Introduction to Abisko

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Why?

- Computations take too long time
  - Use an already parallelized software
  - Doing it yourself
    - Doing it yourself
      - Run each instance on a separate core
      - If inside a loop, maybe suitable for simple parallelization
    - More complex problems requires more explicit parallel programming
- Use your computer for other things
- Requires a lot of memory (up to 256 GB main memory)
- Solve larger (more interesting/realistic) problems

SUPR - SNIC User and Project Repository

1. Get a login at SUPR (`https://supr.snic.se/`)
2. Create a proposal for a project
   (at least: Title, Abstract, Resource Usage, Classification, length of project (1-12 months), which resource(s) you wish to use, and the amount of core hours/month you need.)
3. Get an account at HPC2N

Small level requests

- Max 5000 core hours/month/resource (Abisko)
- Can be submitted at any time (short abstract)
- Applications handled locally at the SNIC centers
- For small projects and new groups that want to gain experience in using HPC systems
- The PI must be employed at a Swedish university (e.g., PhD student or higher)

Medium level requests

- Up to 160000 core hours/month/resource (Abisko)
- Can be submitted at any time
- Applications handled locally at the SNIC centers and assesses the feasibility of using the requested recourses
- Evaluated once a month
- The PI must be a senior scientist in Swedish academia

Large level requests

- Above the medium level (160000 on Abisko)
- Calls for proposals for large level allocations are issued twice a year by SNAC
- Applications are evaluated by SNAC and they also decides on the allocations, based on scientific merit, need for the resources, efficient use of the resources, and impact
- The PI must be a senior scientist in Swedish academia

User Account

- Submit an account application using our online form
  - Name and affiliation
  - Which project you are taking part in (if any)
  - Choose a user name
- Print the final form twice
  - Sign and send one to us together with a copy of your passport (do NOT send by email)
  - Keep one (your initial password is on it)

User Support

- `www.hpc2n.umu.se`
  - Quick-start guides
  - How to access, compile, and submit
  - Installed software
    - Descriptions and how to use them at HPC2N
- `support@hpc2n.umu.se`
  - Problems
  - Requests

User Support

User Support

- Meetings with individuals or groups
  - To see how can HPC2N be of help
  - Help to get started
  - Help to parallelize
- HPC2N Think Tank - Open house
- Courses (0.5 - 3 days)
  - Introduction on how to use our system
  - Parallel programming (MPI, OpenMP)
  - ...

Abisko

- 332 nodes/15936 cores
- 10 fat nodes (512 GB RAM), 318 thin nodes (128 GB RAM)
- CPUs: (thin) 4 x AMD Opteron 6238 (Interlagos) 12 core (2.6 GHz)
- CPUs: (fat) 4 x AMD Opteron 6344 (Abu Dhabi) 12 core (2.6 GHz)
- Interconnect: Infiniband QDR, 40Gb/s, Mellanox
- Installed 2011

Abisko

- Application software: Abinit, Ansys, DDT, Espresso, Gamess, Gaussian, Gromacs, HDF5, Matlab, NetCDF, NWChem, Octave, PETSc, R, Siesta, VASP, WRF, ...
- Num. and Comm. libraries: BLACS, FFTW, BLAS, LAPACK, ScaLAPACK, ACML, Intel MKL, ParMETIS, RECSY, SLICOT, ...
- MPI: OpenMPI, Intel MPI
- Other software on request

Connecting from a Windows System

You need an ssh client to connect.

- PuTTY
- Cygwin

If you want to open graphical displays, you need an X11 server

- Xming
- Cygwin

Transferring files (sftp or scp)

- WinSCP
- FileZilla (only sftp)
- PSCP/PSFTP

Connecting from a UNIX/Linux System

- Login with ssh:
  ```
  local> ssh username@abisko.hpc2n.umu.se
  ```
- If you want to open graphical displays, you need to enable X11 Forwarding:
  ```
  local> ssh -X username@abisko.hpc2n.umu.se
  ```
- Use scp for file transfer:
  ```
  local> scp username@abisko.hpc2n.umu.se:file /tmp
  local> scp file username@abisko.hpc2n.umu.se:file
  ```

Modules

- Many versions of software packages
- Use a tool called modules
  - Can choose a combination of libraries and compilers that will work together
  - Changes the environment
  - User guide and man-page

Modules

- Some useful module commands

help	list all module commands
show	display information on a module
add	add a module to the environment
rm	remove a module from the environment
list	list currently activated modules
avail	list all modules that exist on the system

- Examples
  - `module add pgi`
    will add the latest version of the Portland compilers
  - `module add openmpi/pgi`
    will add the latest version of openmpi (suitable for the current machine) that was built with the Portland compilers

File Systems

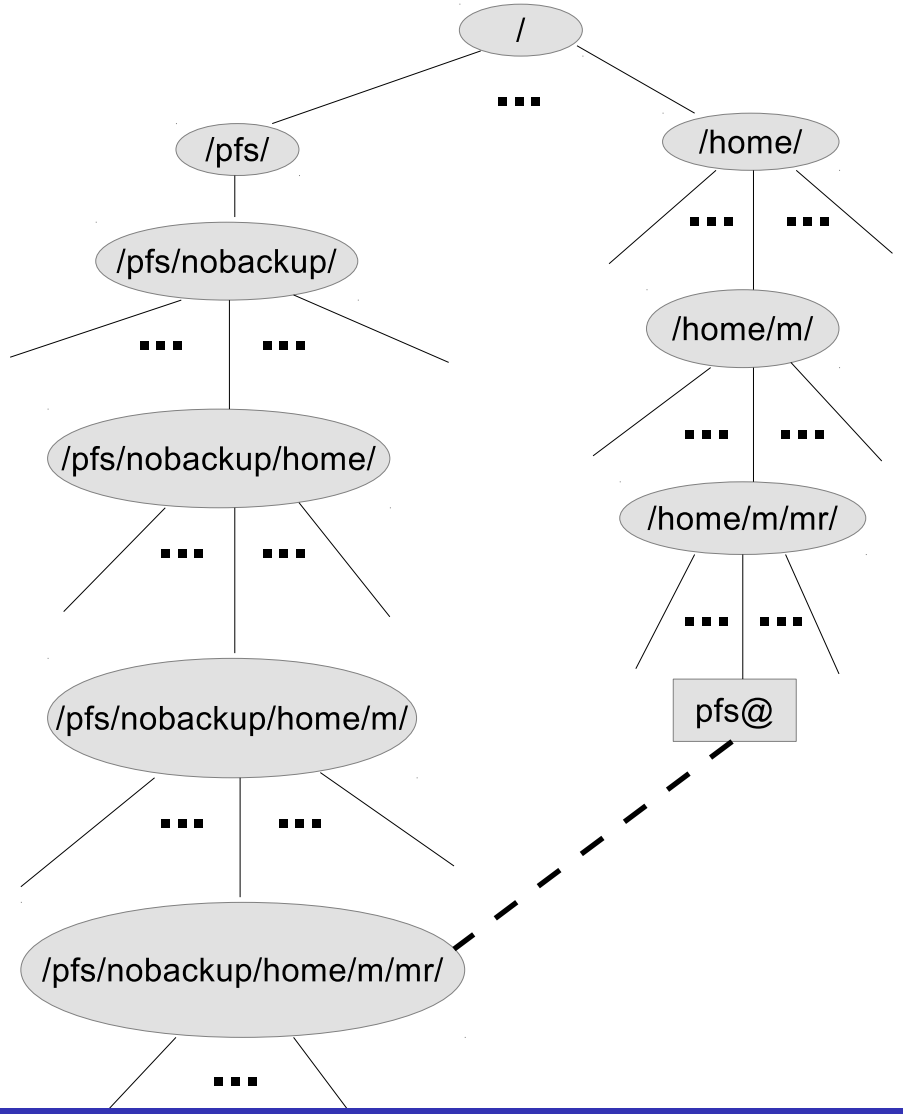
There are 2 file systems

AFS

- Your home directory
- Backed up regularly
- NOT accessable by the batch system

PFS

- Parallel file system
- NO BACKUP
- Accessable by the batch system



PFS

- Offers high performance when accessed from the nodes
- To create soft link from your home directory to your corresponding home on the parallel file system
  `ln -s /pfs/nobackup$HOME $HOME/pfs`
- Then if you use
  `cd pfs`
  from your home directory you will end up in your "parallel" home directory

Batch System (SLURM)

- Large/parallel programs, run through the batch system
- Keeps track of available system resources
- Takes care of scheduling jobs of multiple users, running tasks simultaneously
- Enforces local system resource usage and job scheduling policies
- Users submit to a queue (running, idle, blocked)

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

- Submitting:
  `sbatch <jobscript>`
- Show the job queue:
  `squeue [-u username]`
- Delete a job:
  `scancel <jobid>`

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Your account (-A)

- The account is your project id
- Low priority if not set
- You can find your project id by running: `projinfo`

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Number of tasks (-n)

- The number of tasks is for the most cases the number of processes you want to start.
- The default value is one
- e.g. number of MPI tasks
- e.g. number of serial programs

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Number of cores per task (-c)

- For multi threaded applications (OpenMP/pthreads/...)
- indicates the number of cores each task can use
- The default value is one
- Maximum is 48

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

The run/wallclock time
`D-HH:MM:SS`

- Runtime (wall clock time) of your job
- Try to estimate correctly
  - Hard limit
  - Shorter jobs are more likely to fit into slots of unused space faster.

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Load modules needed or other things. (This is for your program that is compiled with the PathScale compiler and the OpenMPI library.)

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Run your MPI application using `srun`

- Starts the required number of processes
- Note! If your program is serial it will start many instances

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Run your multi threaded application on 36 cores.
Change the marked lines with:

```
#SBATCH -c 32

export OMP_NUM_THREADS=36

./my_OpenMP_program args
```

Job script

```
#!/bin/bash
#SBATCH -A SNICYYYY-XX-NN
#SBATCH -n 48
#SBATCH --time=01:00:00

module add openmpi/psc
srun ./parallel_prog args
```

Output

- Put stdout into the file <*jobid*>.out
  `#SBATCH --output=%J.out`
- Put stderr into the file <*jobid*>.err
  `#SBATCH --error=%J.err`
- By default both to slurm-<*jobid*>.out

Input

- Use `file.txt` as stdin
  `#SBATCH --input=file.txt`

Simple hands-on

1. Log in to Abisko.
2. Go to the parallel file system.
3. Copy executable (threaded program)and submit file:
   `cp ~mr/Public/mandel .`
   `cp ~mr/Public/submit .`
4. Put the submit file into the batch queue.
5. Look at the queue.
6. Where did the output from the program go?
7. Run on 12 cores instead. Does it run twice as fast?
8. The program creates a picture on a file (`mandel.ppm`) as output. Try looking at it (e.g. using the command `display`).