Introduction to HPC2N

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12 September 2017

Overview

- Kebnekaise and Abisko
- Using our systems
- The File System
- The Module System
  - Overview
  - Compiler Tool Chains
  - Examples
- Compiling/linking with libraries
- The Batch System (SLURM)
  - Overview
  - Simple example
  - More examples

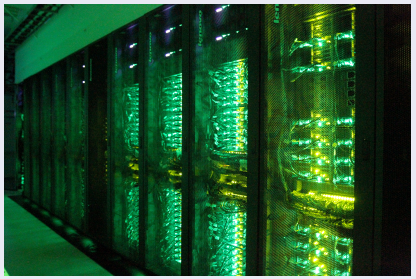
Kebnekaise and Abisko

Abisko

1. 328 nodes / 15744 cores (10 fat, 318 thin)
2. Thin: 4 AMD Opteron 6238, 12 core 2.6 GHz proc.
3. Fat: 4 AMD Opteron 6344, 12 core 2.6 GHz proc.
4. 10 with 512 GB RAM/node, 318 with 128 GB RAM/node
5. Interconnect: Mellanox 4X QSFP 40 Gb/s
6. Theoretical performance: 163.74 TF
7. HP Linpack: 131.9 TF
8. Date installed: Fall 2011. Upgraded Jan 2014

Kebnekaise and Abisko

Kebnekaise



1. 544 nodes / 17552 cores (of which 2448 are KNL)
   - 432 Intel Xeon E5-2690v4, 2x14 cores, 128 GB/node
   - 20 Intel Xeon E7-8860v4, 4x18 cores, 3072 GB/node
   - 32 Intel Xeon E5-2690v4, 2x NVidia K80, 2x14, 2x4992, 128 GB/node
   - 4 Intel Xeon E5-2690v4, 4x NVidia K80, 2x14, 4x4992, 128 GB/node
   - 36 Intel Xeon Phi 7250, 68 cores, 192 GB/node, 16 GB MCDRAM/node
2. 399360 CUDA "cores" (80 * 4992 cores/K80)
3. More than 125 TB memory
4. Interconnect: Mellanox 56 Gb/s FDR Infiniband
5. Theoretical performance: 728 TF
6. HP Linpack: 629 TF
7. Date installed: Fall 2016 / Spring 2017

Using our systems

1. Get an account (https://www.hpc2n.umu.se/documentation/access-and-accounts/users)
2. Connect to:

   `kebnekaise.hpc2n.umu.se`
   or
   `abisko.hpc2n.umu.se`

3. Transfer your files and data (optionally)
4. Compile own code, install software, or run pre-installed software
5. Create batch script, submit batch job
6. Download data/results

- **Linux, OS X:**
  - `ssh username@kebnekaise.hpc2n.umu.se`
    or
    `ssh username@abisko.hpc2n.umu.se`
  - Use `ssh -X ....` if you want to open graphical displays.
- **Windows:**
  - Get an SSH client (PuTTY, Cygwin, MobaXterm ...)
  - Get an X11 server if you need graphical displays (Xming ...)
  - Start the client and login to

    `kebnekaise.hpc2n.umu.se`
    or
    `abisko.hpc2n.umu.se`

  - More information here:

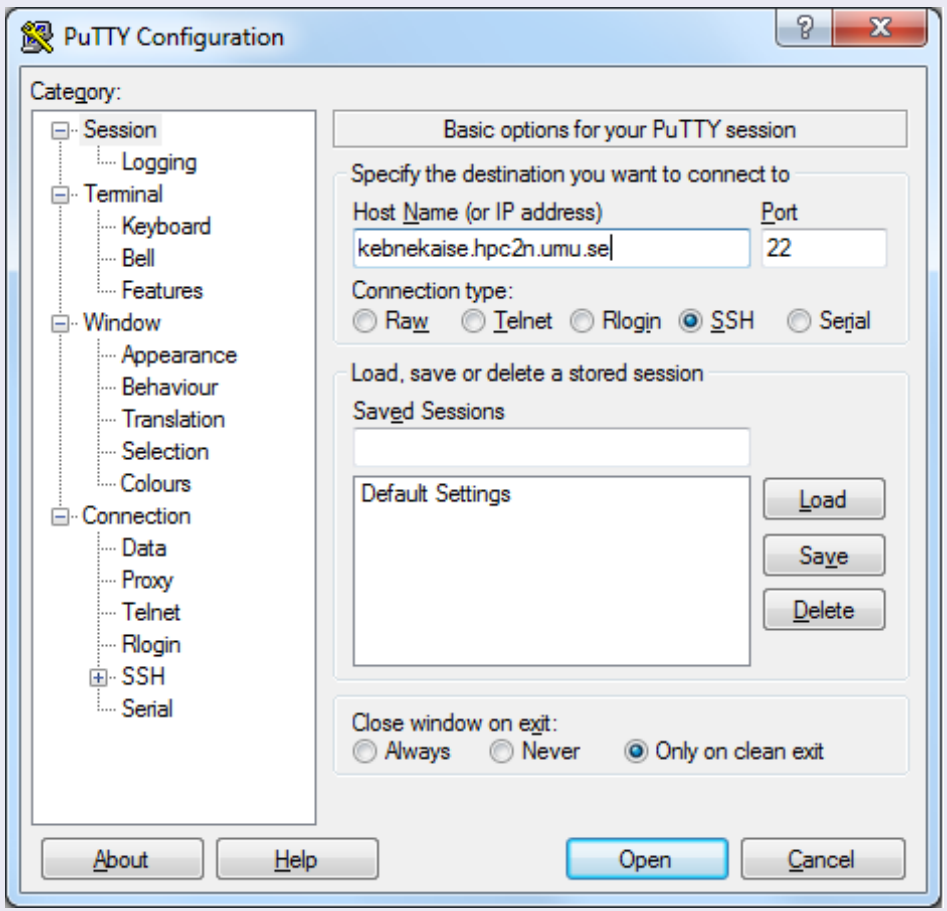
    https://www.hpc2n.umu.se/documentation/guides/windows-connection
- **Mac/OSX:** Guide here:

  https://www.hpc2n.umu.se/documentation/guides/mac-connection

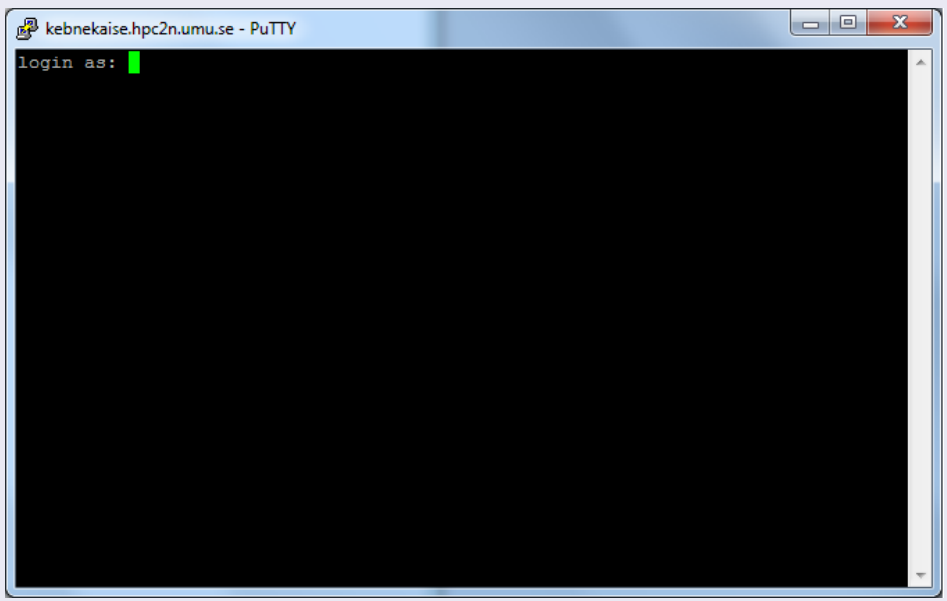
Using our systems

Connecting from a Windows System with PuTTY

Get the Zip file (http://www.putty.org/) with both PuTTY, PSCP, and PSFTP. Unzip, run putty.exe



Enter your username and then your password.



Using our systems

Transfer your files and data

- **Linux, OS X:**
  - Use scp for file transfer:

```
local> scp username@abisko.hpc2n.umu.se:file .
local> scp file username@abisko.hpc2n.umu.se:file
```

or

```
local> scp username@kebnekaise.hpc2n.umu.se:file .
local> scp file username@kebnekaise.hpc2n.umu.se:file
```

- **Windows:**
  - Download client: WinSCP, FileZilla (sftp), PSCP/PSFTP, ...
  - Transfer with sftp or scp
- https://www.hpc2n.umu.se/documentation/filesystems/filetransfer
- **Mac/OSX:**
  - Transfer with sftp or scp (as for Linux) using Terminal
  - Or download client: Cyberduck, Fetch, ...
- More info in guides (see previous slide) and here:

  https://www.hpc2n.umu.se/documentation/filesystems/filetransfer

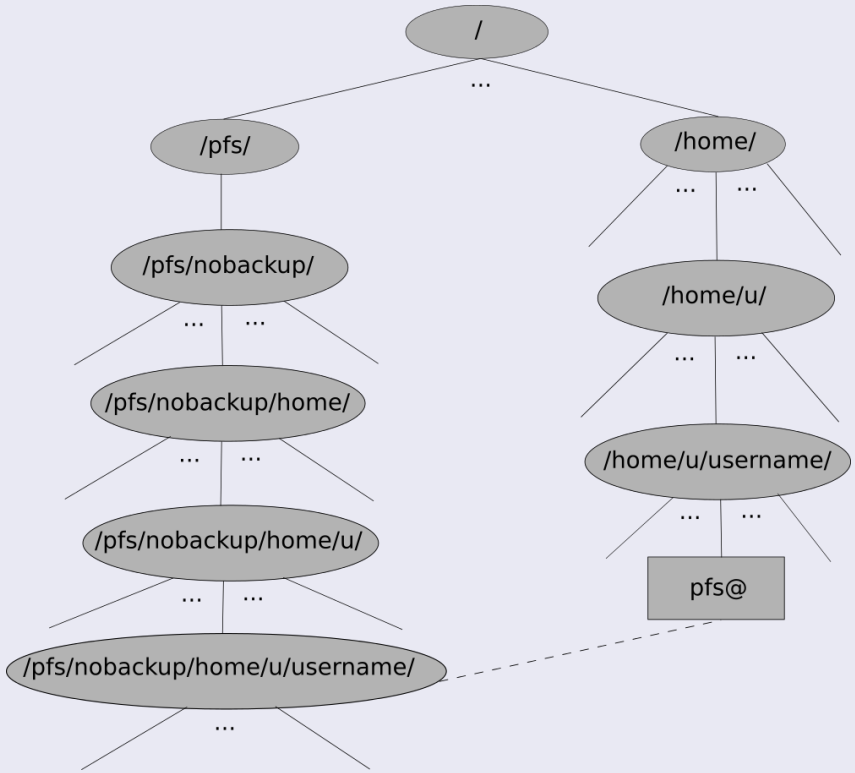
Editing your files

- Various editors: vi, vim, nano, emacs ...
- Example, nano:
  - `nano <filename>`
  - Save and exit nano: `Ctrl-x`
- Example, Emacs:
  - Start with: emacs
  - Open (or create) file: Ctrl-x Ctrl-f
  - Save: Ctrl-x Ctrl-s
  - Exit Emacs: Ctrl-x Ctrl-c

The File System

There are 2 file systems
More info here: http://www.hpc2n.umu.se/filesystems/overview

- **AFS**
  - This is where your home directory is located (cd $HOME)
  - Regularly backed up
  - NOT accesseable by the batch system (except the folder Public with the right settings)
- **PFS**
  - Parallel File System
  - NO BACKUP
  - Accessible by the batch system



The File System

AFS

- Your home directory is located in /home/u/username and can also be accessed with the environment variable $HOME
- It is located on the AFS (Andrew File System) file system
- Important! The batch system cannot access AFS since ticket-forwarding to batch jobs do not work
- AFS does secure authentification using Kerberos tickets

The File System

PFS

- The 'parallel' file system, where your 'parallel' home directory is located in /pfs/nobackup/home/u/username (/pfs/nobackup/$HOME)
- Offers high performance when accessed from the nodes
- The correct place to run all your batch jobs
- NOT backed up, so you should not leave files there that cannot easily be recreated
- For easier access, create a symbolic link from your home on AFS to your home on PFS:

  ```
  ln -s /pfs/nobackup/$HOME $HOME/pfs
  ```

  You can now access your pfs with `cd pfs` from your home directory on AFS

The Module System (Lmod)

Most programs are accessed by first loading them as a 'module'

- See which modules exists:
  `ml spider`
- Modules depending only on what is currently loaded:
  `module avail` or `ml av`
- See which modules are currently loaded:
  `module list` or `ml`
- Example: loading a compiler toolchain, here for GCC:
  `module load foss` or `ml foss`
- Example: Unload the above module:
  `module unload foss` or `ml -foss`
- More information about a module:
  `ml show <module>`
- Unload all modules except the 'sticky' modules:
  `ml purge`

The Module System

Compiler Toolchains

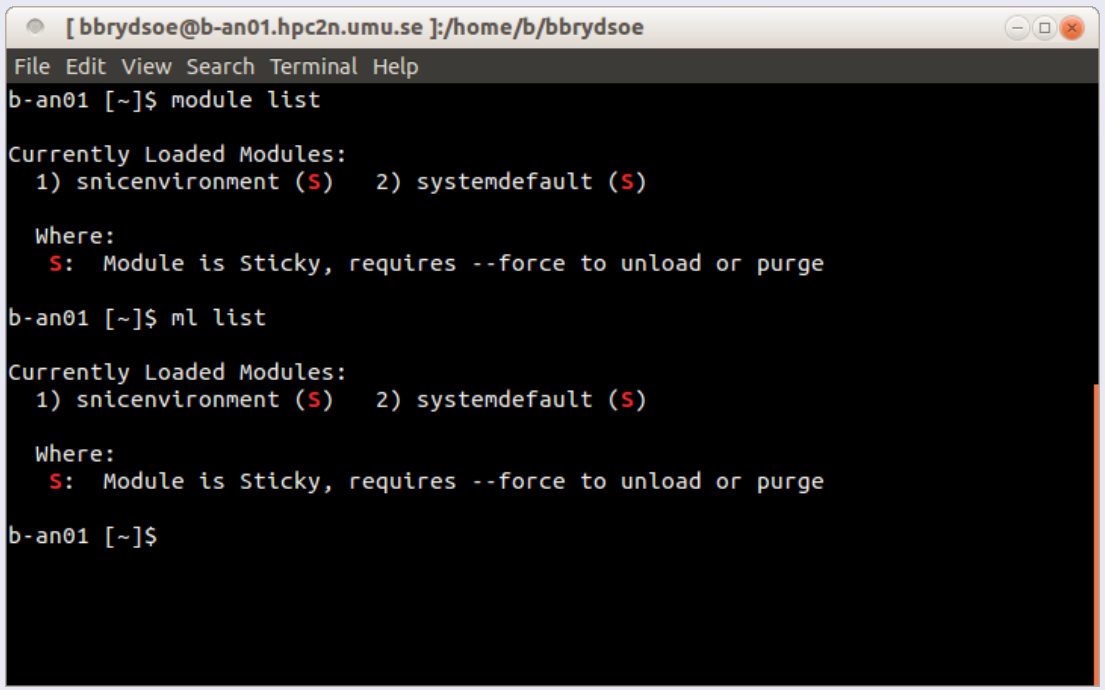
Compiler toolchains load bundles of software making up a complete environment for compiling/using a specific prebuilt software. Includes some/all of: compiler suite, MPI, BLAS, LAPACK, ScaLapack, FFTW, CUDA.

- Currently available toolchains (check `ml av` for versions):
  - **GCC**: GCC only
  - **gcccuda**: GCC and CUDA
  - **foss**: GCC, OpenMPI, OpenBLAS/LAPACK, FFTW, ScaLAPACK
  - **gimkl**: GCC, IntelMPI, IntelMKL
  - **gimpi**: GCC, IntelMPI
  - **gompi**: GCC, OpenMPI
  - **gompic**: GCC, OpenMPI, CUDA
  - **goolfc**: gompic, OpenBLAS/LAPACK, FFTW, ScaLAPACK
  - **icc**: Intel C and C++ only
  - **iccifort**: icc, ifort
  - **iccifortcuda**: icc, ifort, CUDA
  - **ifort**: Intel Fortran compiler only
  - **iimpi**: icc, ifort, IntelMPI
  - **intel**: icc, ifort, IntelMPI, IntelMKL
  - **intelcuda**: intel and CUDA
  - **iomkl**: icc, ifort, Intel MKL, OpenMPI
  - **pomkl**: PGI C, C++, and Fortran compilers, IntelMPI
  - **pompi**: PGI C, C++, and Fortran compilers, OpenMPI

The Module System

Examples

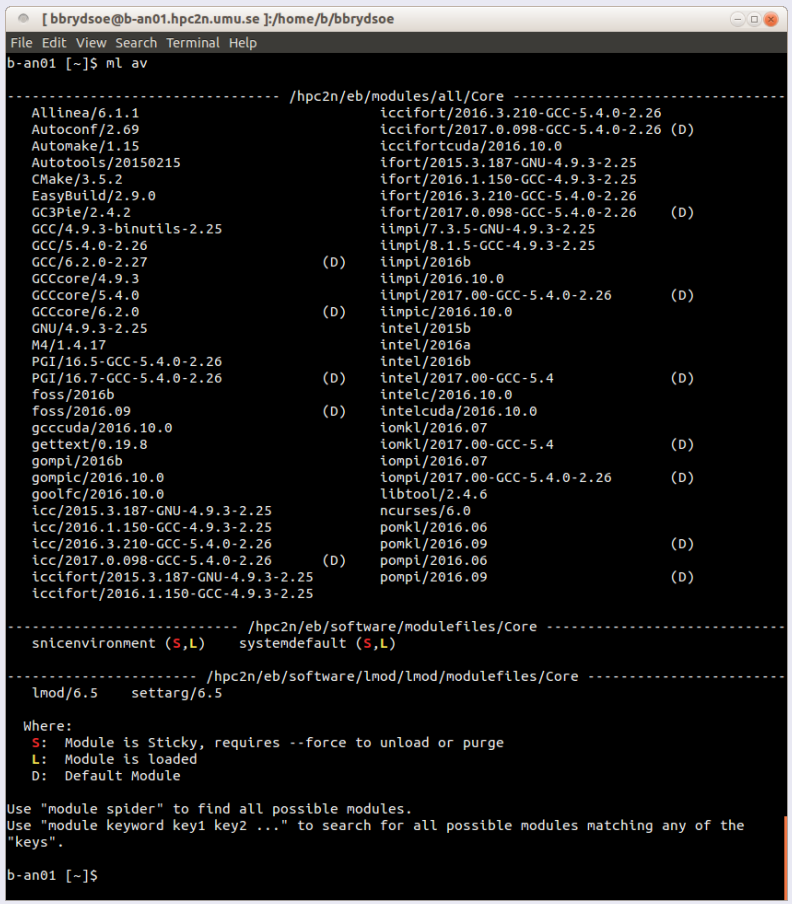
```
module list
ml list
ml
```



The Module System

Examples

```
module avail
ml avail
ml av
```



The Module System

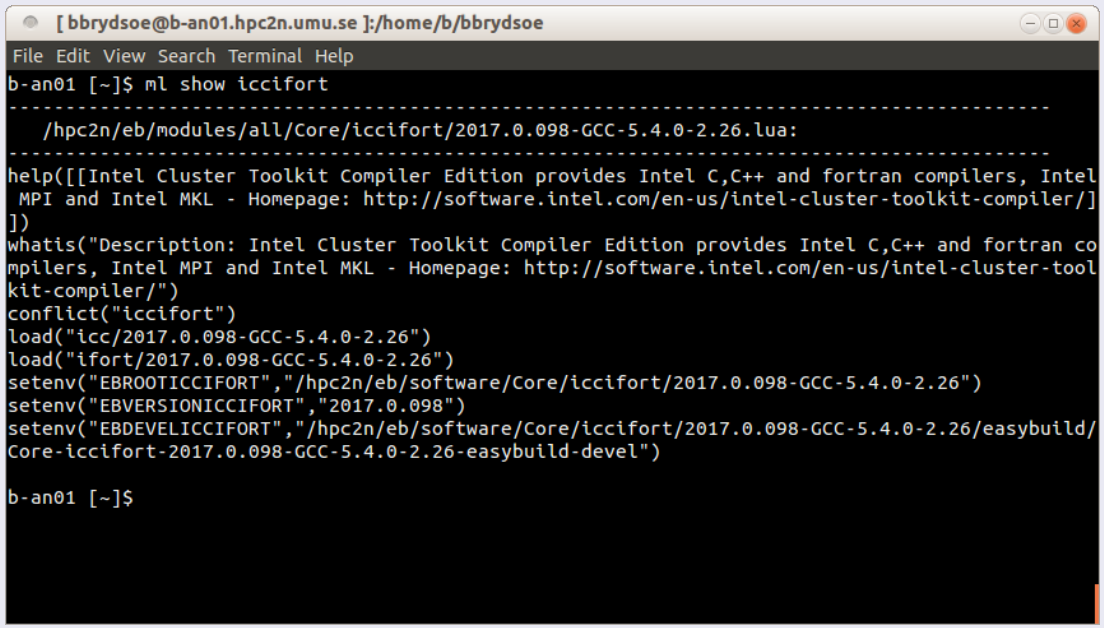
Examples

```
module spider
ml spider
```

The Module System

Examples

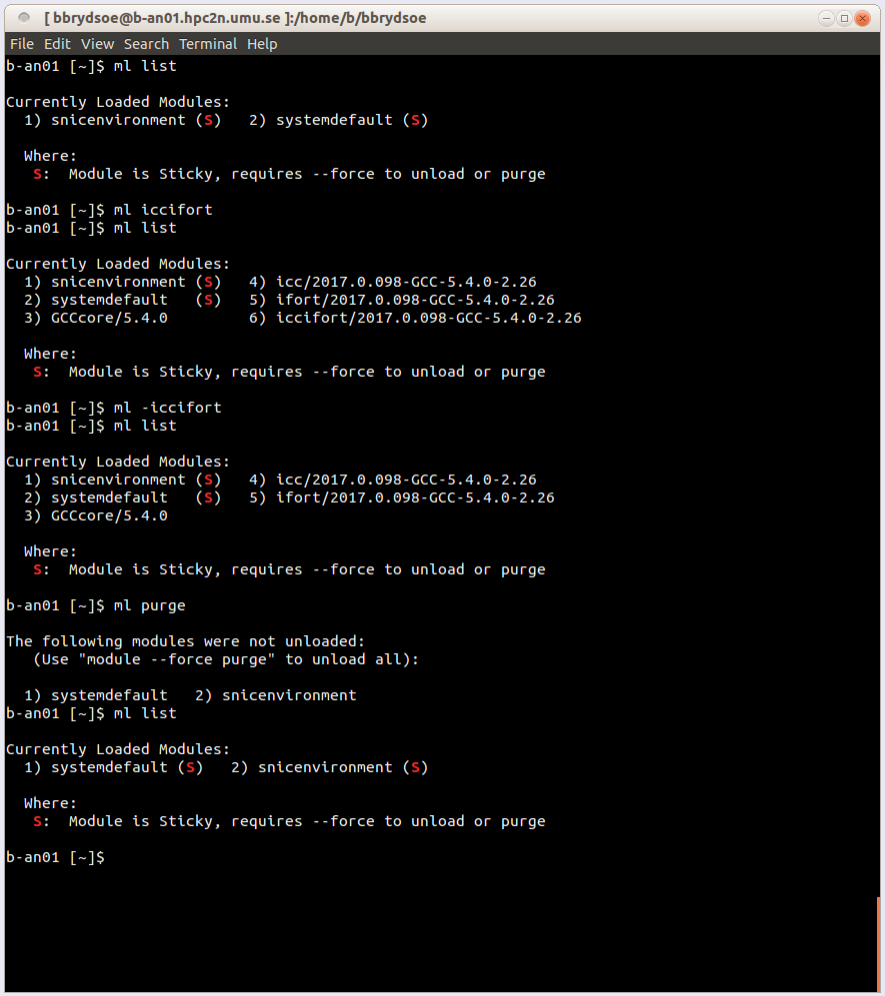
```
module show <module>
ml show <module>
```



The Module System

Examples

`module load <module>` / `module unload <module>`
`ml <module>` / `ml -<module>`



Compiling and Linking with Libraries

Some examples

- MPI C program:
  - Intel compilers, Intel MPI:
    ```
    ml iimpi
    mpicc <program.c> -o <outfile>
    ```
  - GCC compilers, OpenMPI:
    ```
    ml gompi
    mpicc <program.c> -o <outfile>
    ```
- OpenMP Fortran program:
  - Intel compilers:
    ```
    ml iccifort
    ifort -qopenmp <program.f90> -o <outfile>
    ```
  - GCC compilers:
    ```
    ml GCC
    gfortran -fopenmp <program.f90> -o <outfile>
    ```

Compiling and Linking with Libraries

Continued

Examples

- C program, BLAS, LAPACK:
  - Intel compilers, Intel MKL:
    `ml intel/version`

    ```
    -L${MKLROOT}/lib/intel64 -lmkl_intel_ilp64 \
    -lmkl_sequential -lmkl_core -lpthread -lm -ldl
    ```
  - GCC compilers, OpenBLAS/LAPACK:
    ```
    ml foss/version
    gcc -o program.c program.o -lopenblas
    ```

Compiling and Linking with Libraries

Continued

Examples

- Fortran program, ScaLAPACK, OpenMPI:
  - GCC, OpenBLAS/LAPACK, ScaLAPACK, OpenMPI:

    ```
    ml foss/version
    gcc -o program program.o -lscalapack -lopenblas
    ```
  - Intel, MKL, Intel MPI:

    ```
    ml intel/version
    -L${MKLROOT}/lib/intel64 -lmkl_scalapack_ilp64 \
    -lmkl_intel_ilp64 -lmkl_sequential -lmkl_core \
    -lmkl_blacs_intelmpi_ilp64 -lpthread -lm -ldl
    ```
- C program, OpenMPI, CUDA:
  - GCC:

    ```
    ml goolfc
    -lcuda -lcudart
    ```

    or `nvcc program.cu -o program`

Figuring out how to link

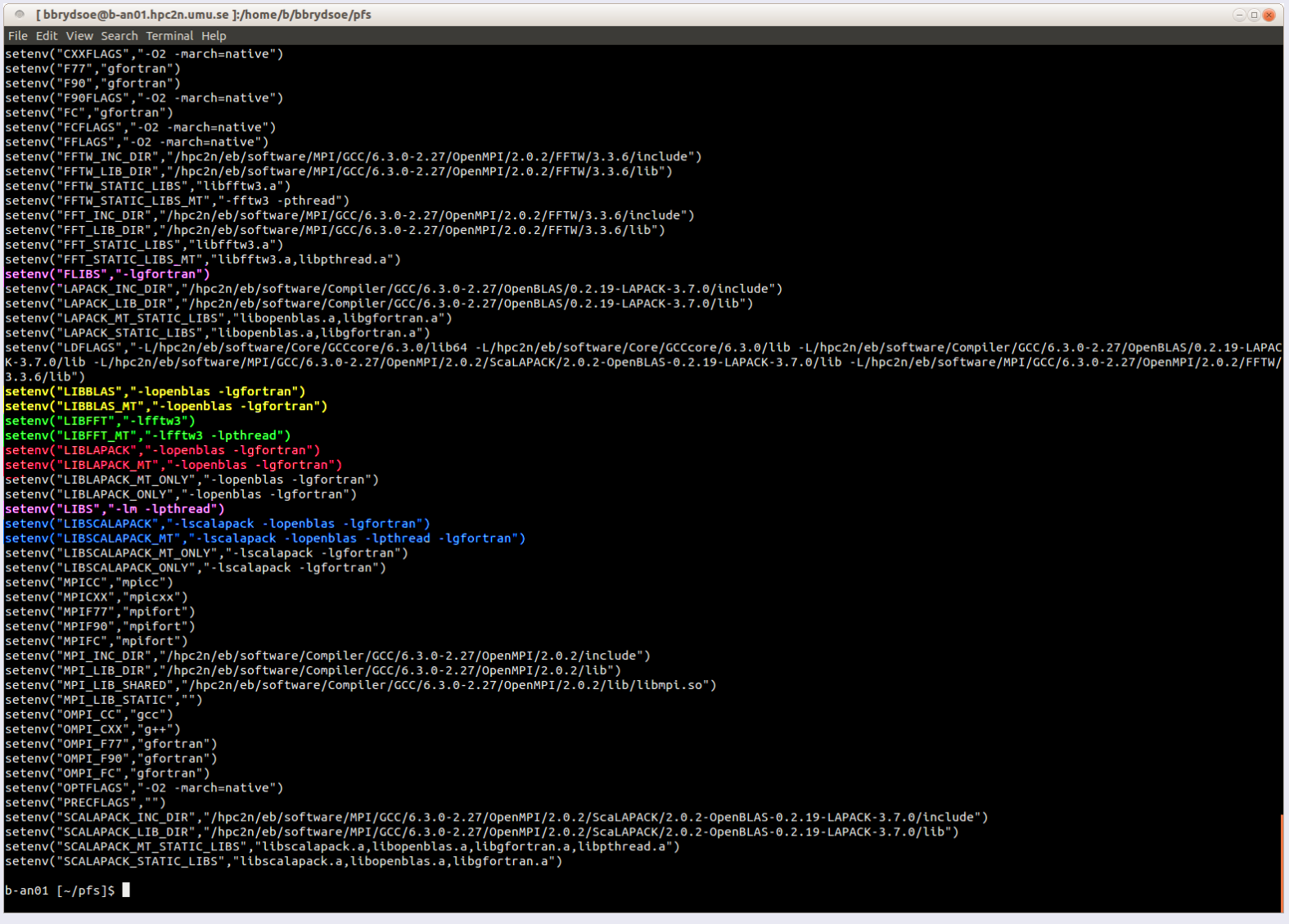
- Intel and Intel MKL linking:

  `https://software.intel.com/en-us/articles/intel-mkl-link-line-advisor`
- Buildenv
  - After loading a compiler toolchain, load `'buildenv'` and use `'ml show buildenv'` to get useful linking info
  - Example, foss (add relevant version):

    ```
    ml foss/version
    ml buildenv
    ml show buildenv
    ```
  - Using the environment variable (prefaced with $) is highly recommended!

Compiling and Linking with Libraries

Example: ml foss, ml buildenv, ml show buildenv



The Batch System (SLURM)

- Large/long/parallel jobs must be run through the batch system
- SLURM is an Open Source job scheduler, which provides three key functions
  - Keeps track of available system resources
  - Enforces local system resource usage and job scheduling policies
  - Manages a job queue, distributing work across resources according to policies
- Same batch system on Abisko and Kebnekaise. The differences are that there are GPUs and KNLs which can be allocated on Kebnekaise
- Guides and documentation at: http://www.hpc2n.umu.se/support

The Batch System

Accounting, Compute nodes, Abisko

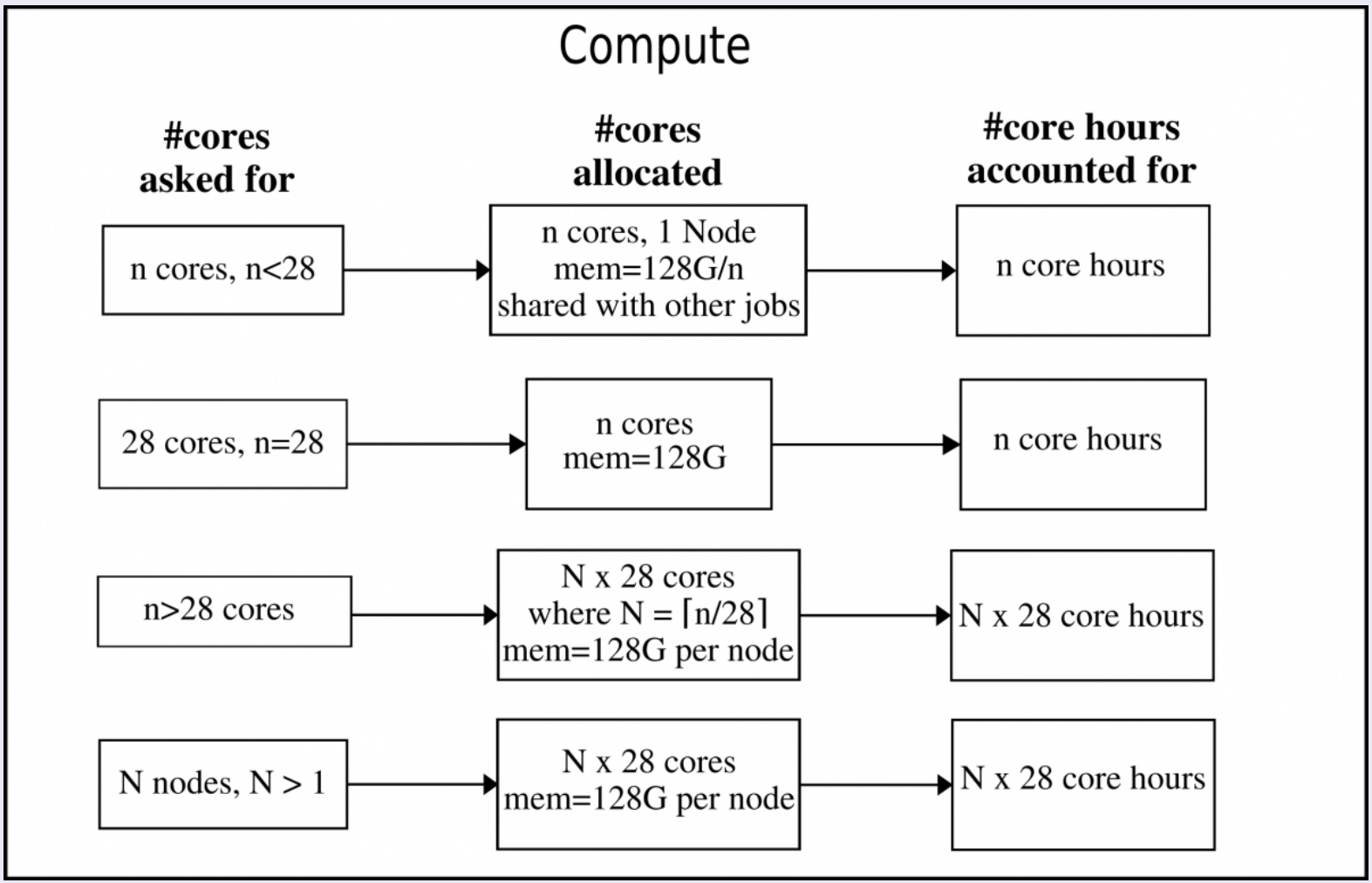
- Physically, a socket is 12 cores, but for SLURM allocation purposes a socket is 6 cores (a NUMA node)
- Thus allocation is in groups of 6 cores (one NUMA island). This also means 6 cores is the smallest unit you can allocate.
- This is how your project is charged, depending on how many cores you ask for:

You ask for	Cores you get	Project is charged
1 core	6 cores	6 cores
6 cores	6 cores	6 cores
7 cores	12 cores	12 cores
c cores	ceil(c/6) cores	ceil(c/6) cores

If you request resources using **#SBATCH -c** you request c cores per task, and SLURM only allocates cores on a single node.
If you request resources using **#SBATCH -n** you request tasks which can be allocated on multiple nodes.

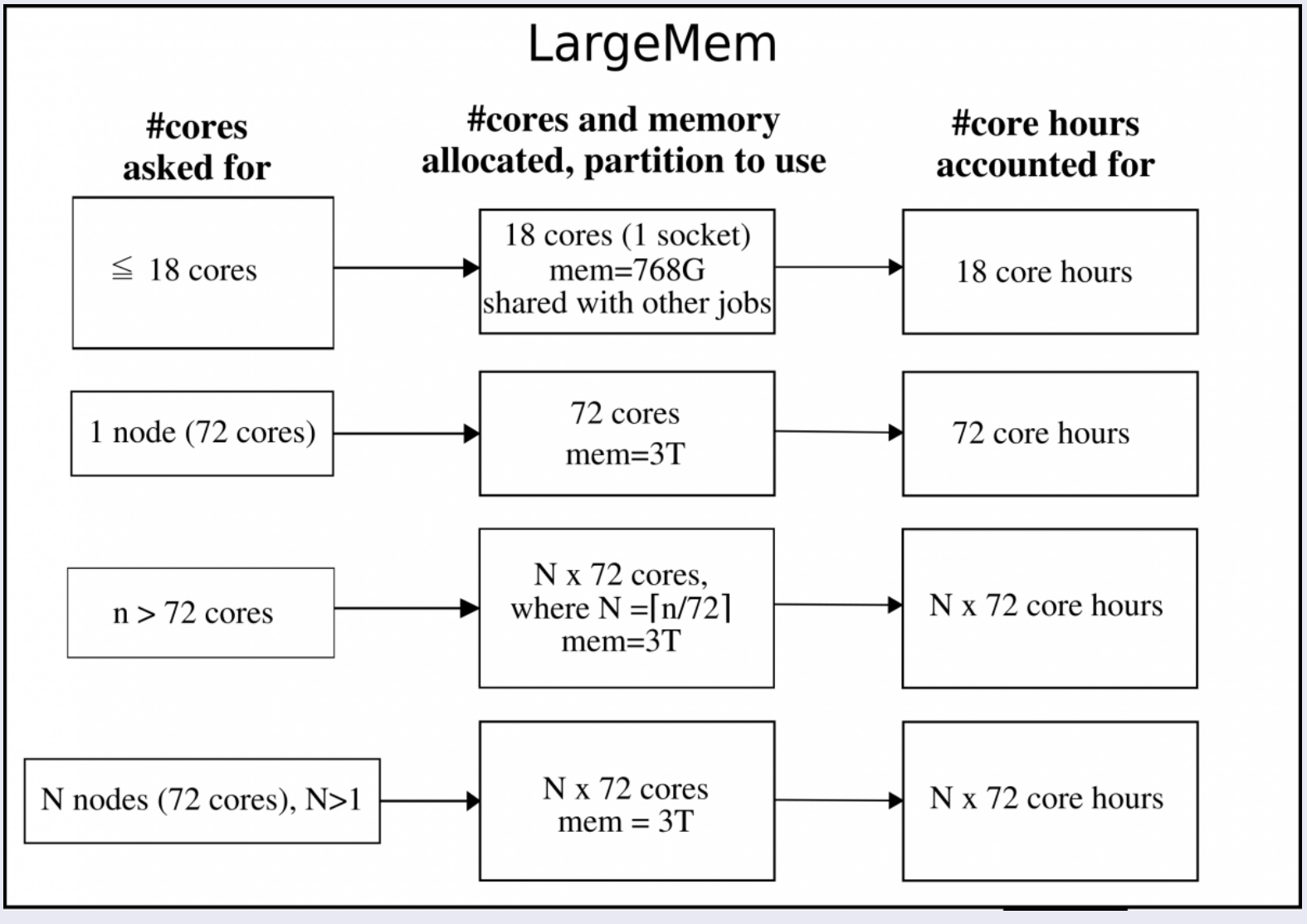
The Batch System

Accounting, Compute nodes, Kebnekaise



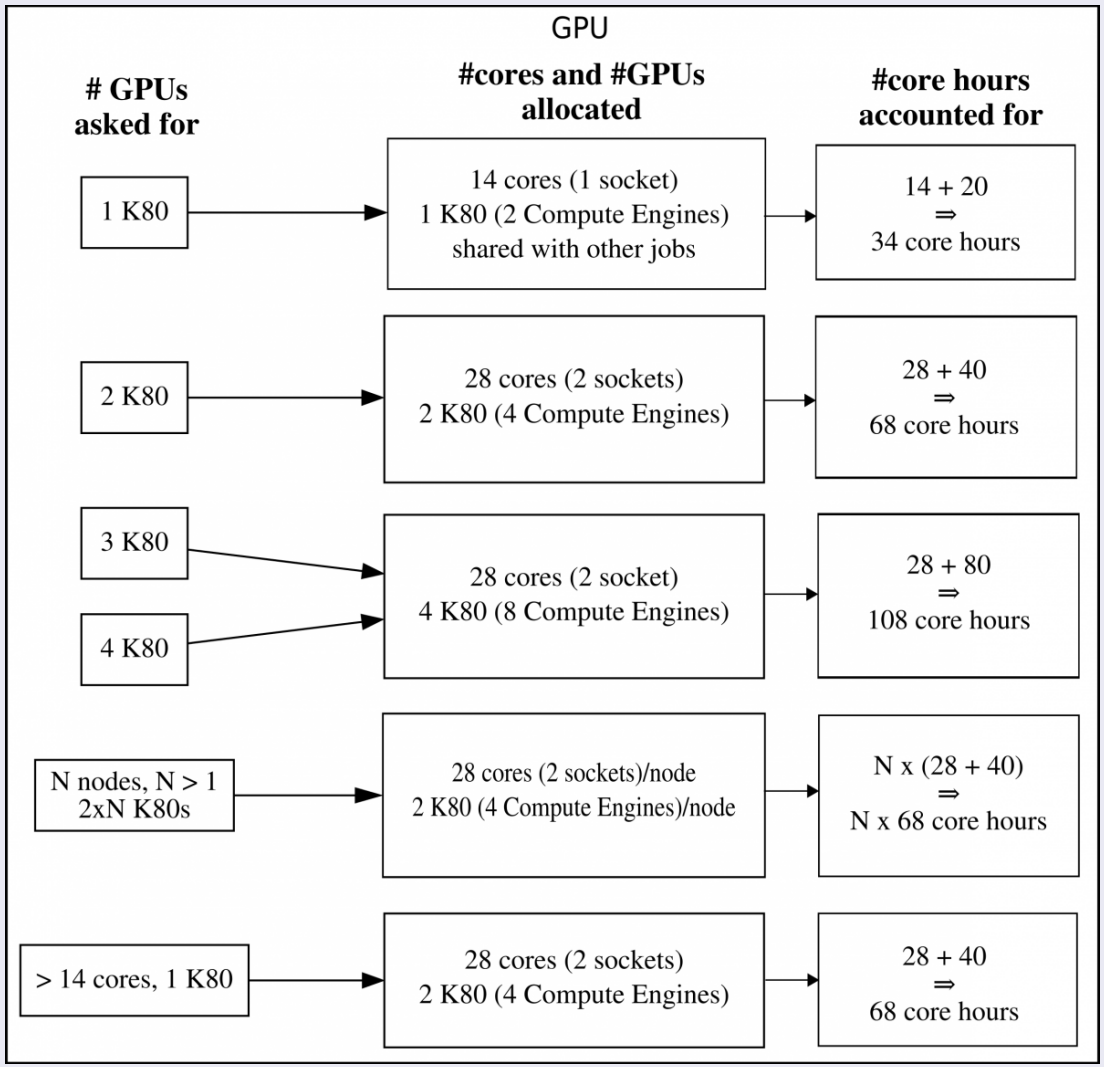
The Batch System

Accounting, largemem nodes, Kebnekaise



The Batch System

Accounting, GPU nodes, Kebnekaise



The Batch System (SLURM)

Useful Commands

- Submit job: `sbatch <jobscript>`
- Get list of your jobs: `squeue -u <username>`
- `srun <commands for your job/program>`
- `salloc <commands to the batch system>`
- Check on a specific job: `scontrol show job <job id>`
- Delete a specific job: `scancel <job id>`

The Batch System (SLURM)

Job Output

- Output and errors in:
  `slurm-<job id>.out`
- Look at it with vi, nano, emacs, cat, less...
- To get output and error files split up, you can give these flags in the submit script:
  `#SBATCH --error=job.%J.err`
  `#SBATCH --output=job.%J.out`
- To run on the 'fat' nodes, add this flag to your script:
  `#SBATCH -p largemem` (Kebnekaise - largemem does not have general access)
  `#SBATCH -p bigmem` (Abisko)

The Batch System (SLURM)

Simple example, serial

Example: Serial job on Kebnekaise, compiler toolchain 'foss'

```
#!/bin/bash
# Project id - change to your own after the course!
#SBATCH -A SNIC2017-3-81
# Asking for 1 core
#SBATCH -n 1
# Asking for a walltime of 5 min
#SBATCH --time=00:05:00

# Always purge modules before loading new ones in a
script.   module purge
ml foss/2017b

./my_serial_program
```

Submit with:

`sbatch <jobscript>`

The Batch System (SLURM)

Example, MPI C program

```
#include <stdio.h>
#include <mpi.h>

int main (int argc, char *argv[])

int myrank, size;

MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Comm_size(MPI_COMM_WORLD, &size);

printf("Processor %d of %d:  Hello World!\n", myrank,
size);

MPI_Finalize();
```

The Batch System (SLURM)

Simple example, parallel

Example: MPI job on Kebnekaise, compiler toolchain 'foss'

```
#!/bin/bash
#SBATCH -A SNIC2017-3-81
#SBATCH -n 14
#SBATCH --time=00:05:00
##SBATCH --exclusive
#SBATCH --reservation=hpc2n-intro

module purge
ml foss/2017b

srun ./my_parallel_program
```

The Batch System (SLURM)

Simple example, output

Example: Output from a MPI job on Kebnekaise, run on 14 cores (one NUMA island)

```
b-an01 [~/pfs/slurm]$ cat slurm-15952.out

The following modules were not unloaded:
   (Use "module --force purge" to unload all):

  1) systemdefault   2) snicenvironment
Processor 12 of 14: Hello World!
Processor 5 of 14: Hello World!
Processor 9 of 14: Hello World!
Processor 4 of 14: Hello World!
Processor 11 of 14: Hello World!
Processor 13 of 14: Hello World!
Processor 0 of 14: Hello World!
Processor 1 of 14: Hello World!
Processor 2 of 14: Hello World!
Processor 3 of 14: Hello World!
Processor 6 of 14: Hello World!
Processor 7 of 14: Hello World!
Processor 8 of 14: Hello World!
Processor 10 of 14: Hello World!
```

The Batch System (SLURM)

Requesting GPU nodes

Currently there is no separate queue for the GPU nodes

- You request GPU nodes by adding the following to your batch script:
  `#SBATCH --gres=gpu:k80:x` where `x=1, 2, 4`
- x = the number of K80 cards, each with 2 GPU engines
- There are 32 nodes with dual K80 cards and 4 nodes with quad K80 cards

Note: This is only valid on Kebnekaise. Abisko has no GPUs.

The Batch System (SLURM)

Longer example

```
#!/bin/bash
#SBATCH -A SNIC2017-3-81
#SBATCH -n 14
#SBATCH --time=00:05:00
#SBATCH --reservation=hpc2n-intro

module purge
ml foss/2017b

echo "Running on hosts:  $SLURM_NODELIST"
echo "Running on $SLURM_NNODES nodes."
echo "Running on $SLURM_NPROCS processors."
echo "Current working directory is `pwd`"

echo "Output of srun hostname:"
srun /bin/hostname

srun ./mpi_hello
```