Introduction to HPC2N

Course: R in an HPC environment

Overview

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Connecting to Kebnekaise

1. **ThinLinc** is recommended
2. Download the client from https://www.cendio.com/thinlinc/download
3. Install the client and start it.
4. Enter the servername: *kebnekaise-tl.hpc2n.umu.se*. Enter your username under ”Username”.
5. Go to ”Options” -> ”Security” and check that authentication method is set to password.
6. Go to ”Options” -> ”Screen”. Uncheck ”Full screen mode”.
7. Enter your HPC2N password. Click ”Connect”
8. More information here: https://www.hpc2n.umu.se/documentation/guides/thinlinc

Connecting to Kebnekaise - other SSH clients

1. Linux, macOS:

- Connect with `ssh username@kebnekaise.hpc2n.umu.se`
- Opening a gui? Use `ssh -Y username@kebnekaise.hpc2n.umu.se`
- For macOS you may need to install XQuartz first

2. Windows:

- Get SSH client (MobaXterm, PuTTY, Cygwin ...)
- Get X11 server if you need graphical displays (Xming, ...)
- Start client. Login with HPC2N username to `kebnekaise.hpc2n.umu.se`

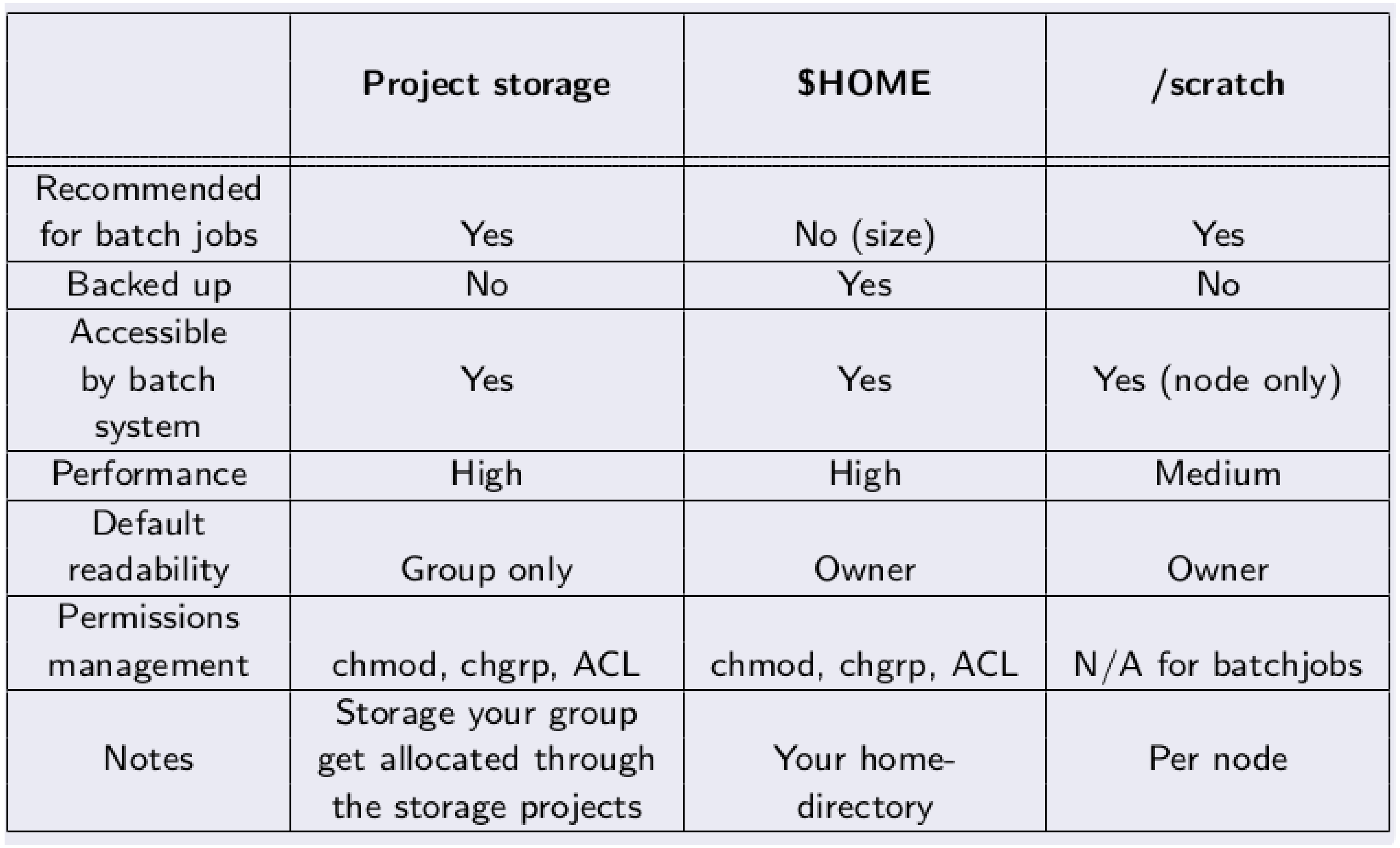
Editors

Editing your files on Kebnekaise (OS: Linux Ubuntu)

- Several editors available; vi/vim, nano, emacs...
- vi/vim:
  - Open/create file: `vi <filename>`
  - Insert before: `i`
  - Save and exit: Press ESC and then type ```:wq``
- nano:
  - Open/create file: `nano filename`
  - Save and exit: Ctrl-x (Press CTRL and x together)

File system

More info: http://www.hpc2n.umu.se/filesystems/overview



	Project storage	$HOME	/scratch
Recommended for batch jobs	Yes	No (size)	Yes
Backed up	No	Yes	No
Accessible by batch system	Yes	Yes	Yes (node only)
Performance	High	High	Medium
Default readability	Group only	Owner	Owner
Permissions management	chmod, chgrp, ACL	chmod, chgrp, ACL	N/A for batchjobs
Notes	Storage your group get allocated through the storage projects	Your home-directory	Per node

The module environment

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

Modules:

- are used to set up your environment (paths to executables, libraries, etc.) for a particular (set of) software package(s)
- help users manage their Unix/Linux shell environment, allows groups of related environment-variable settings to be made/removed dynamically
- allows access to multiple versions of a program/package by loading a module
- are installed in a hierarchial layout; some modules are only available after loading a specific compiler and/or MPI version

Compiler toolchains: software-bundles for complete environments (compilers, prebuilt software). Includes: compiler suite, MPI, BLAS, LAPACK, ScaLapack, FFTW, CUDA.

Loading the R module

Check existing modules (versions): `ml spider R`

- We recommend `R 4.0.4` on Kebnekaise
- To check how to load this and any prerequisites: `ml spider R/4.0.4`
- Load the module: `ml GCC/10.2.0 OpenMPI/4.0.5 R/4.0.4`
- Loading (with CUDA support): `ml GCC/10.2.0 CUDA/11.1.1 OpenMPI/4.0.5 R/4.0.4`
- To see other available R versions: `ml spider R`
- To see available modules in general: `ml spider` and `ml avail`

You start R by typing `R` on the command line.

R packages needed for this course

- **parallel**
- **Rmpi**
- **foreach**
- **doParallel**
- **cluster**
- **boot**
- knor (now called clusternor)

Most of these packages (marked above in **bold**) are available as extensions to the R module on Kebnekaise and so are loaded together with the R module. You can see a list of extensions with `ml spider R/4.0.4`.

Available R packages

In general: to see which packages are available in your R version, start R and enter this:

```
installed.packages()
```

In some cases entering these four lines will give a more thorough result:

```
ip <- as.data.frame(installed.packages()[,c(1,3:4)])
rownames(ip) <- NULL
ip <- ip[is.na(ip$Priority),1:2,drop=FALSE]
print(ip, row.names=FALSE)
```

Installing your own R packages - setup

First create a folder for installing your own R libraries:

```
mkdir $HOME/<path-to-folder>/R-packages-4.0.4/
export R_LIBS_USER=$HOME/<path-to-folder>/R-packages-4.0.4/
```

Change to the location of your R package folder (or remove if no subdir). There should be a folder for each version of R - in this case R 4.0.4 if on Kebnekaise.

Installing your own R packages

Installing from inside R (once per package):

- Find the name of the package. Load the "R" module. Start the "R" program
- Type “install.packages(“RPACKAGE”)”, where RPACKAGE should be changed to the name of the package in question. Press the Enter/Return key.
- If you have not installed other packages during this session, you will be prompted to choose a mirror to download from.
- When the prompt is again ">" the package has finished downloading and installing.

From command line (if no dependencies and R module loaded):

-
```
R --quiet --no-save --no-restore -e "install.packages('RPACKAGE',
repos='http://ftp.acc.umu.se/mirror/CRAN/')"
```

Installing your own R packages

Manual download and install

- Download from the package from http://cran.r-project.org/ or elsewhere (GitHub etc.)
- Load the "R" module
- Install with `R CMD INSTALL -l $HOME/R-packages-4.0.4 RPACKAGE.tar.gz` (change to your chosen R package directory and name of R package in question)

Regardless of how you installed the R package, you can now use it the same way as other R packages: by loading it inside R with the command `library("RPACKAGE")`

Installing other R packages

While clsuternor is the only one of the needed packages not installed on Kebnekaise, there will likely be several to install on your own computer.

NOTE: if you are using Linux Ubuntu (R installed with `sudo apt-get install r-base`), some packages can be installed from the Ubuntu repo:

- r-cran-rmpi r-cran-foreach r-cran-doparallel r-cran-cluster r-cran-boot

Install the "parallel" package with `install.packages(c("parallel"))` from within R.

Check with `installed.packages()` (from inside R) which are installed.

Installing R packages for the course

- Install help, all OS: https://www.hpc2n.umu.se/events/courses/2022/R-in-HPC/setup
- Specific for Linux Ubuntu: https://umeauniversity.sharepoint.com/:w:/s/HPC2N630/EeLAM89iSrhHuMbduJkzjDwBoqxTHNo5TF6b0TplvaoLPw?e=gxgW4p

Installing the R package "clusternor" on Kebnekaise

"clusternor" package (https://github.com/neurodata/knorR)

- Setup a directory for R packages (already done if you have installed packages).
  - Add `R_LIBS_USER="path/to/rpackages"` to the file .Renviron (change "path/to/rpackages" to actual location)
  - Example: `R_LIBS_USER="/proj/nobackup/support-hpc2n/bbrydsoe/R-packages-%V"`
- Since "clusternor" is no longer on CRAN, we have to install from their GitHub.
- `git clone --recursive https://github.com/flashxio/knorR.git`
- cd knorR
- ./install.sh

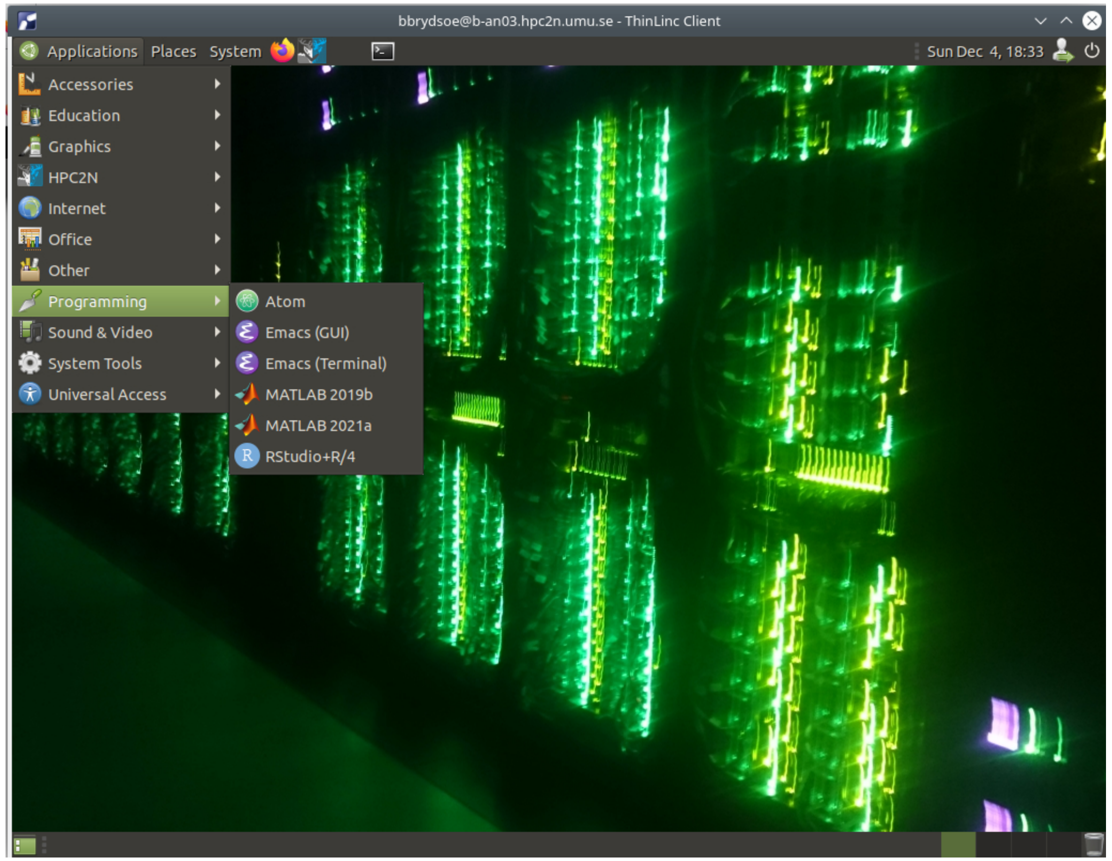
Installing Rstudio - own computer

To install Rstudio on your own computer, see the links on setup:

- https://www.hpc2n.umu.se/events/courses/2022/R-in-HPC/setup
- Specific for Linux Ubuntu: https://umeauniversity.sharepoint.com/:w:/s/HPC2N630/EeLAM89iSrhHuMbduJkzjDwBoqxTHNo5TF6b0TplvaoLPw?e=gxgW4p

Accessing Rstudio on Kebnekaise

To use Rstudio on Kebnekaise, you need to connect using ThinLinc as it is not installed on the regular login nodes. It matches R 4.0.4.



Running longer/paralle R programs

- Large/long/parallel jobs **must** be run through the batch system
- SLURM is an Open Source job scheduler. It 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
- To run a batch job, you need a SLURM submit file (batch submit file, batch script, job script ...)
- When submitting jobs to the batch system, you **must** use the course project!
- Guides and documentation at: http://www.hpc2n.umu.se/support

Useful commands to the Batch System

- Submit job: `sbatch <jobscript.sh>` (successful submission returns a job-id number)
- As default, output/errors are found in `slurm-<job-id>.out`
- Get list of all jobs: `squeue`
- Get list of only your jobs: `squeue -u <username>`
- Adding the flag `--start` gives the estimated job start time. This can change depending on other people's jobs.
- Check on a specific job: `scontrol show job <job id>`
- Delete a specific job: `scancel <job id>`
- Delete all your jobs: `scancel -u <username>`

SLURM batch script for a serial R job

```
#!/bin/bash
#SBATCH -A SNIC2022-22-1012 #Project id
#SBATCH -J my-serial-R-job #Name of job
#SBATCH --time=00:10:00 #Jobtime (HH:MM:SS) Max: 168H
#SBATCH -o Rjob_%j.out #Naming the output file
#SBATCH -e Rjob_%j.err #Naming the error file
#SBATCH -n 1 #Number of tasks (Default is 1 CPU/task. Change with --cpus-per-task)

ml purge > /dev/null 2>&1
ml GCC/10.2.0 OpenMPI/4.0.5 R/4.0.4

R --no-save --quiet < input.R > Rexample.out
```

SLURM batch script for a parallel R job, using Rmpi

NOTE that you need to load the Rmpi library within your R script for this to work. NOTE also that you can NOT spawn slaves with mpi.spawn.Rslaves()!

```
#!/bin/bash
#SBATCH -A SNIC2022-22-1012
#SBATCH -n 8
#SBATCH --time=00:30:00

ml purge > /dev/null 2>&1
ml GCC/10.2.0 OpenMPI/4.0.5 R/4.0.4

mpirun R -q -f <program>.R
```

SLURM batch script for a parallel R job, using doParallel

Assume we have a small R program, "doParallel.R":

```r
library(doParallel)
cl <- makeCluster(4)
registerDoParallel(cl)

# code that we want executed in parallel

stopCluster(cl)
```

SLURM batch script for a parallel R job, using doParallel - continued

Batch script to submit the R program on the previous slide:

```
#!/bin/bash
#SBATCH -A SNIC2022-22-1012
#SBATCH -t 00:10:00
#SBATCH -N 1
#SBATCH -c 4

ml purge > /dev/null 2>&1
ml GCC/10.2.0 OpenMPI/4.0.5 R/4.0.4

R -q --slave -f doParallel.R
```

Various useful info

- A project has been set up for the workshop: `SNIC2022-22-1012`
- You use it in your batch submit file by adding:
  - `#SBATCH -A SNIC2022-22-1012`
- Kebnekaise ThinLinc login node: `kebnekaise-tl.hpc2n.umu.se`
- Kebnekaise "regular" login node: `kebnekaise.hpc2n.umu.se`