Week 8: Introduction to Xsede and Stampede2

Computational Tools and Techniques in STEM

Mar 26-28, 2019

Learning Goals

- **L1**: Logging into Xsede.
- **L2**: Quick intro to Stampede2.
- **L3**: Navigating in Stampede2.
- **L4**: Filesystem in Stampede2.
- **L5**: Login and compute nodes.
- **L6**: Interactive jobs.
- **L7**: Modules.
- **L8**: Transferring files.

Logging into Xsede

```
$ ssh <username>@login.xsede.org -X
```

```
$ gsissh stampede2
```

Cluster Diagram

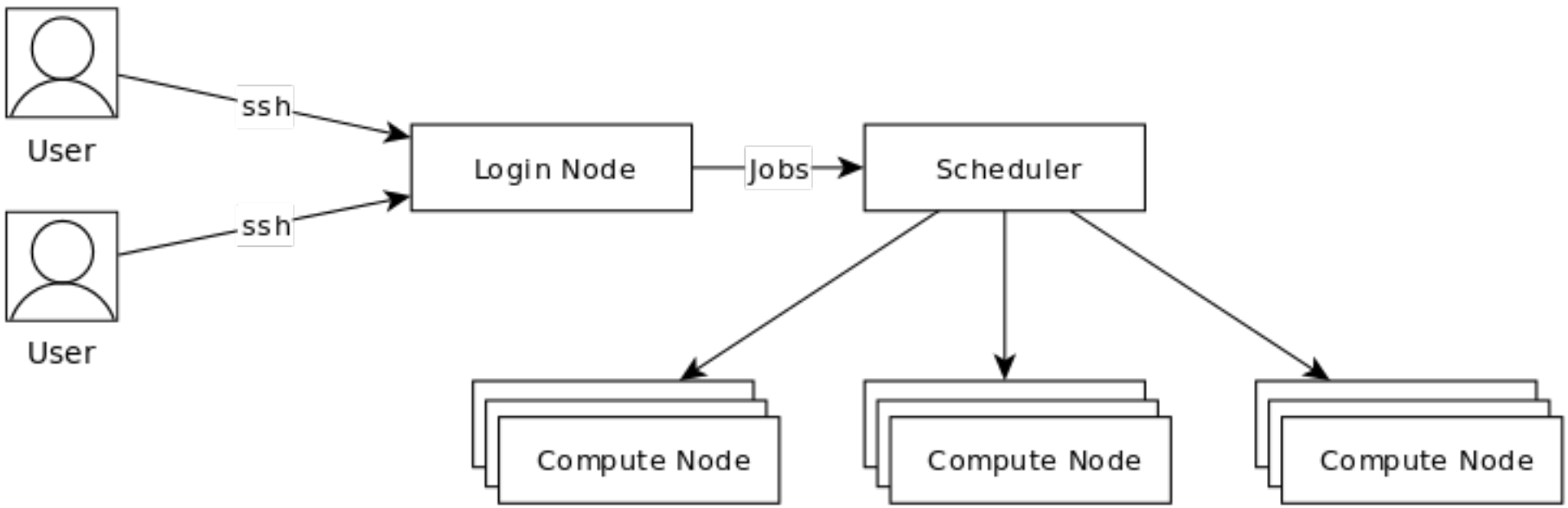

Figure: Picture source: `https://docs.hpc.qmul.ac.uk/intro/`

Quick intro to Stampede2

- Peak performance: 18 petaflops.
- Two types of computes nodes: Intel Knights Landing (KNL) and Intel Xeon Skylake (SLX) nodes.
- **KNL nodes: 4200, cores per node: 68 cores**, 96GB of DDR RAM, 16GB of MCDRAM.
- SKX nodes: 1736, cores per node: 48 cores, 192GB RAM.

Note: We will be using KNL nodes (available are usually 64 cores per node). Even if you request less than 64 nodes, you get charged for the whole node.

Stampede2 Cluster

- Manufacturer: Dell
- Platform: TACC Dell/Intel Knights Landing, Skylake System (Stampede2)
- CPU Type: Intel Xeon Phi Knights Landing, Intel Xeon Skylake
- Operating System: Linux Centos 7
- Processor Cores: 368280
- Nodes: 5940
- Memory: 359 TB
- Peak Performance: 12800 TFlops
- CPU Cores Per Node 62
- Memory Per CPU: 1 GB

Filesystem in Stampede2

File System	Quota	Key Features
$HOME	10GB, 200,000 files	**Not intended for parallel or high-intensity file operations.** Backed up regularly. Overall capacity ~1PB. Two Meta-Data Servers (MDS), four Object Storage Targets (OSTs). Defaults: 1 stripe, 1MB stripe size. Not purged.
$WORK	1TB, 3,000,000 files across all TACC systems, regardless of where on the file system the files reside.	**Not intended for high-intensity file operations or jobs involving very large files.** On the Global Shared File System that is mounted on most TACC systems. See Stockyard system description for more information. Defaults: 1 stripe, 1MB stripe size Not backed up. Not purged.
$SCRATCH	no quota	Overall capacity ~30PB. Four MDSs, 66 OSTs. Defaults: 1 stripe, 1MB stripe size. Not backed up. **Subject to purge** if access time* is more than 10 days old.

Figure: Picture source:
`https://www.tacc.utexas.edu/systems/stampede2`

Requesting an interactive job

To request an interactive single-core job on the compute node:

$idev

This will lead to a few messages. Wait until the command prompt ($) shows up again.

Once you are on the interactive node, this is where you will do all your compilation, test runs for the serial code, etc.

Modules

To see the list of currently loaded modules:
$module list

To see all the modules available:
$module avail

To load a module:
$module load <modulename>

E.g. to load python3:
$module load python3

Transferring files to Stampede2 via scp

Two-step process.

First step: Transfer to Xsede from local.

$scp myfile.txt <username>@login.xsede.org:

Second step: Transfer to Stampede2 from Xsede.

$gsiscp myfile.txt stampede2: