used in batch jobs
- If a tamulauncher job gets killed, you can resubmit the same job to complete the unfinished commands in the input file
- Preferred over LSF job arrays

https://hprc.tamu.edu/wiki/index.php/Ada:Tamulauncher

Common Job Problems

- Control characters (`^M`) in job files or data files edited with Windows editor
  - remove the `^M` characters with: `dos2unix my_job_file`

```
$ file jobfile.txt
jobfile.txt: ASCII text, with CRLF line terminators
$ dos2unix abc.txt
dos2unix: converting file jobfile.txt to UNIX format ...
$ file abc.txt
jobfile.txt: ASCII text
```

- Did not load the required module(s)
- Insufficient walltime specified in #BSUB -W parameter
- Insufficient memory specified in #BSUB -M and -R "rusage[mem=xxx]" parameters
- No matching resource (-R rusage[mem] too large)
- Running OpenMP jobs across nodes
- Insufficient SU: See your SU balance: `myproject -l`
- Insufficient disk or file quotas: check quota with `showquota`
- Using GUI-based software without setting up X11 forwarding
  - Enable X11 forwarding at login `ssh -X user@ada.tamu.edu`
  - Or use VNC
- Software license availability `license_status -a`

FAQ: https://hprc.tamu.edu/wiki/index.php/HPRC:CommonProblems

Need Help?

- Check the FAQ (https://hprc.tamu.edu/wiki/index.php/HPRC:CommonProblems) or the Ada User Guide (https://hprc.tamu.edu/wiki/index.php/Ada) for possible solutions first.
- Email your questions to **help@hprc.tamu.edu**. (Now managed by a ticketing system)
- Help us, help you -- we need more info
  - Which Cluster
  - UserID/NetID (*UIN is not needed!*)
  - Job id(s) if any
  - Location of your jobfile, input/output files
  - Application used if any
  - Module(s) loaded if any
  - Error messages
  - Steps you have taken, so we can reproduce the problem
- Or visit us @ 114A Henderson Hall
  - Making an appointment is recommended.

Upcoming Programming Short Courses

Topics	**Date/Time**
Introduction to Using Ada Cluster (encore)	3-5 PM, Wed, Feb 8
Introduction to Using Terra Cluster	3-5 PM, Fri, Feb 10
Introduction to Python	3-5 PM, Wed, Feb 15
Introduction to Perl	3-5 PM, Wed, Feb 22
Intermediate MATLAB Programming	3-5 PM, Wed, Mar 1
Next Generation Sequencing Data Analysis on the Ada Cluster	3-5 PM, Wed, Mar 22
Introduction to Code Parallelization using OpenMP	3-5 PM, Wed, Mar 29
Introduction to Code Parallelization using MPI	3-5 PM, Wed, Apr 5

- Register or see a full list of short courses at:
  - https://hprc.tamu.edu/register/classlist.php

HIGH PERFORMANCE RESEARCH COMPUTING
TEXAS A&M UNIVERSITY

Thank you.

Any question?

Backup slides

Brief Introduction to Parallel Computing

Parallelism

Parallelism means doing multiple things at the same time: you can get more work done in the same time.

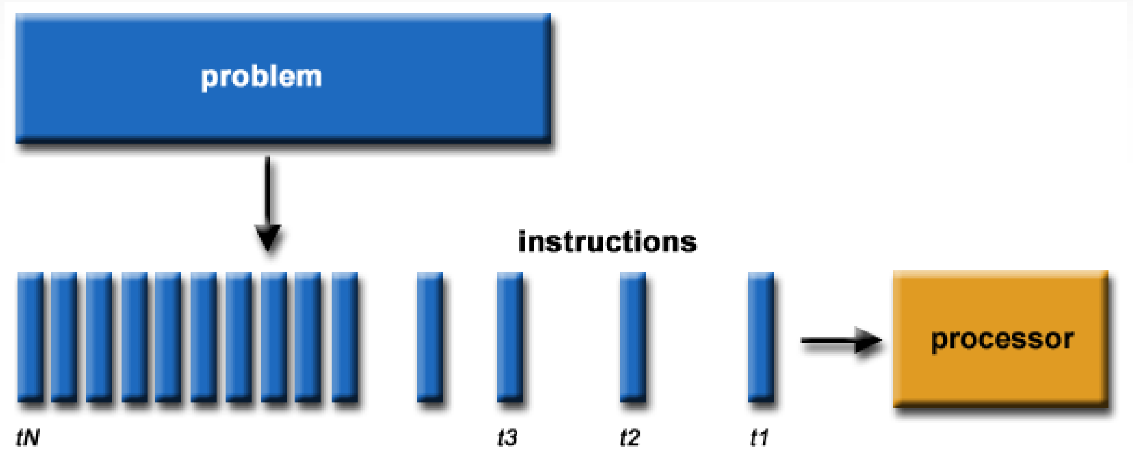
Less fish …

More fish!

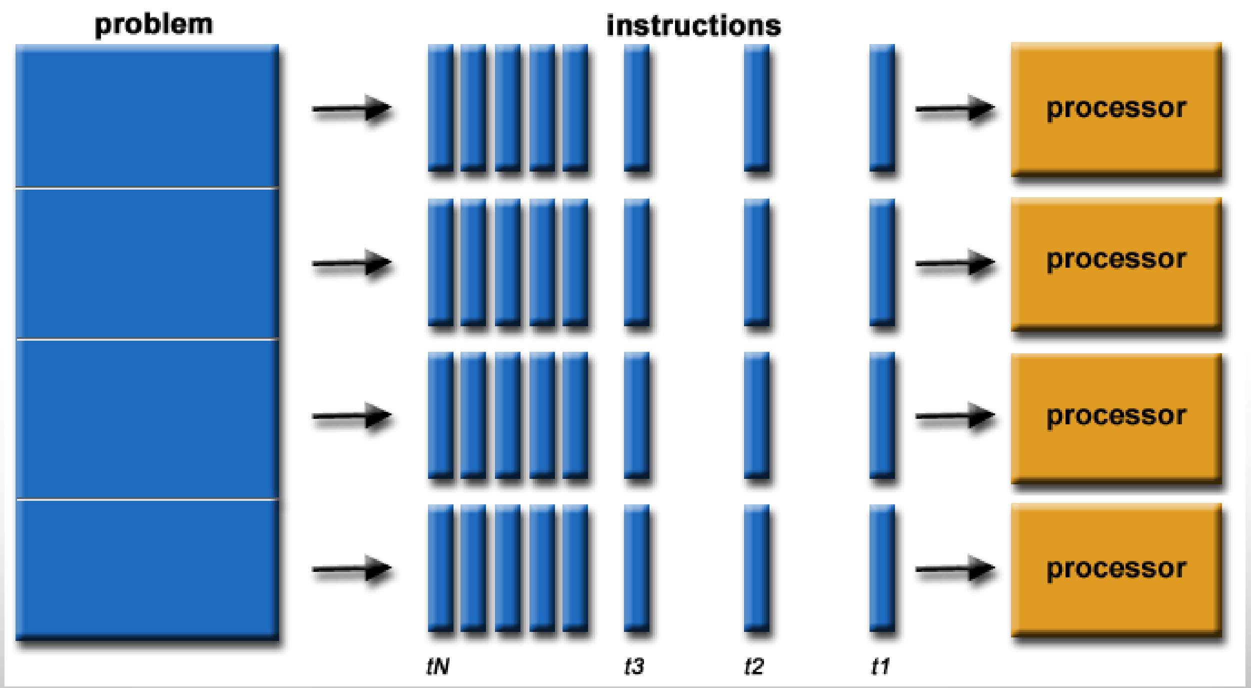
Source: http://oscer.ou.edu/Workshops/Overview/sipe_overview_20090201.ppt

Serial vs Parallel Computing

Serial Computing



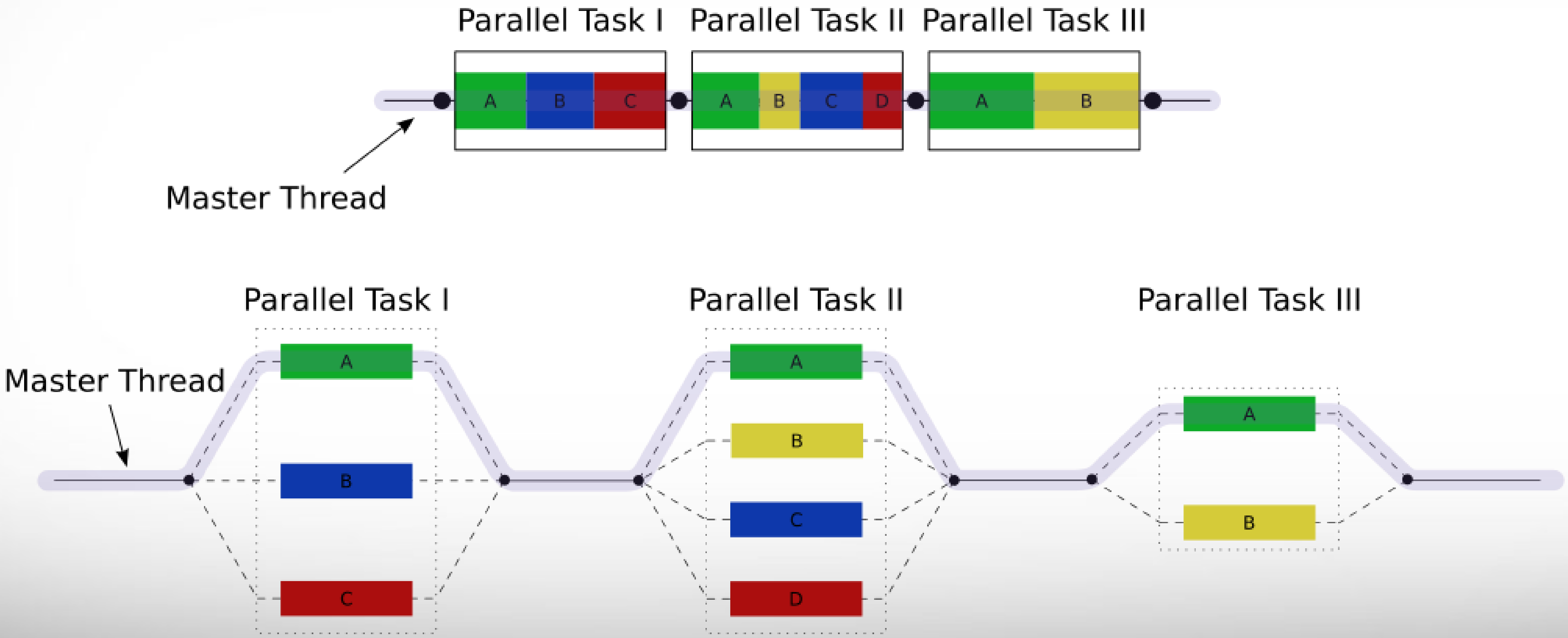
Parallel Computing



Source: https://computing.llnl.gov/tutorials/parallel_comp/

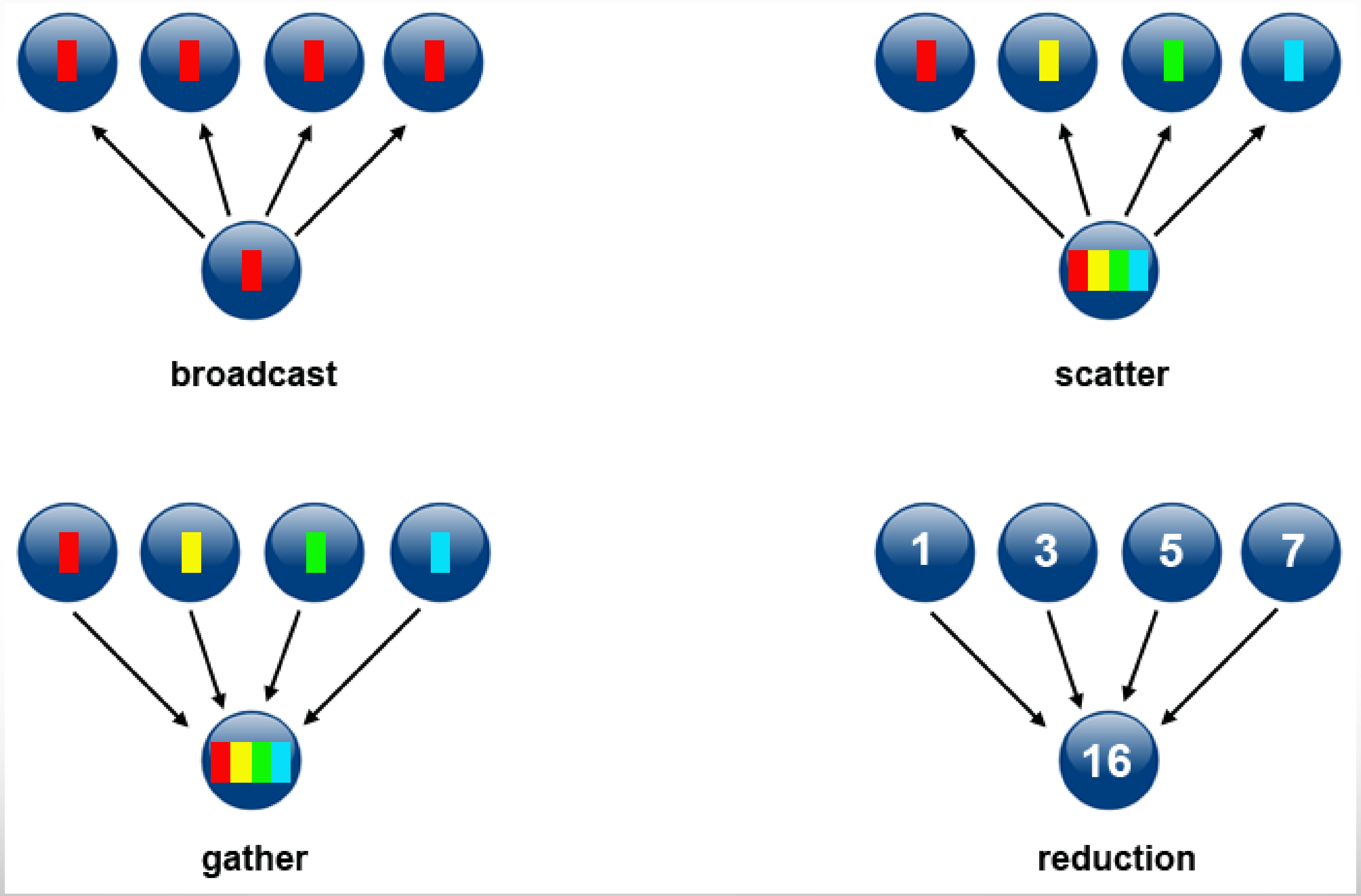
Multi-threading

Some tasks can be split and executed on process cores in a compute node.



Source: https://en.wikipedia.org/wiki/OpenMP

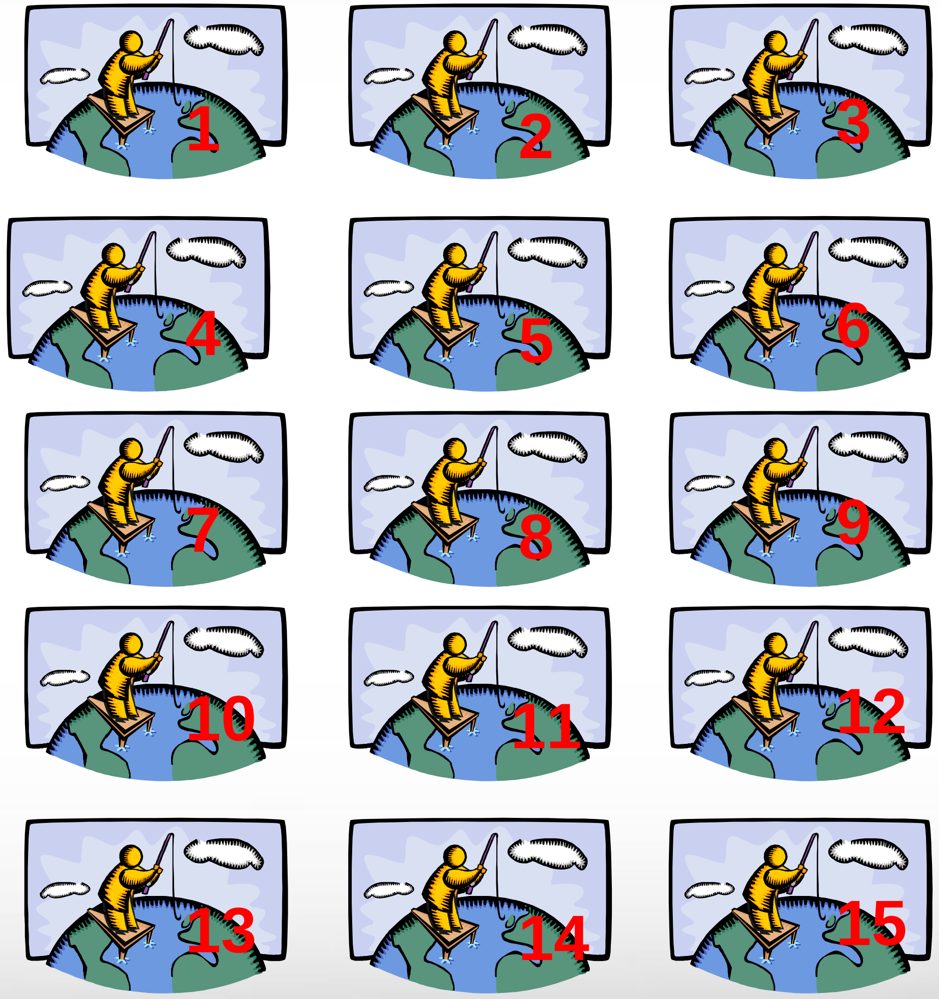
Distributed Computing - Collective Communication



Source: https://computing.llnl.gov/tutorials/mpi/

High Throughput Computing

- Each worker solve a subset of problems
- No dependency/communication among workers
- Parameter sweeping
- Script is your friend
- ***tamulauncher***



Still More fish!

Compiling Programs on Ada

Compiling Basics

- Generally provide the compiler:
  - source file(s) and/or object file(s)
  - compilation option(s)
  - optionally a name for the resulting executable. Default executable name is *a.out* if no name provided.
- Example:

```
icc objfile.o subroutine.c main.c
```

Basic Compiler Flags

Flag	Description
-help [category]	Shows all available compiler options or all options under a specified category
-o <file>	Specifies the name for an object file. For an executable, the -output filename will be <file> instead of a.out
-c	Only compile the source file(s). Linking phase will be skipped.
-L <dir>	Tells the linker to search for libraries in directory <dir> ahead of the standard library directories.
-l<name>	Tells the linker to search for library named lib**name**.so or lib**name**.a

Examples:

```
icc -o mprog.x subroutine.c myobjs.o main.c
icc -L mylibs -lmyutils main.c
```

https://hprc.tamu.edu/wiki/index.php/Ada:Compile:All#Basic_compiler_flags

Compiler Optimization Flags

Flag	Description
-O2	Default optimization level (includes inlining, constant/copy propagation, loop unrolling,peephole optimizations, etc)
-O3	Enables more aggressive loop transformations in addition to *-O2* optimizations.
-xHost	Tells the compiler to generate vector instructions for the highest instruction set available on the host machine.
-fast	Shortcut for *-ipo*, *-O3*, *-no-prec-div*, *-static*, and *-xHost* flags.
-ip	Perform inter-procedural optimization within the same file.
-ipo	Perform inter-procedural optimization between files.
-parallel	Enable automatic parallelization by the compiler (very conservative)
-opt-report=[n]	Generate optimization report. n represent the level of detail (0 ..3, 3 being most detailed)
-vec-report[=n]	Generate vectorization report. n represents the level of detail (0..7 , 7 being most detailed)

For more information, consult the *opt*, *advanced*, and *ipo* compiler help categories.

Other Compiler Flags

- Debugging flags:
  - https://hprc.tamu.edu/wiki/index.php/Ada:Compile:All#Debugging_flags
  - See also the ***`icc -help command`*** which includes debugging and other flags.
- Flags affecting floating point operations:
  - https://hprc.tamu.edu/wiki/index.php/Ada:Compile:All#Flags_affecting_floating_point_operations
  - See also the ***`icc -help float help`*** or the ***`ifort -help float`*** commands. Some floating point flags are specific to Fortran.
- Many more compiler flags. Consult each compiler's man page or the output from the compiler's ***-help*** option.

Compiling OpenMP Programs

- OpenMP programming:
  - Use compiler directives to specify which code regions to run in parallel
  - Compiler generates multi-threaded code for these code regions
- Example:

```
module load intel/2015B
ifort -qopenmp -o omp_helloWorld.exe omp_helloWorld.f90
```

https://hprc.tamu.edu/wiki/index.php/Ada:Compile:OpenMP

Running OpenMP Programs

- Common environment variables:
  - OMP_NUM_THREADS:
    - Sets the maximum number of threads per nesting level
    - Default value is 1
  - OMP_STACKSIZE:
    - Sets the size for the private stack of each worker thread. Suffix can be B,K,M,G
    - Default value is 4 MB
- Example using 4 threads and 16 MB stack size per thread

```
$ export OMP_NUM_THREADS=4
$ export OMP_STACKSIZE=16M
$ ./omp_helloWorld.exe
```

- **Do not use more than 8 cores on the login nodes!**

Compiling MPI Programs

- Use a MPI compiler wrapper to compile MPI codes.
  - Wrapper invokes underlying compiler and adds linker flags specific for MPI programs
  - Intel MPI provides wrappers for both Intel and GNU compilers
  - Any flags not recognized by the wrapper are passed to the underlying compiler.
- Example to compile MPI C program with the Intel compiler's *-O3* optimization flag

```
mpiicc -o mpi_prog.x -O3 mpi_prog.c
```

https://hprc.tamu.edu/wiki/index.php/Ada:Compile:MPI

Running MPI Programs

- Requires a MPI launcher (mpirun) to run MPI programs

  mpirun [mpi_flags] executable [executable params]

- Example:

```
module load intel/2015B
mpirun -np 4 ./mpi_helloWorld.exe
```

- **Do not use more than 8 cores on the login nodes!**

Other Programming Methods

- Compiling programs to use GPU accelerators
  - https://hprc.tamu.edu/wiki/index.php/Ada:Compile:CUDA
- Compiling programs to use Phi coprocessors
  - https://hprc.tamu.edu/wiki/index.php/Ada:Compile:PHI

Intel Math Library (MKL)

- Provides optimized and threaded math routines such as BLAS, LAPACK, sparse solvers, FFTs, vector math, and more.
- Offers sequential, parallel, and cluster versions.
- Examples:

```
module load intel/2015B
ifort example.f -mkl=sequential -o example.exe
icc example.c -mkl=parallel -o example.exe
mpiifort example.f -mkl=cluster -o example.exe
```

- Consult Intel MKL Link advisor for usage help: https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor

https://hprc.tamu.edu/wiki/index.php/Ada:MKL

Remote Visualization

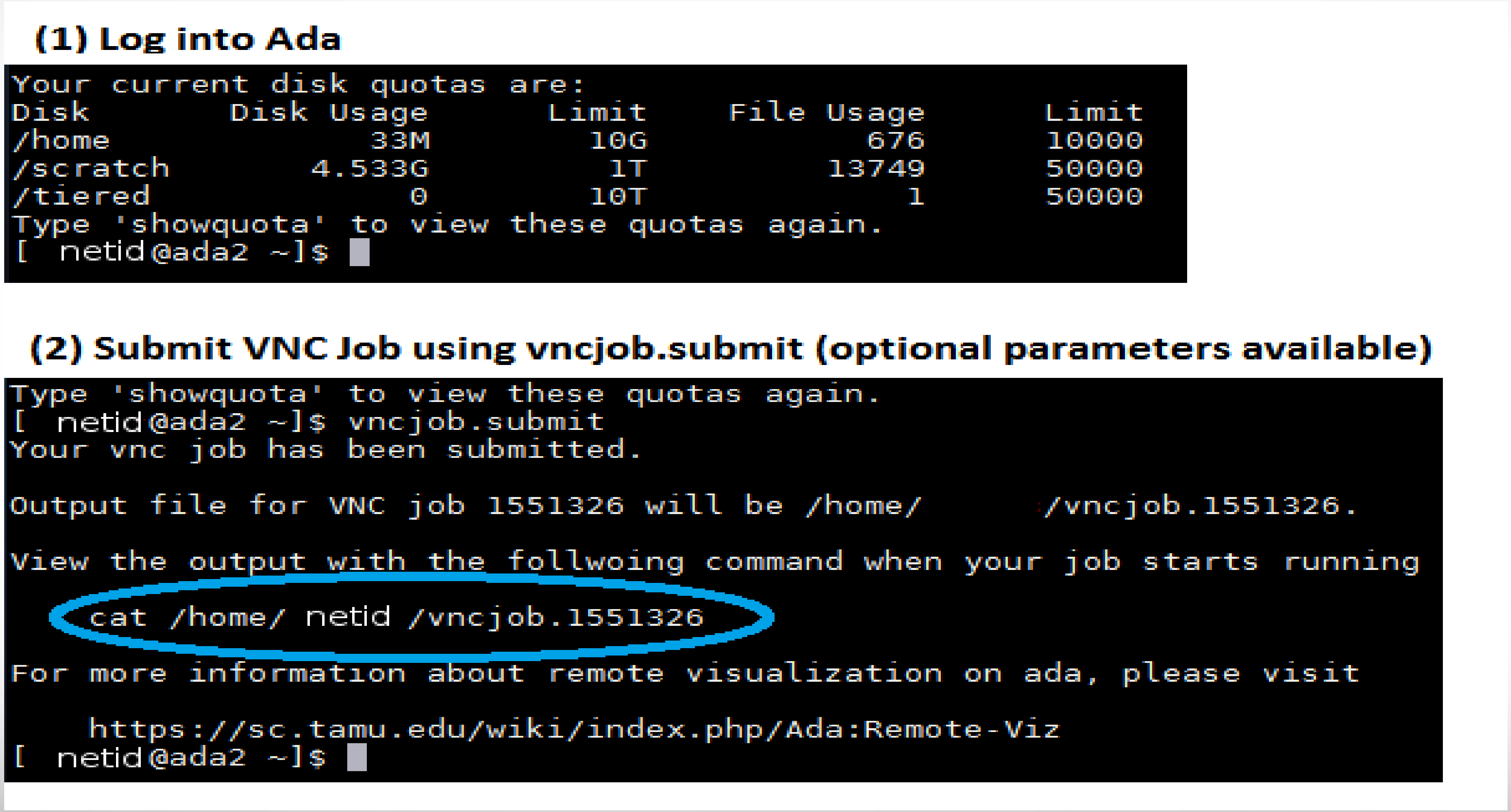
Remote Visualization Jobs

- Use to run programs with graphical interfaces on Ada and display them on your computer:
- Can leverage GPU nodes for better graphics performance
- Better than X11 forwarding (especially when using VPN)

Command	Description
vncjob.submit [-h] [-g MxN] [-t type]	Submit a VNC job. Type 'vncjob.submit -h' for help
vncjob.kill JOBID	Kill a VNC job whose id is JOBID
vncjob.list	List all your VNC jobs currently in the batch system

https://hprc.tamu.edu/wiki/index.php/Ada:Remote_Visualization

Remote Visualization Job Example



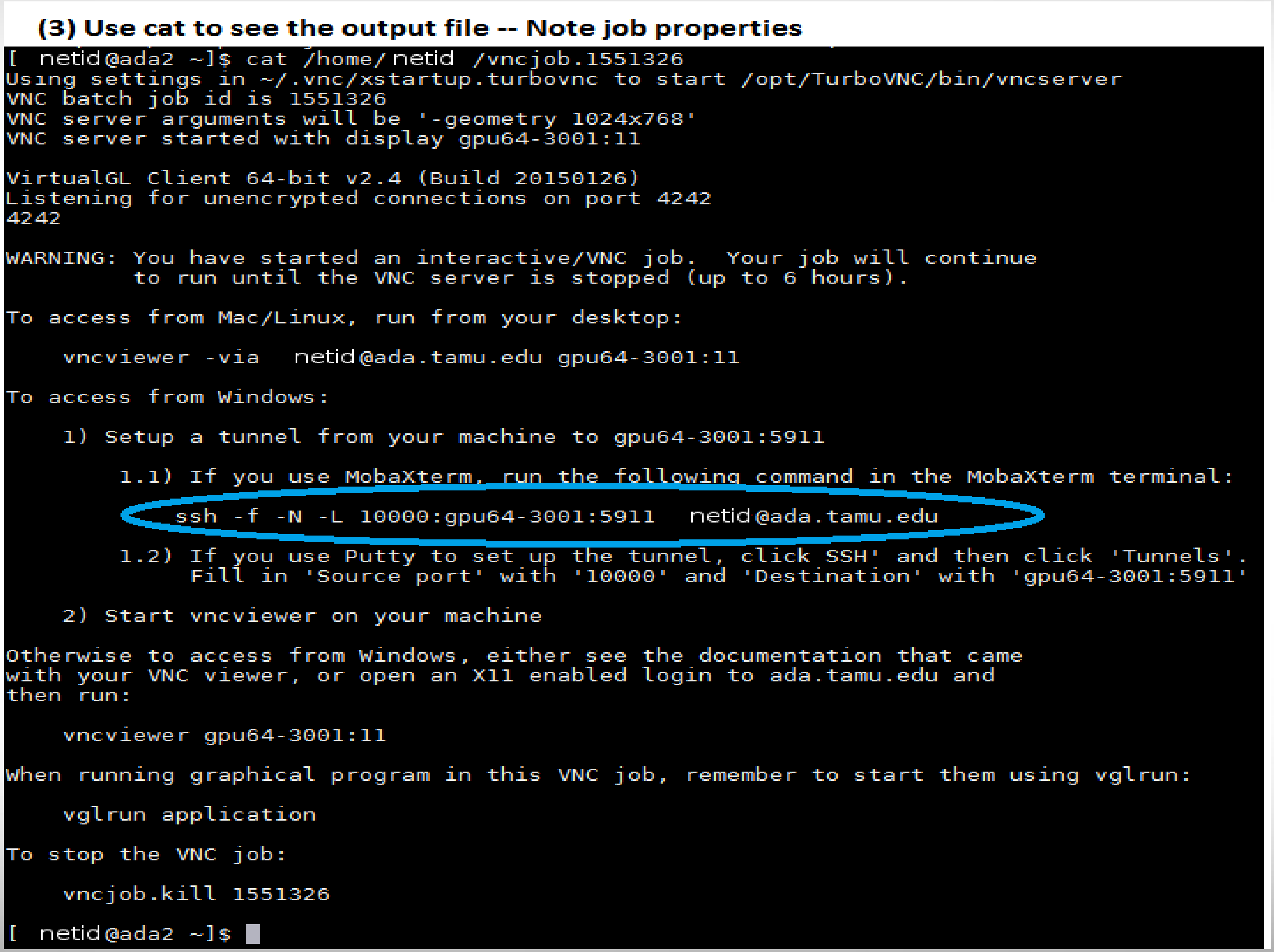
(1) Log into Ada

```
Your current disk quotas are:
Disk        Disk Usage      Limit    File Usage      Limit
/home              33M        10G           676      10000
/scratch        4.533G         1T         13749      50000
/tiered              0        10T             1      50000
Type 'showquota' to view these quotas again.
[ netid@ada2 ~]$ 
```

(2) Submit VNC Job using vncjob.submit (optional parameters available)

```
Type 'showquota' to view these quotas again.
[ netid@ada2 ~]$ vncjob.submit
Your vnc job has been submitted.

Output file for VNC job 1551326 will be /home/      /vncjob.1551326.

View the output with the follwoing command when your job starts running

    cat /home/ netid /vncjob.1551326

For more information about remote visualization on ada, please visit

    https://sc.tamu.edu/wiki/index.php/Ada:Remote-Viz
[ netid@ada2 ~]$ 
```

Remote Visualization Job Example

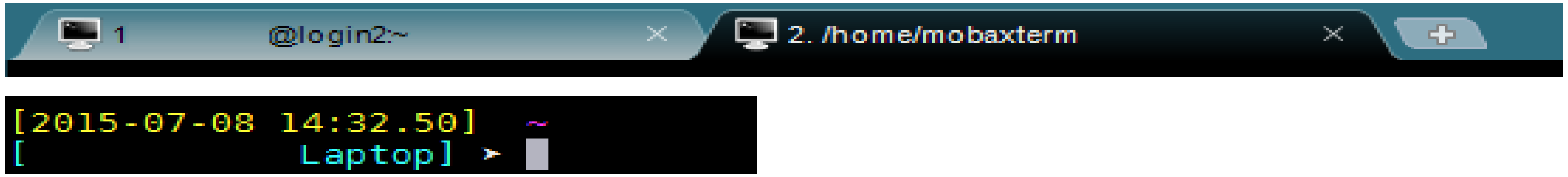


(3) Use cat to see the output file -- Note job properties

```
[ netid@ada2 ~]$ cat /home/ netid /vncjob.1551326
Using settings in ~/.vnc/xstartup.turbovnc to start /opt/TurboVNC/bin/vncserver
VNC batch job id is 1551326
VNC server arguments will be '-geometry 1024x768'
VNC server started with display gpu64-3001:11

VirtualGL Client 64-bit v2.4 (Build 20150126)
Listening for unencrypted connections on port 4242
4242

WARNING: You have started an interactive/VNC job.  Your job will continue
         to run until the VNC server is stopped (up to 6 hours).

To access from Mac/Linux, run from your desktop:

    vncviewer -via  netid@ada.tamu.edu gpu64-3001:11

To access from Windows:

    1) Setup a tunnel from your machine to gpu64-3001:5911

        1.1) If you use MobaXterm, run the following command in the MobaXterm terminal:

            ssh -f -N -L 10000:gpu64-3001:5911  netid@ada.tamu.edu

        1.2) If you use Putty to set up the tunnel, click SSH' and then click 'Tunnels'.
             Fill in 'Source port' with '10000' and 'Destination' with 'gpu64-3001:5911'

    2) Start vncviewer on your machine

Otherwise to access from Windows, either see the documentation that came
with your VNC viewer, or open an X11 enabled login to ada.tamu.edu and
then run:

    vncviewer gpu64-3001:11

When running graphical program in this VNC job, remember to start them using vglrun:

    vglrun application

To stop the VNC job:

    vncjob.kill 1551326

[ netid@ada2 ~]$ █
```

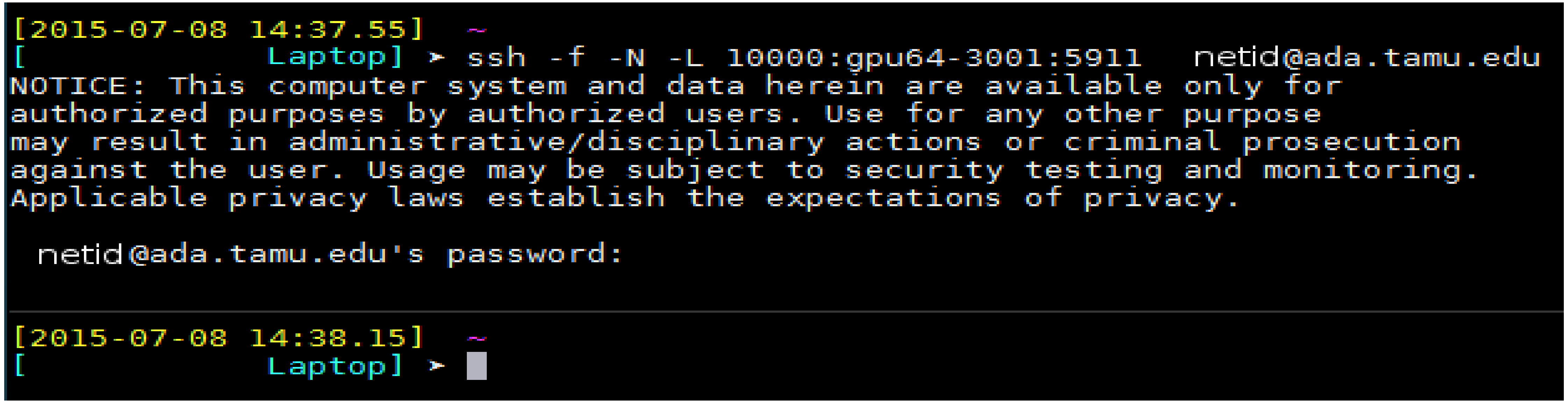
Remote Visualization Job Example

(4) Start new tab/terminal pointed to local machine



```
[2015-07-08 14:32.50]  ~
[              Laptop] ➤ 
```

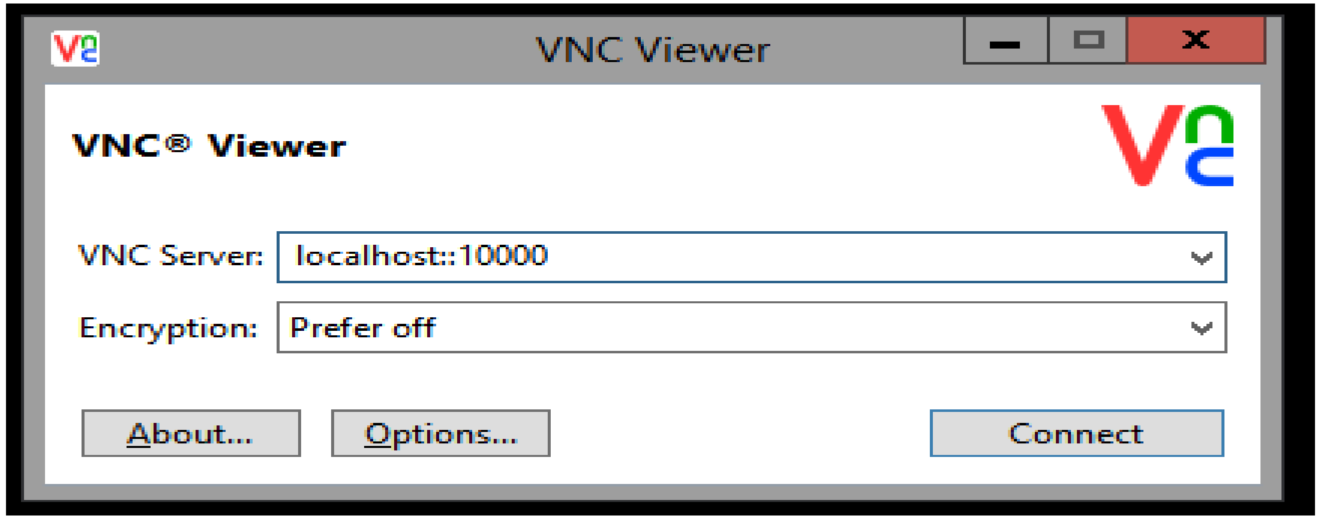
(5) Use command from (3) to create tunnel -- Local port 10000 must be free



```
[2015-07-08 14:37.55]  ~
[              Laptop] ➤ ssh -f -N -L 10000:gpu64-3001:5911  netid@ada.tamu.edu
NOTICE: This computer system and data herein are available only for
authorized purposes by authorized users. Use for any other purpose
may result in administrative/disciplinary actions or criminal prosecution
against the user. Usage may be subject to security testing and monitoring.
Applicable privacy laws establish the expectations of privacy.

 netid@ada.tamu.edu's password:

[2015-07-08 14:38.15]  ~
[              Laptop] ➤ 
```

Remote Visualization Job Example

(6) Open VNC Viewer and enter connection information



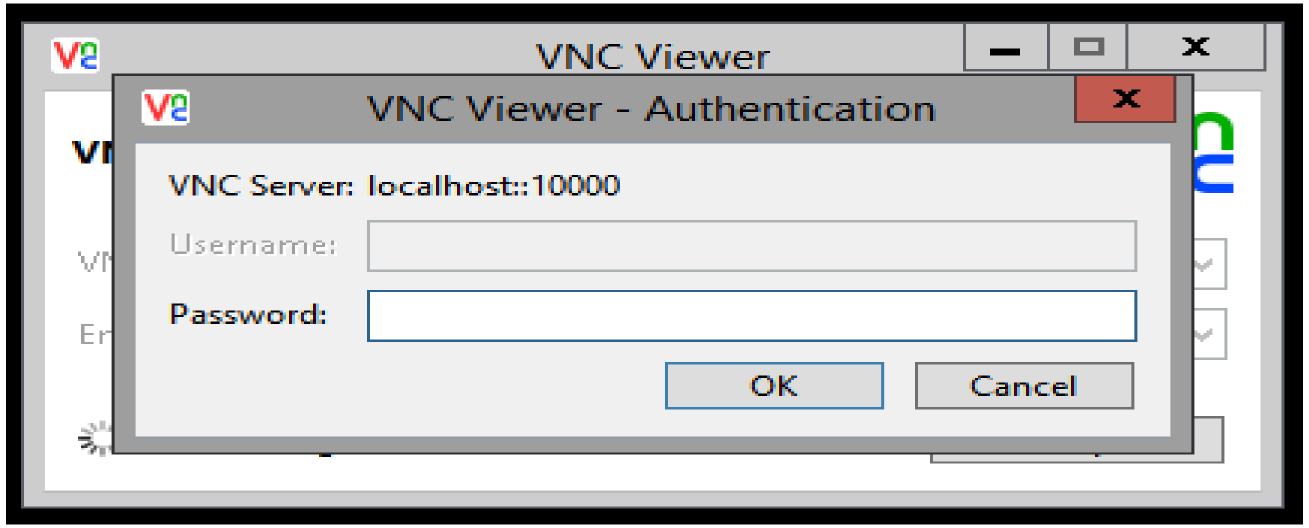
VNC Viewer

VNC® Viewer

VNC Server: localhost::10000

Encryption: Prefer off

(7) Enter your *VNC* password



VNC Viewer - Authentication

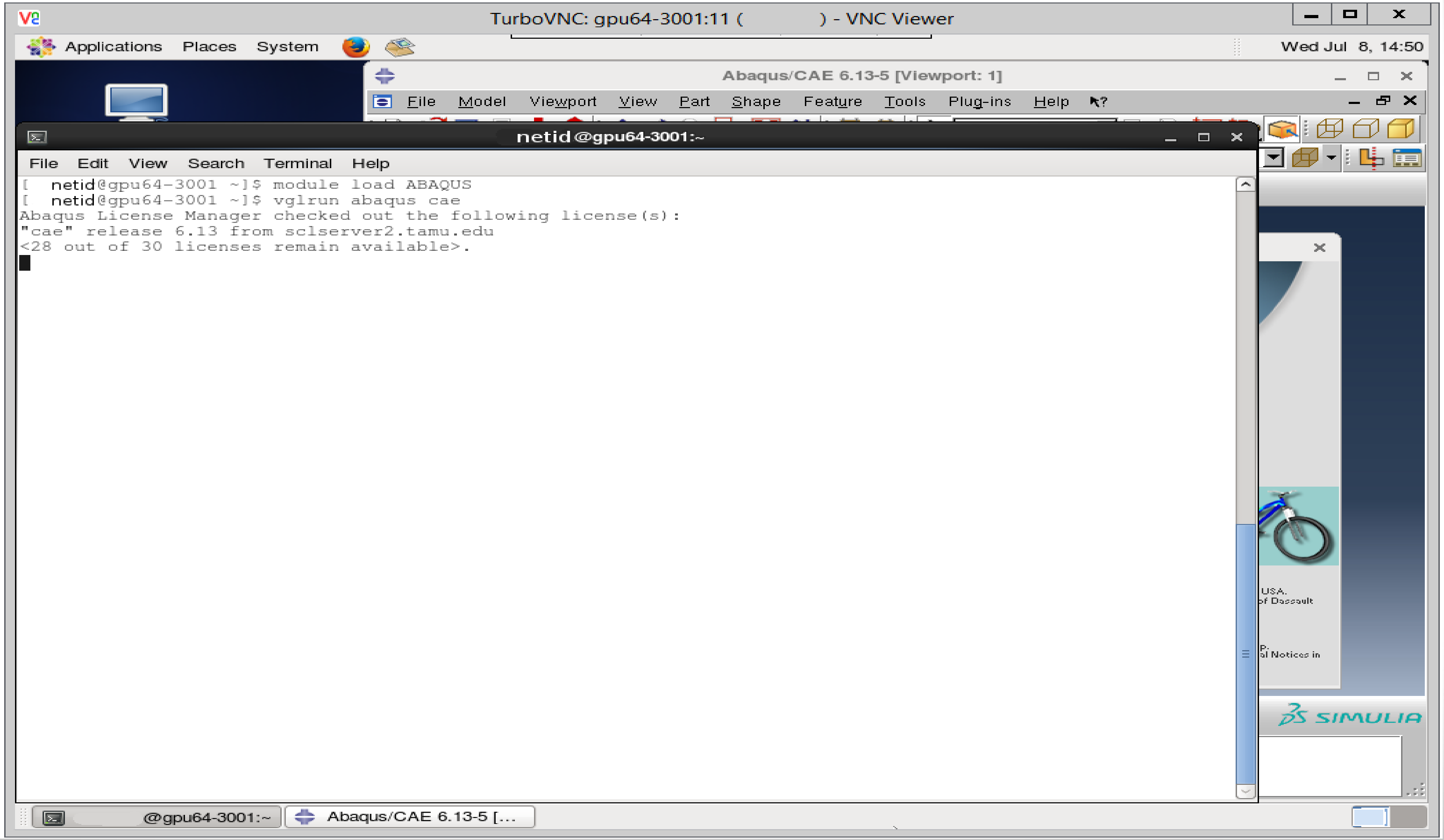
VNC Server: localhost::10000

Username:

Password:

Remote Visualization Job Example

(8) VNC window opens -- load modules -- use vglrun to launch GUI


TurboVNC: gpu64-3001:11 ( ) - VNC Viewer
Applications Places System
Wed Jul 8, 14:50
Abaqus/CAE 6.13-5 [Viewport: 1]
File Model Viewport View Part Shape Feature Tools Plug-ins Help
netid@gpu64-3001:~
File Edit View Search Terminal Help
SIMULIA
@gpu64-3001:~
Abaqus/CAE 6.13-5 [...

```
[  netid@gpu64-3001 ~]$ module load ABAQUS
[  netid@gpu64-3001 ~]$ vglrun abaqus cae
Abaqus License Manager checked out the following license(s):
"cae" release 6.13 from sclserver2.tamu.edu
<28 out of 30 licenses remain available>.
```