Using a supercomputer
Hands-on introduction

Benjamin Czaja, Marco Verdicchio
HPC Advisors, SURFsara

Linux and Cluster Computing

1) Introduction

a. What is a computer?

b. What is a supercomputer?

c. How is a supercomputer different from the cloud

d. Access and usage

2) Introduction to Linux

a. Getting started

b. Usage and basic commands

c. Shell script programming

3) Running jobs on the HPC system

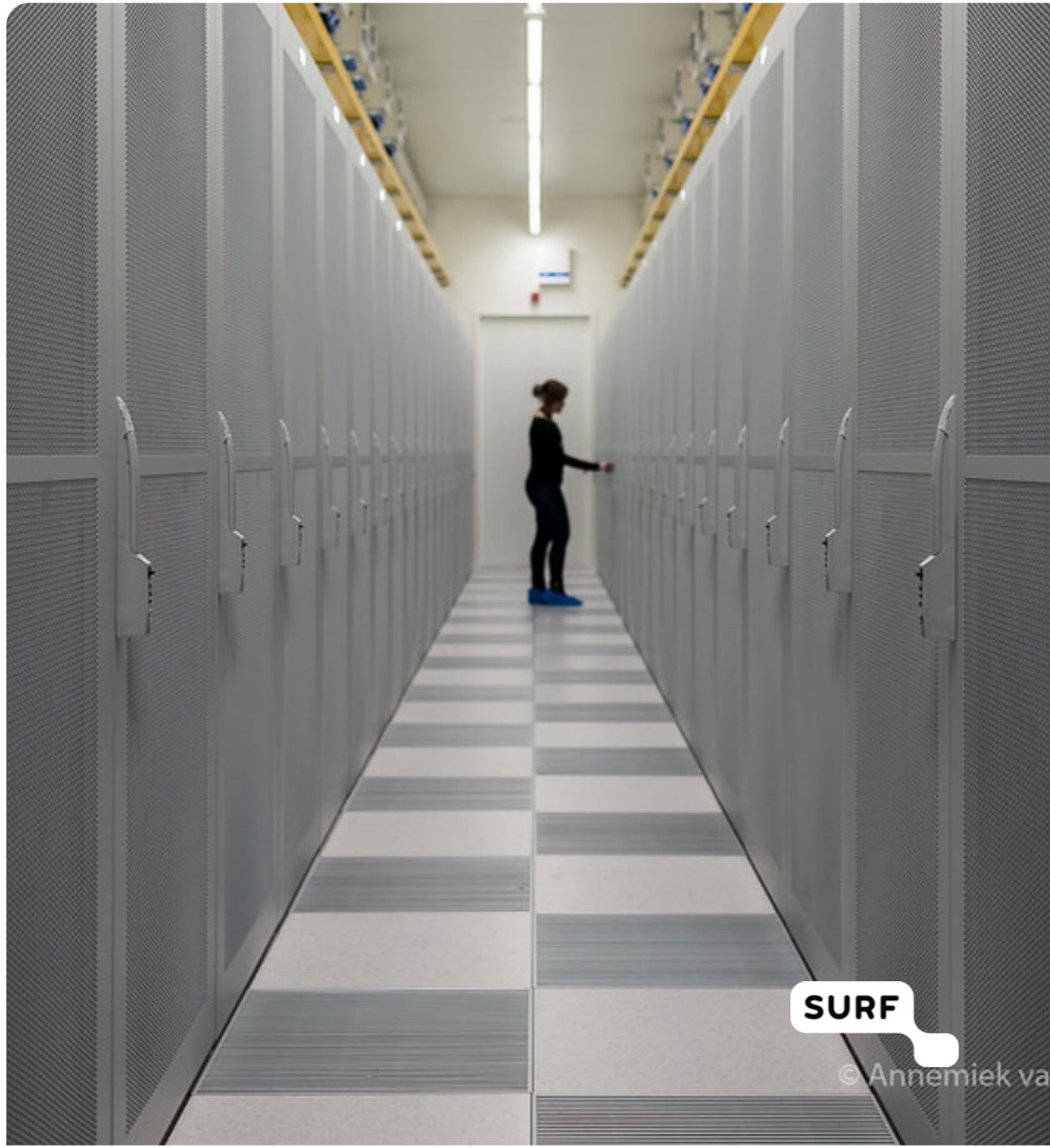
a) Interact with the batch scheduler

b) Run a “real” scientific workflow

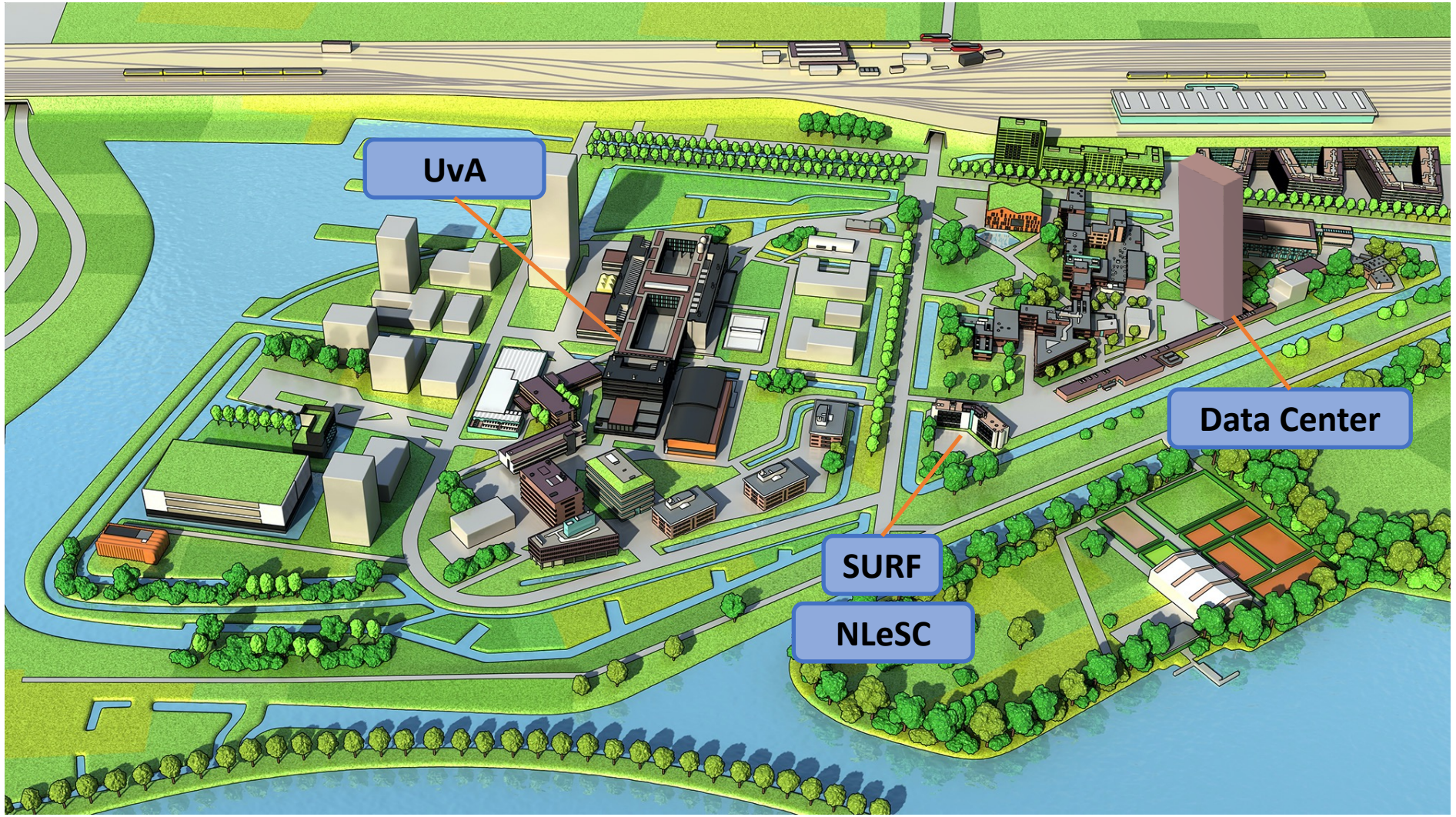
SURF Bootcamp
Hands-on introduction using a supercomputer

- **Slides and exercises**

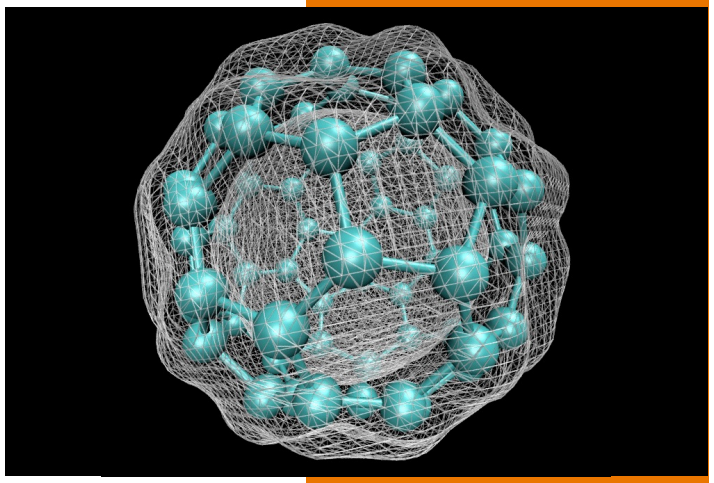
https://github.com/sara-nl/Intro-to-HPC



Location of SURF Amsterdam



High-performance computing (HPC) is …



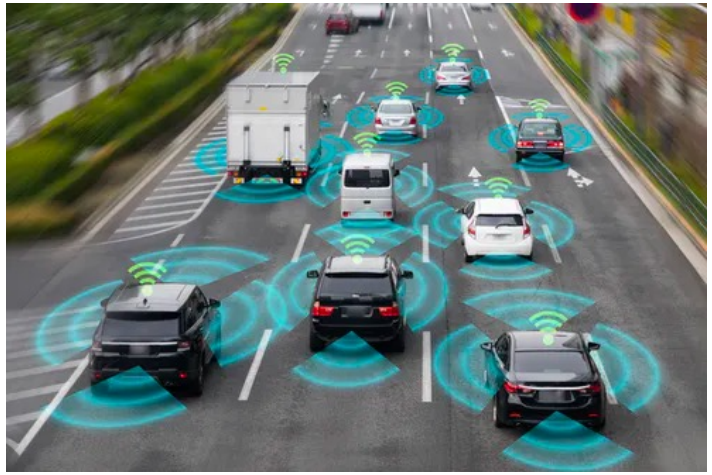


Image source: https://www.trustedreviews.com/news/gran-turismo-ps5-will-complete-form-series-3895762
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Image source: https://thestrategybridge.org/the-bridge/2016/8/16/a-new-plan-using-complexity-in-the-modern-world

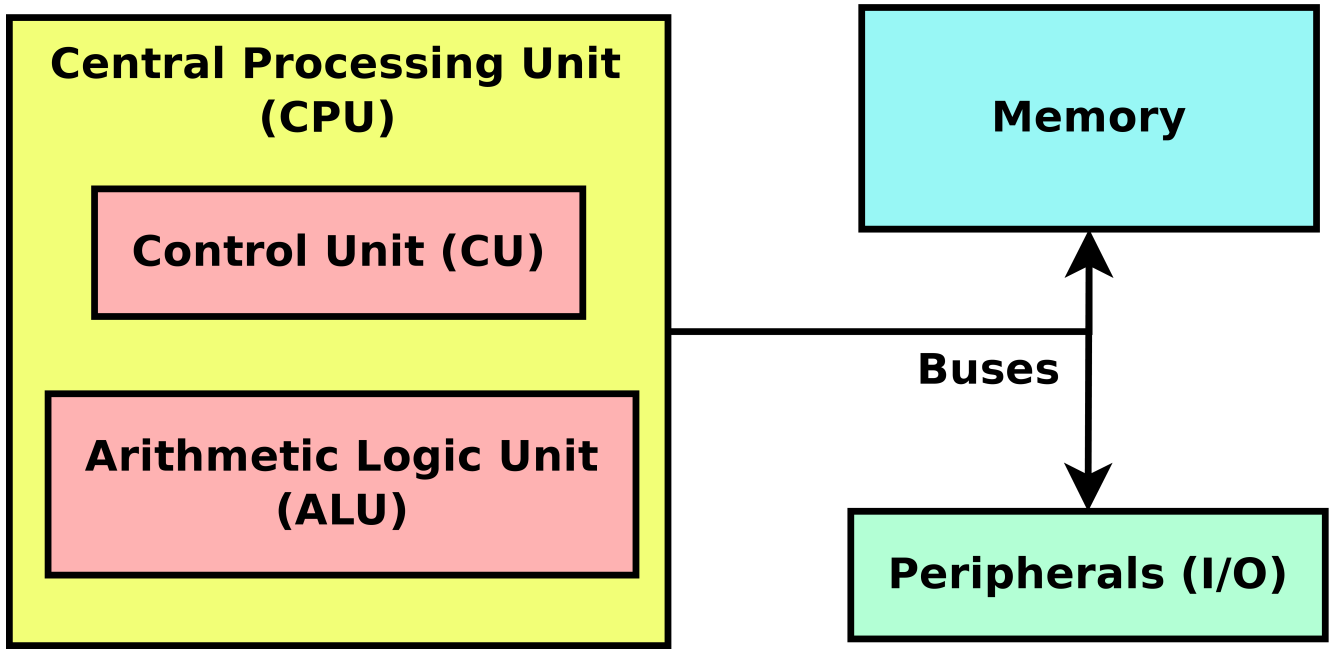
High-performance computing (HPC) …

- *… is an area of computer-based computation. It includes all computing work that requires a high computing capacity or storage capacity.*
- *… is the use of parallel processing for running advanced application programs efficiently, reliably and fast.*
- *… refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business.*
- *… is the use of super computers and parallel processing techniques for solving complex computational problems.*

WORKING WITH A SUPERCOMPUTER

a. What is a computer?
b. What is a supercomputer?
c. Access and usage

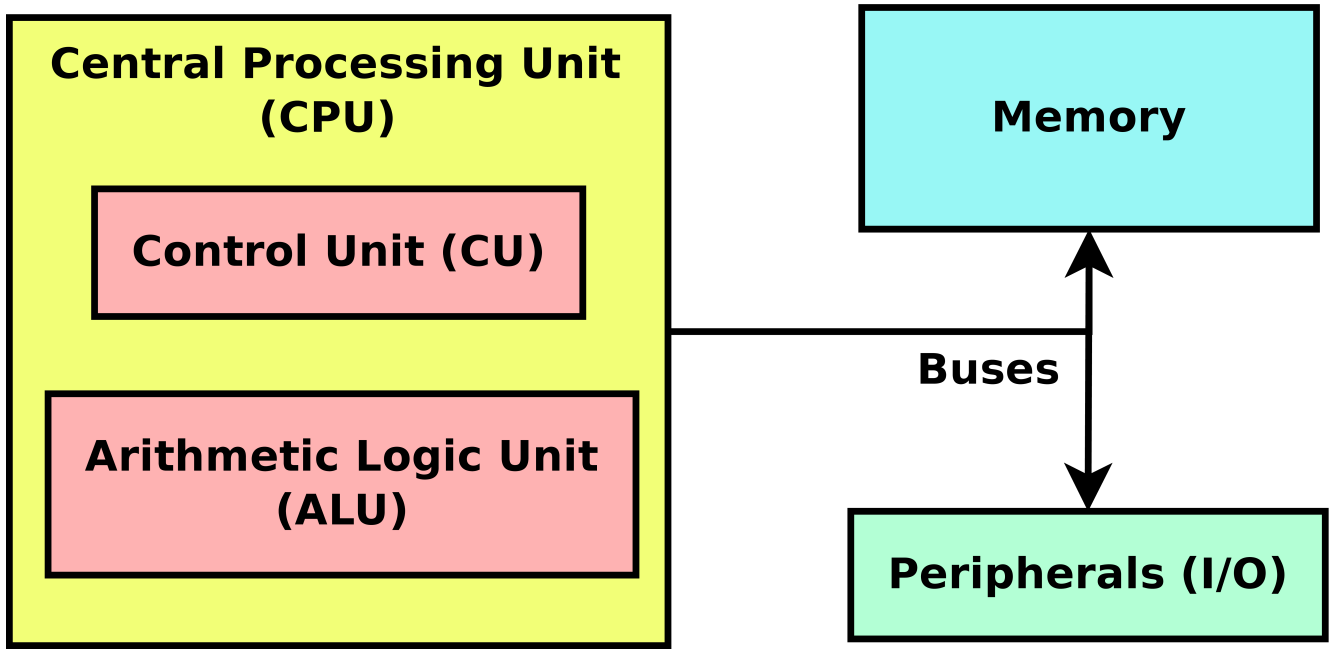
A computer is …



Peripherals (I/O) are …

Image source: https://media.sciencephoto.com/image/t4150120/800wm/T4150120-Piles_of_discarded,_redundant_computer_keyboards.jpg
Image source: https://static.guim.co.uk/sys-images/Guardian/Pix/pictures/2014/2/10/1392028631237/Pile-of-computer-monitors-008.jpg

A computer is …



A memory is …

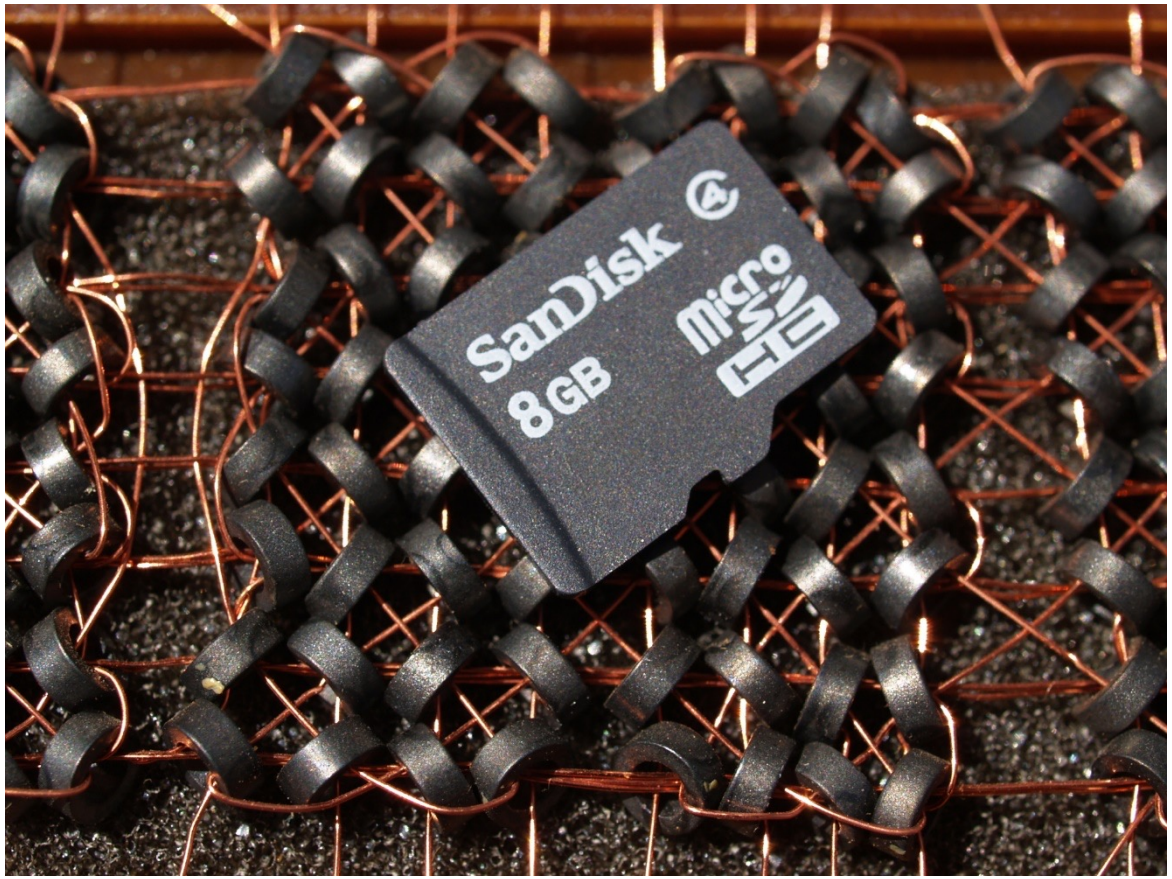
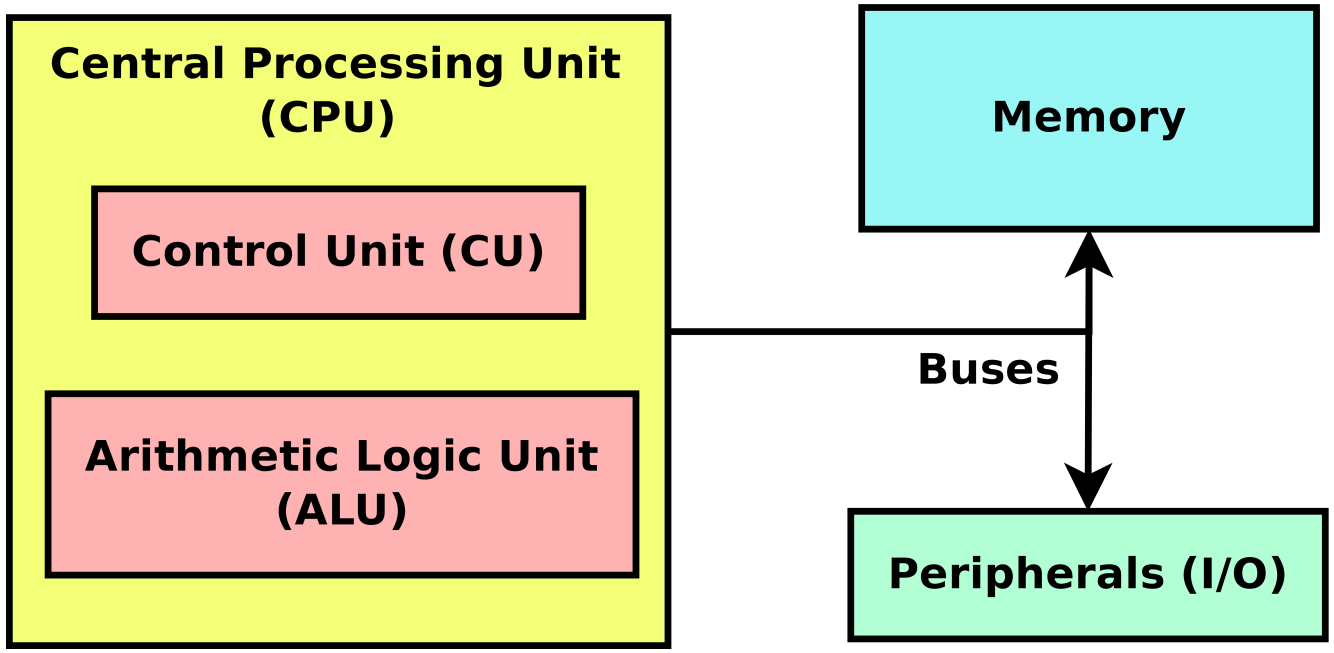
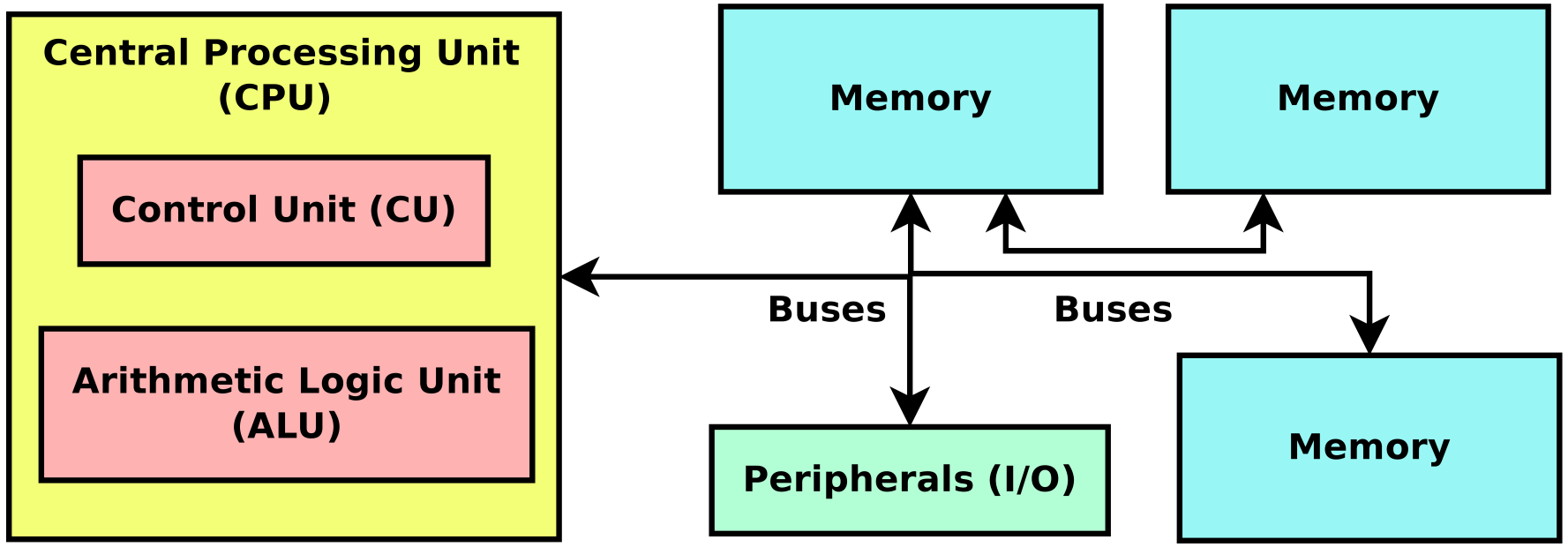


Image source: https://upload.wikimedia.org/wikipedia/commons/c/c0/8 bytes vs. 8Gbytes.jpg

A computer is …



A larger computer could be …



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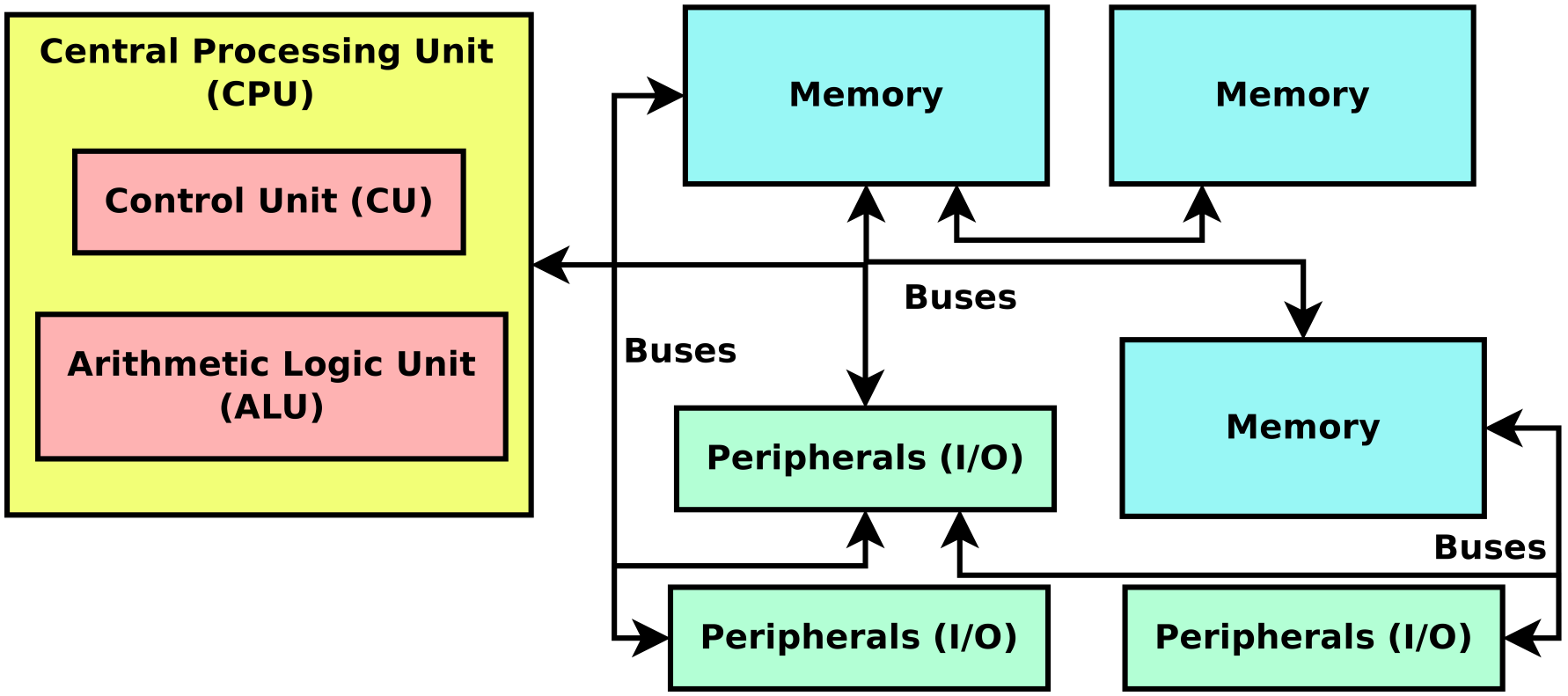

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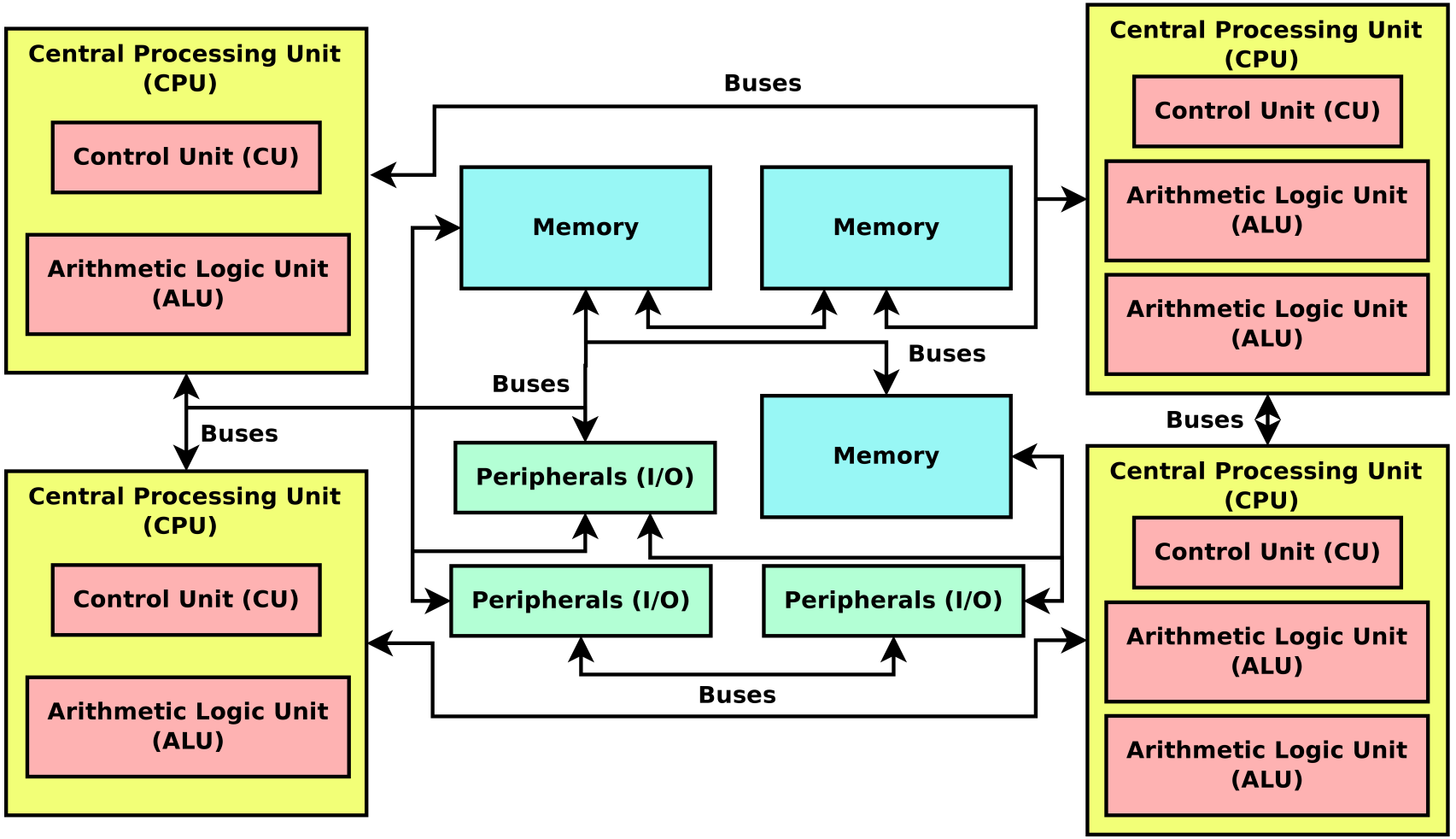

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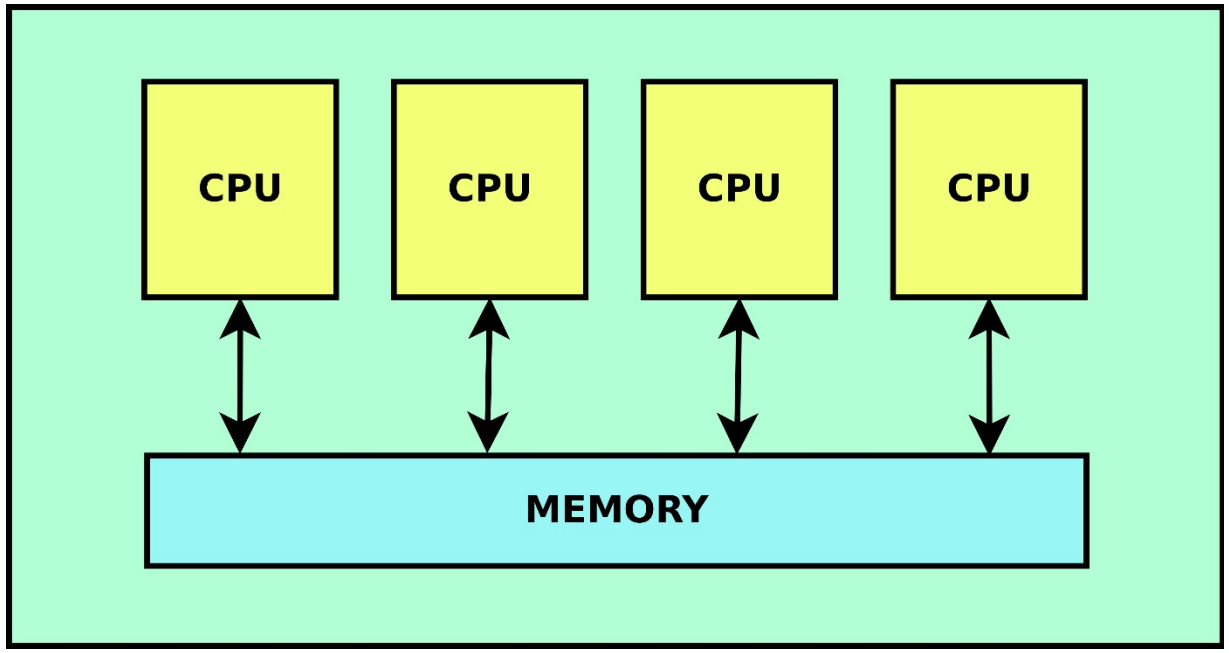

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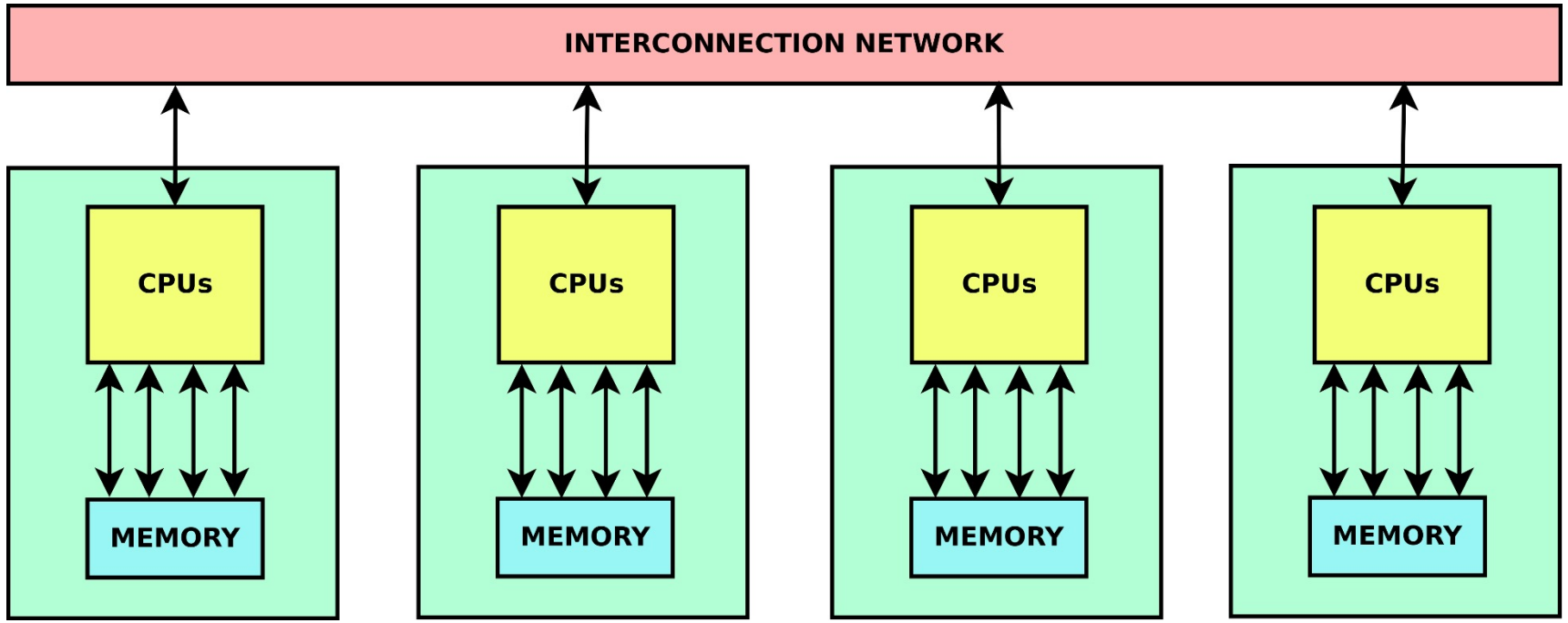

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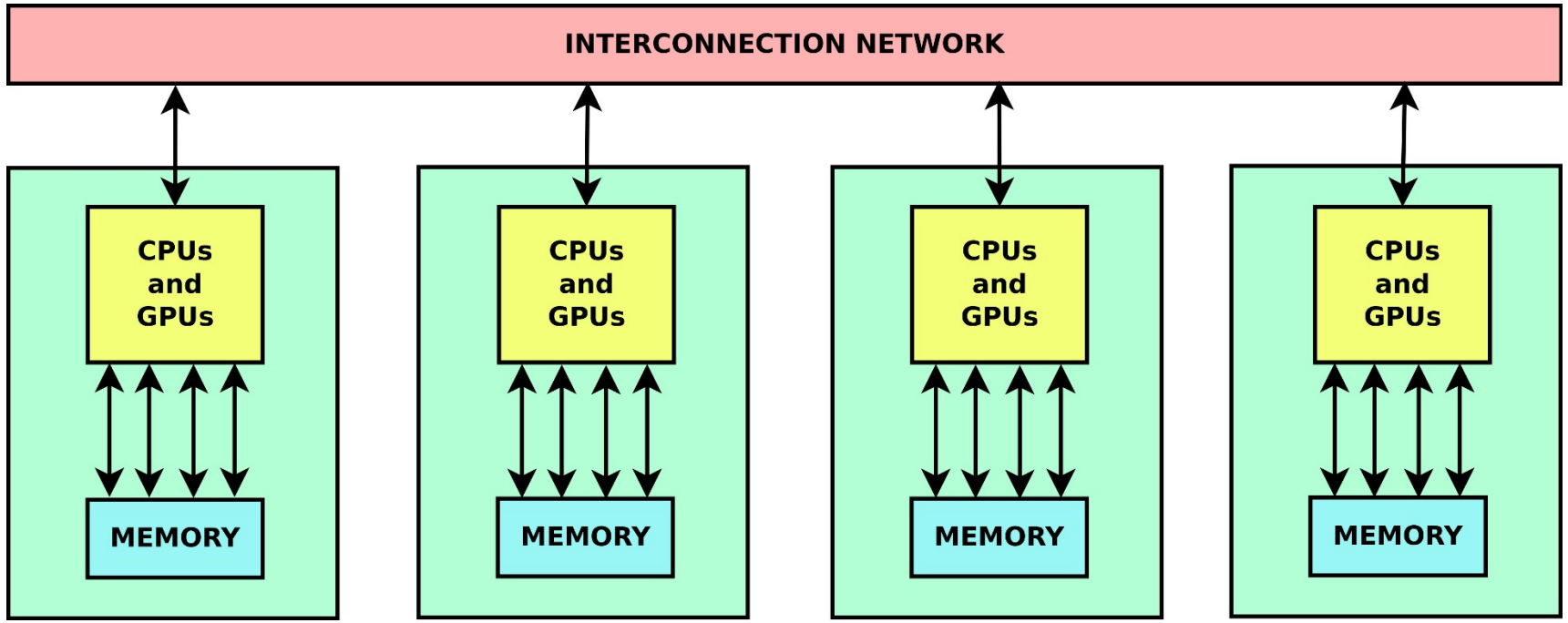


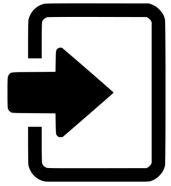
Schematic overview of a supercomputer

A compute cluster is a group of tightly couple operating system insteances that work together so closely that it can be seen as a single computer

Dutch national supercomputers: performance increase

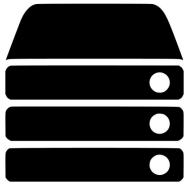
Year	Machine	R_{peak} (GFlop/s)	kW	GFlop/s/ kW
1984	CDC Cyber 205 1-pipe	0.1	250	0.0004
1988	CDC Cyber 205 2-pipe	0.2	250	0.0008
1991	Cray Y-MP/4128	1.33	200	0.0067
1994	Cray C98/4256	4	300	0.0133
1997	Cray C916/121024	12	500	0.024
2000	SGI Origin 3800	1,024	300	3.4
2004	SGI Origin 3800 +SGI Altix 3700	3,200	500	6.4
2007	IBM p575 Power5+	14,592	375	40
2008	IBM p575 Power6	62,566	540	116
2009	IBM p575 Power6	64,973	560	116
2013	Bull bullx DLC	250,000	260	962
2014	Bull bullx DLC	~ 1,000,000	520	1923
2017	Bull bullx DLC + KNL	~ 1,840,000	850	2168
2021	Lenovo AMD (1st phase)	~ 6,100,000	610	10000
2016	Raspberry PI 3 (35 euro)	0.44	0.004	110

Working with a Supercomputer



Login node(s)

- Editing and transferring files
- Compile programs
- Prepare simulations



Compute nodes

- Multicore nodes
- Large memories
- High-speed interconnections

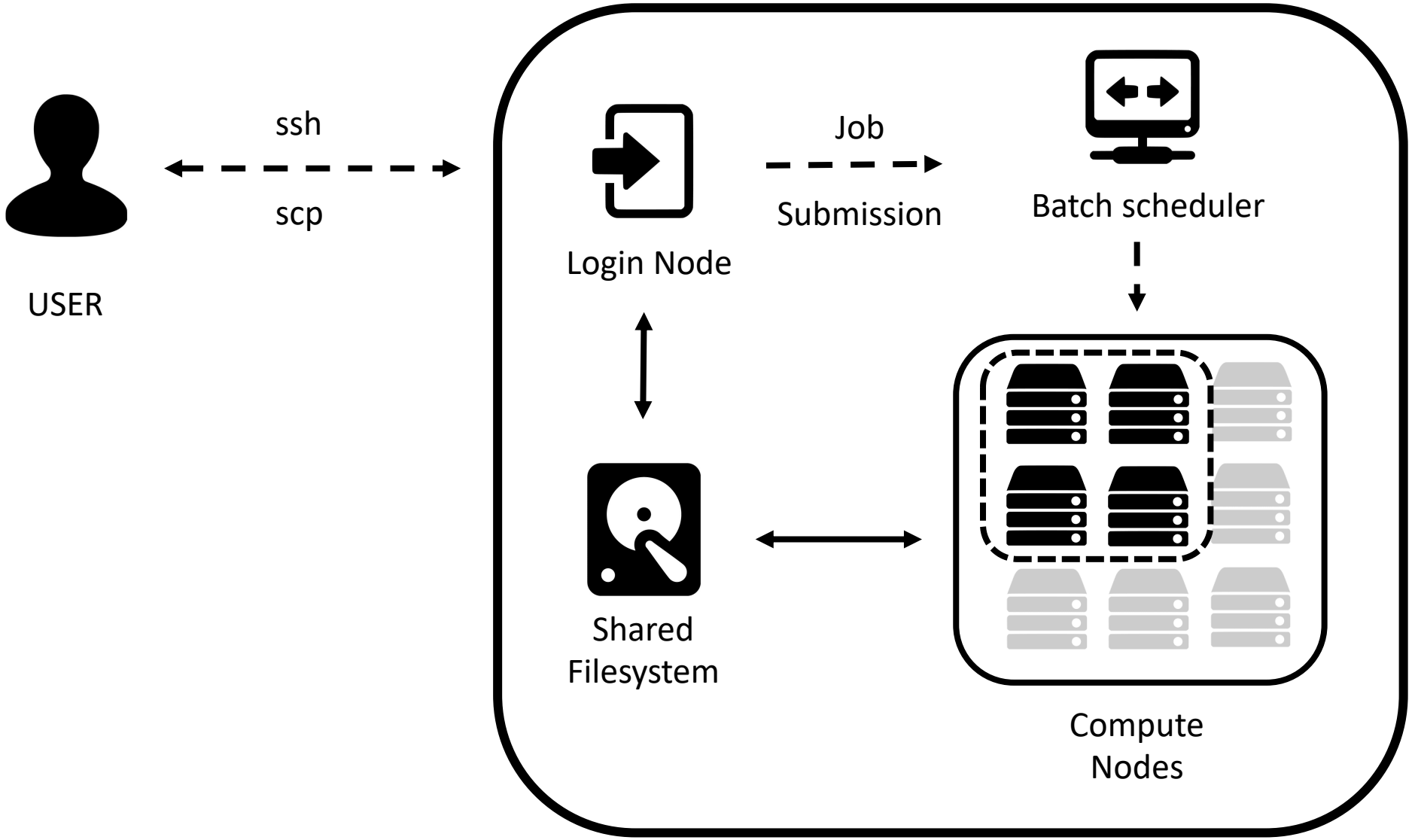
Batch scheduler

- Resource allocation
- Job queueing
- Accounting and

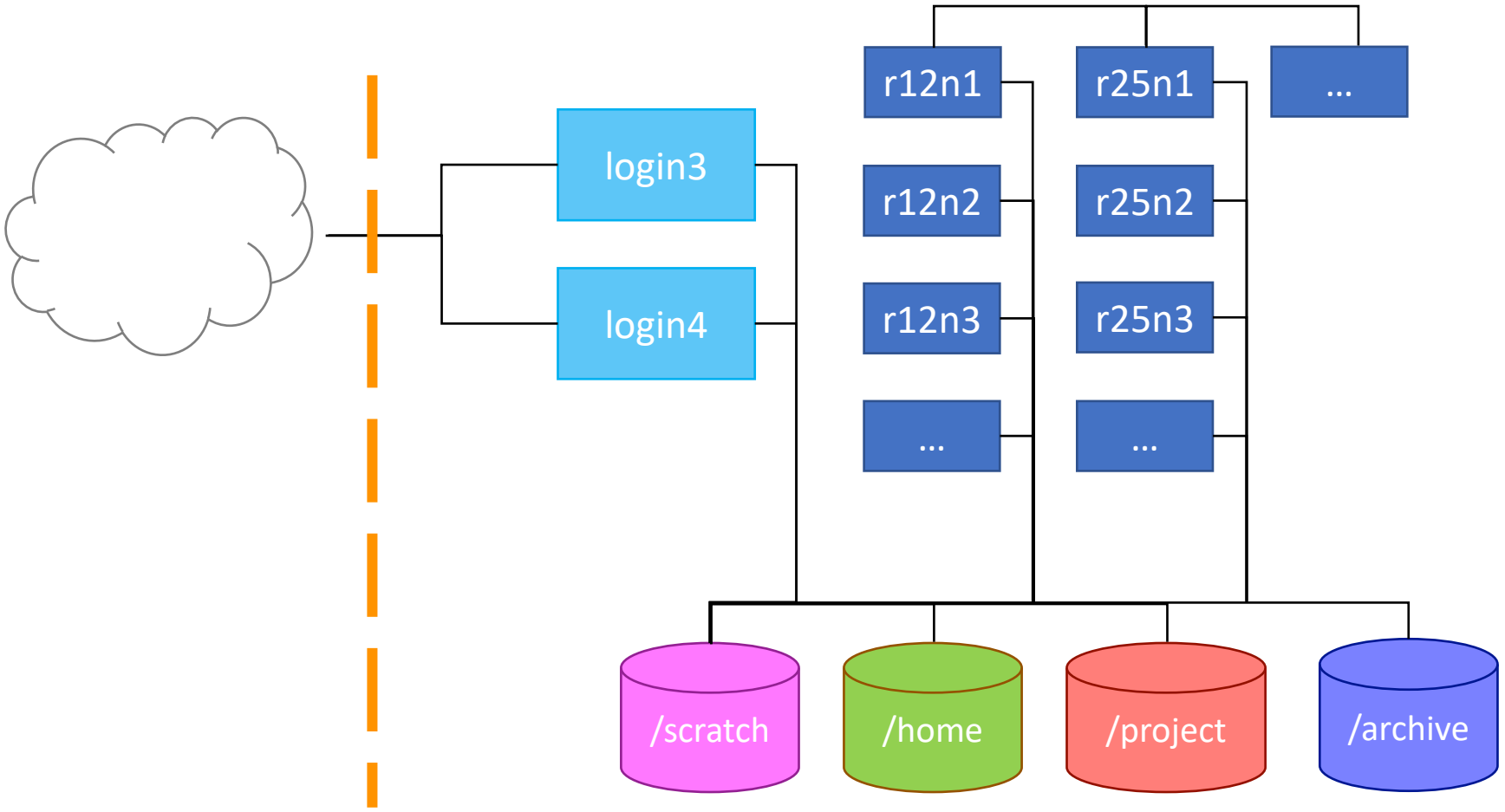
File system

- Parallel FS
- Efficient I/O
- Node local disks

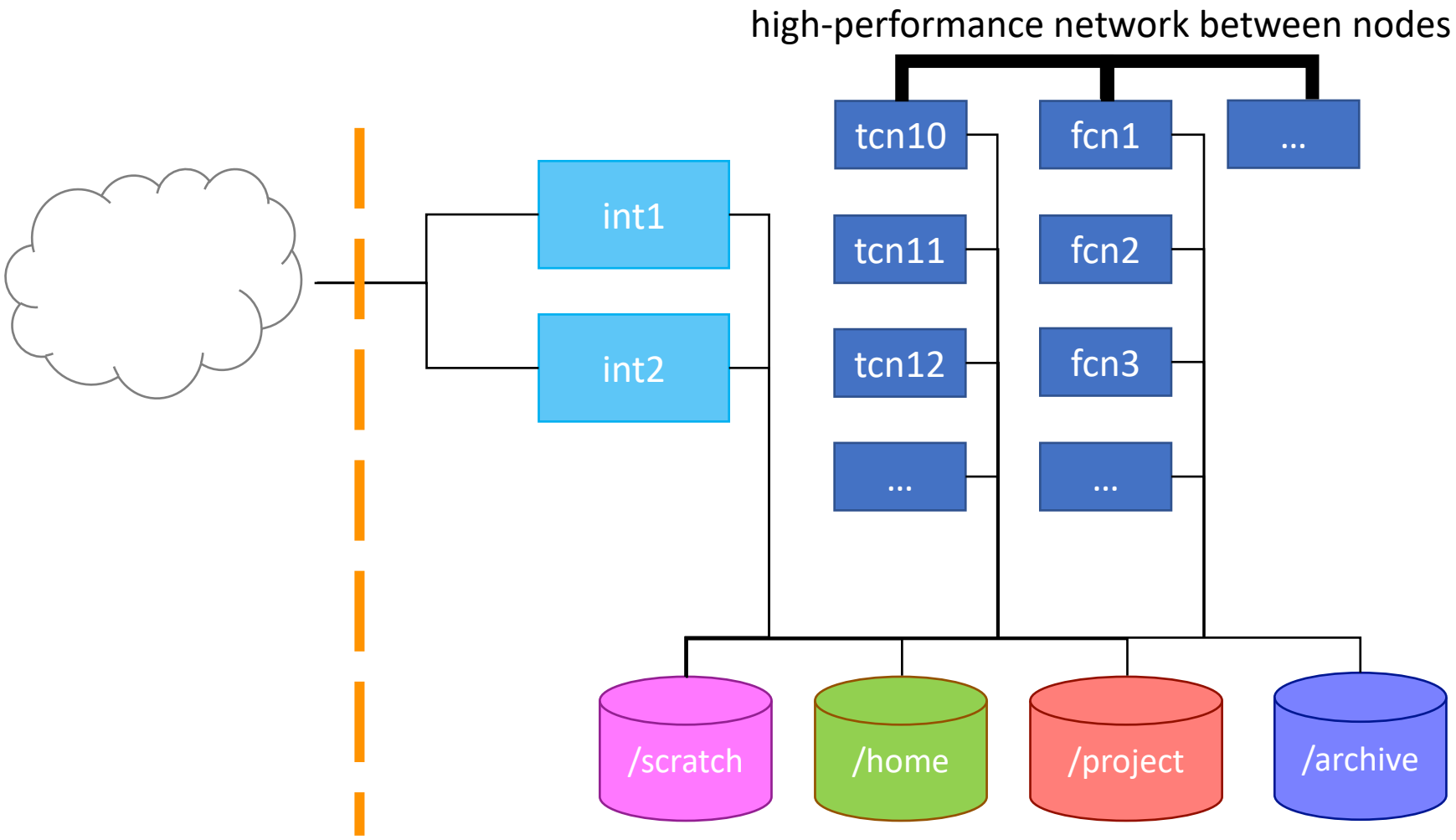
Working with a Supercomputer



Specific example: Lisa architecture



Specific example: Snellius architecture



Compute power on Snellius (Phase 1)

Node name	Number of nodes	Cores per node	CPU	Accelerator	Clock	Memory
tcn	504	2 x 64	AMD Rome 7H12		2.6 GHz	256 GB
fcn	72	2 x 64	AMD Rome 7H12		2.6 GHz	1 TB
hcn	4	2 x 64	AMD Rome 7H12		2.6 GHz	4 TB & 8 TB
gcn	36	2 x 36	Intel Xeon Platinum 8360Y	4 x Nvidia A100	2.5 GHz	512 / 160 GB (7 GB/core)
int	3	2 x 8	AMD EPYC 7F32		3.2 GHz	256 GB
srv	7	2 x 8	AMD EPYC 7F32		3.2 GHz	256 GB

- 76,992 cores + 144 GPUs: **6.1 Pflop/s** (peak performance) + 236 TB memory
- Low-latency interconnection network: InfiniBand HDR100 (100 Gb/s), fat tree
- File systems: 720 TB for home directories and 12.4 PB for scratch and project spaces (GPFS)
- Specific policy for software installation and maintenance

Working with a Supercomputer

Is NOT like this….

Working with a Supercomputer

Working with a Supercomputer

Get access to the system

- EU funded projects (PRACE, CompBioMed, etc.)
- National initiatives
  - NWO, Computing Time on National Computer Facilities
- Special agreements with Universities or research centers
- Contact the HPC center
  - Pilot applications
  - helpdesk@surfsara.nl

INTRODUCTION TO LINUX

a. ACCESSING THE SYSTEM (SSH)

b. BASIC COMMANDS AND USAGE

c. SHELL SCRIPTING

Working with a Supercomputer

Login to LISA system

- Email from helpdesk@surfsara.nl

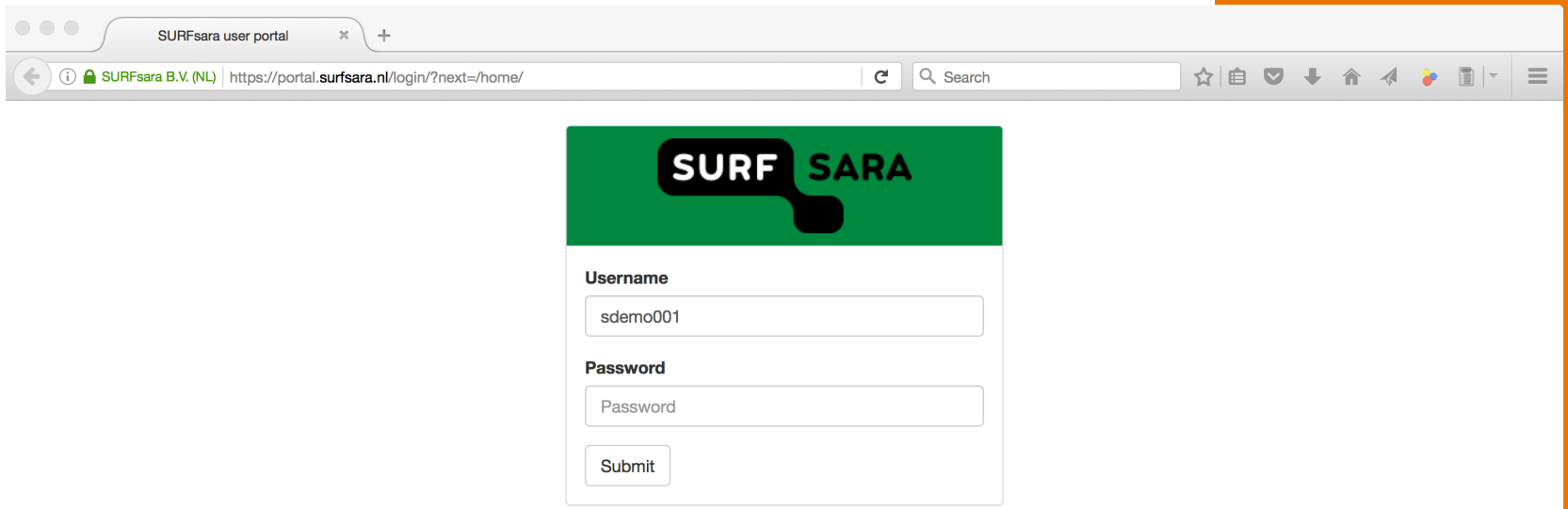
  with credentials (lcurXXXX)

- Login to SURFsara portal

- Accept usage agreement

- Change password

- Check systems status



https://portal.surfsara.nl

Working with a Supercomputer

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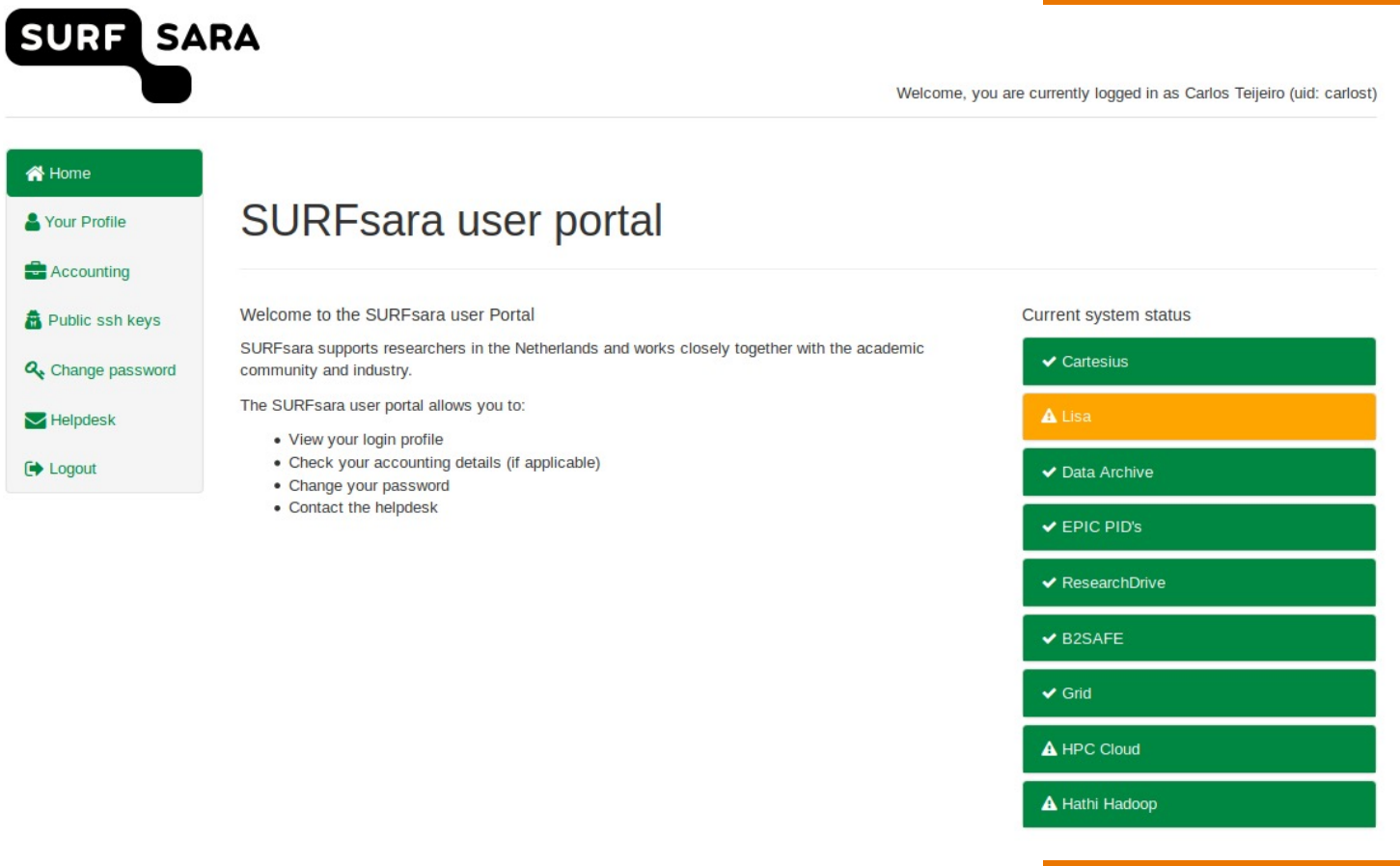
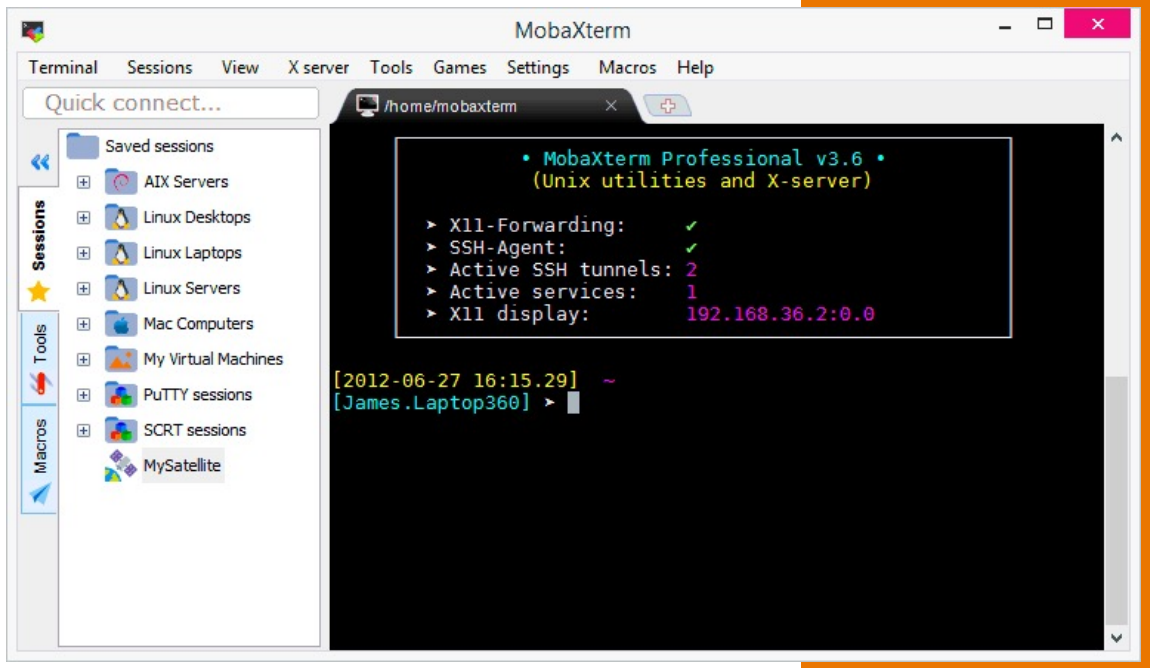


Working with a Supercomputer

Install UNIX tools on your local machine

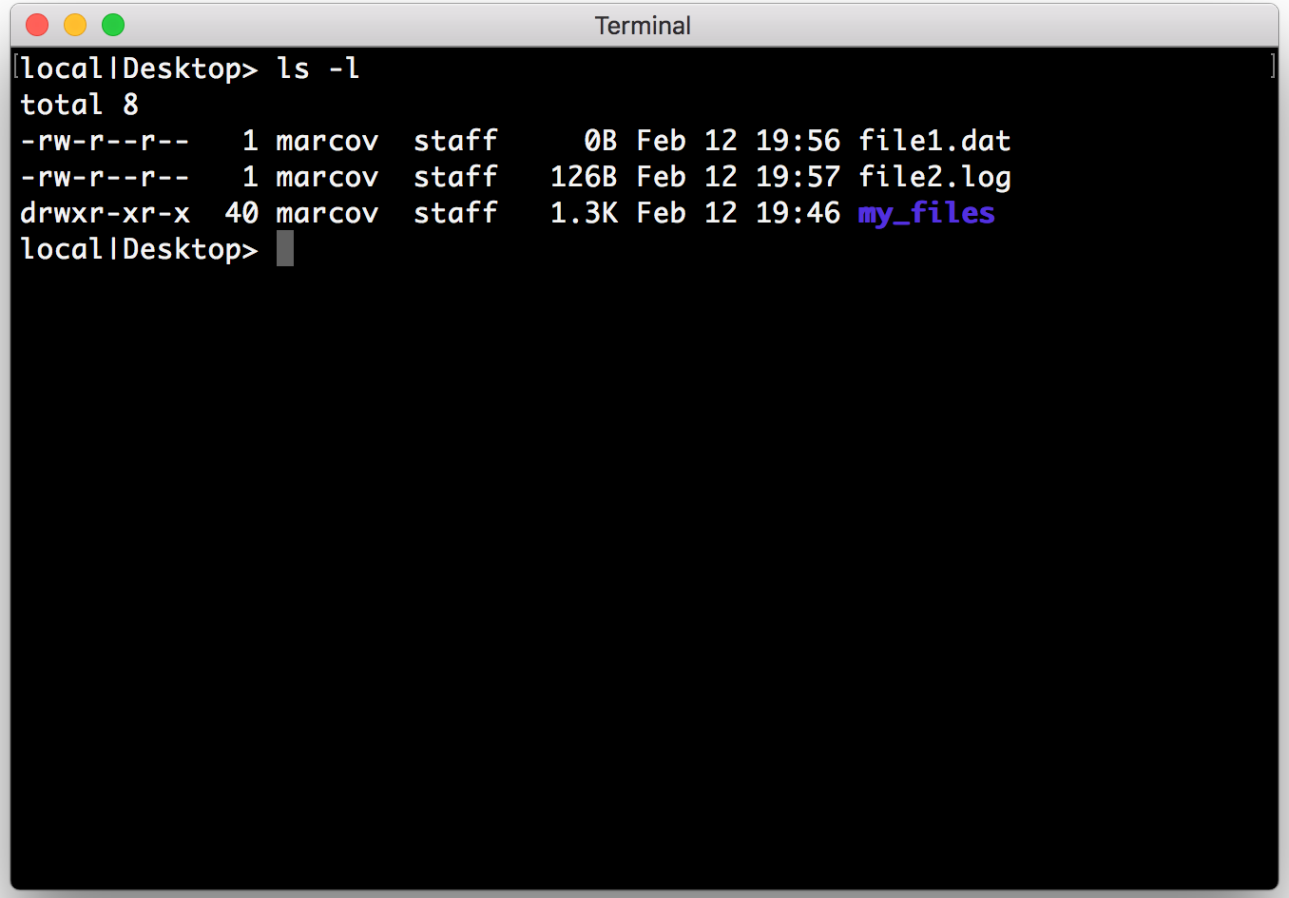
- Windows
  - Putty (https://www.putty.org/)
  - MobaXterm (http://mobaxterm.mobatek.net)
- Mac OSX
  - Terminal (pre-installed)
  - iTerm2 (https://iterm2.com)
- Linux
  - You are already well equipped!



MobaXterm interface

Working with a Supercomputer

The Terminal and the command line



Working with a Supercomputer

SSH, or Secure SHell

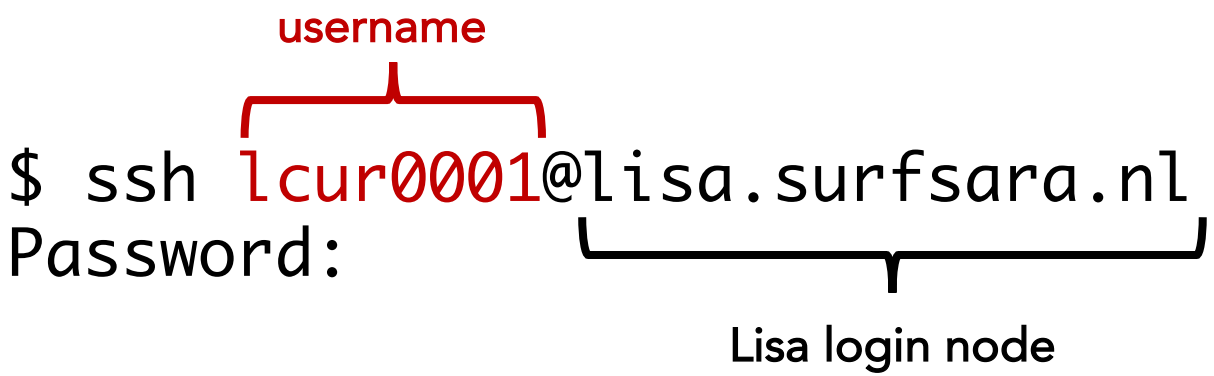
- establishing a cryptographically secured connection
- authenticating each side to the other
- passing commands and output back and forth

```
$ ssh lcur0001@lisa.surfsara.nl
Password:
```

Working with a Supercomputer

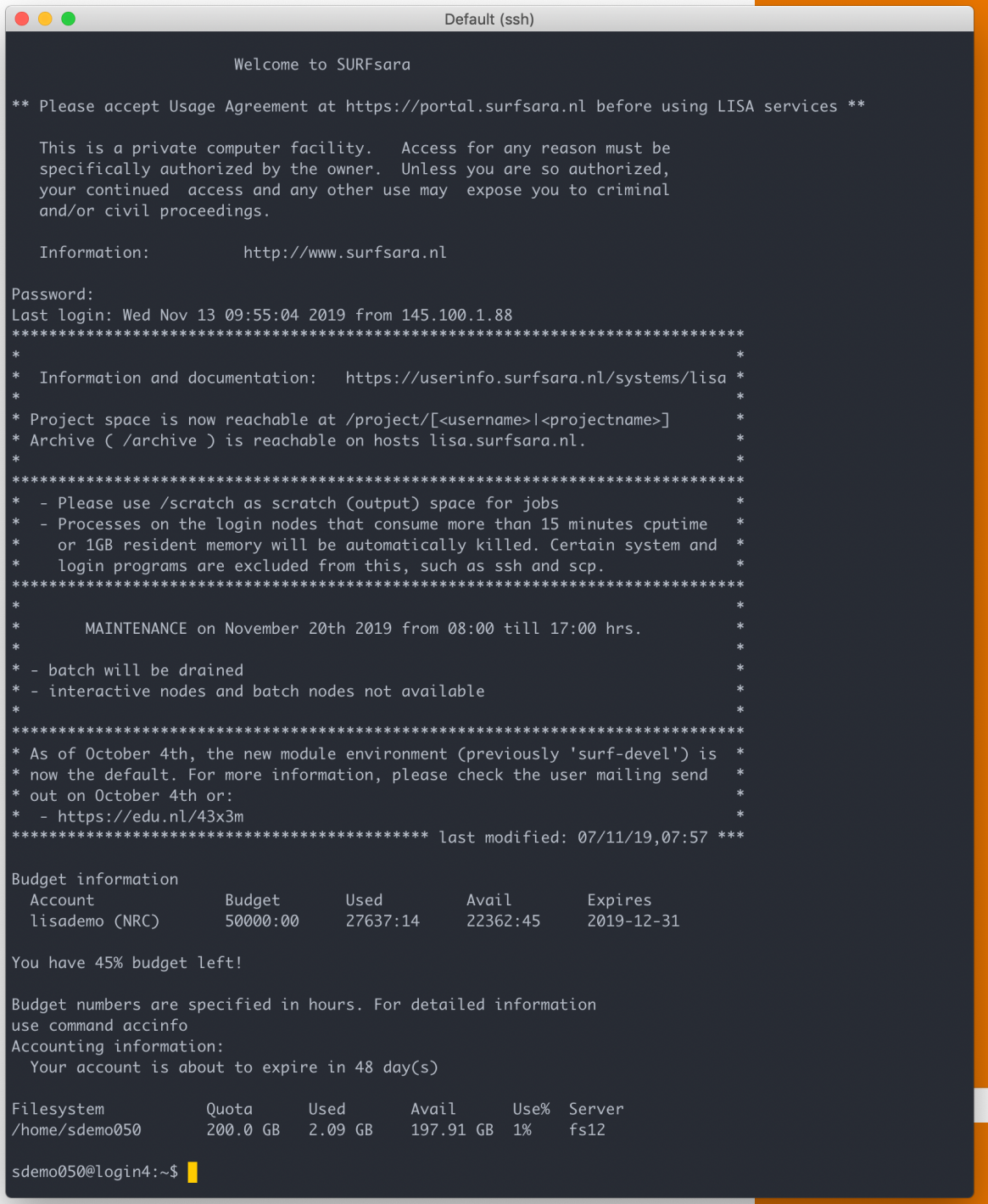
SSH, or Secure SHell

- establishing a cryptographically secured connection
- authenticating each side to the other
- passing commands and output back and forth



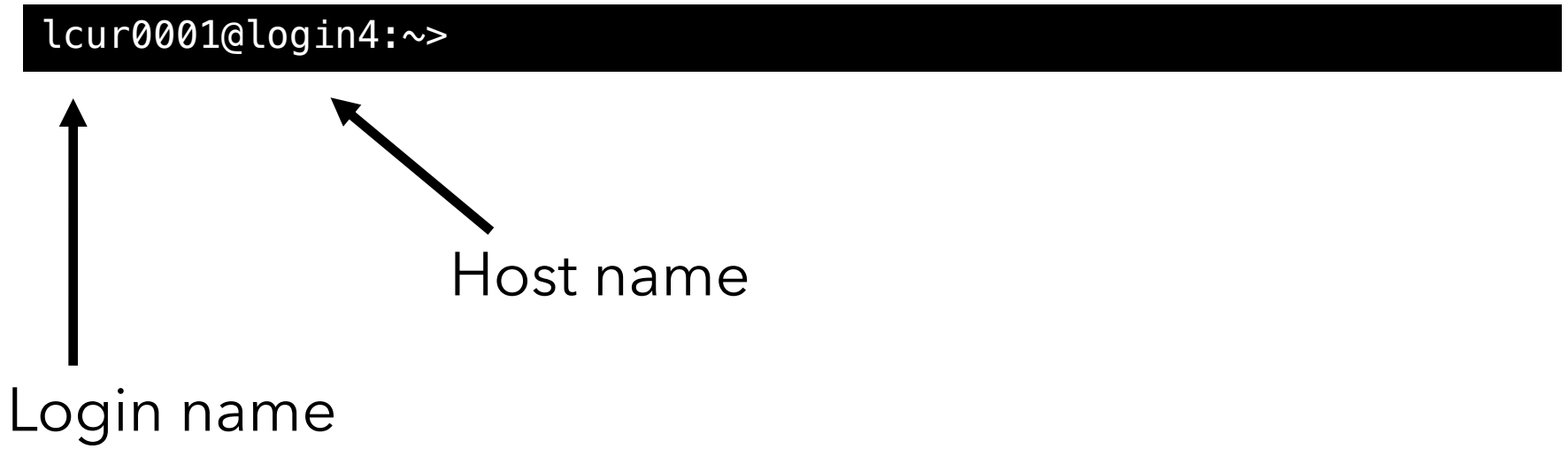
Working with a Supercomputer

You are logged in!!!



Introduction to Linux

- After successful login



- Now the system is ready to accept commands

Introduction to Linux - Exercise

- **Explore the file system**
  - ls, cd, pwd
- **Create and edit files and directories**
  - mkdir, touch, cp, mv, nano, less, vi
- **Use variable (env. variables)**
  - $USER, $HOME
- **System tools**
  - history, find, zip, tar

```
cd VU_HPC-master

:~> ls
bin file1.txt file2.log

nano README.md

:~> echo $USER
```

SURF SARA

Introduction to Linux

- First command

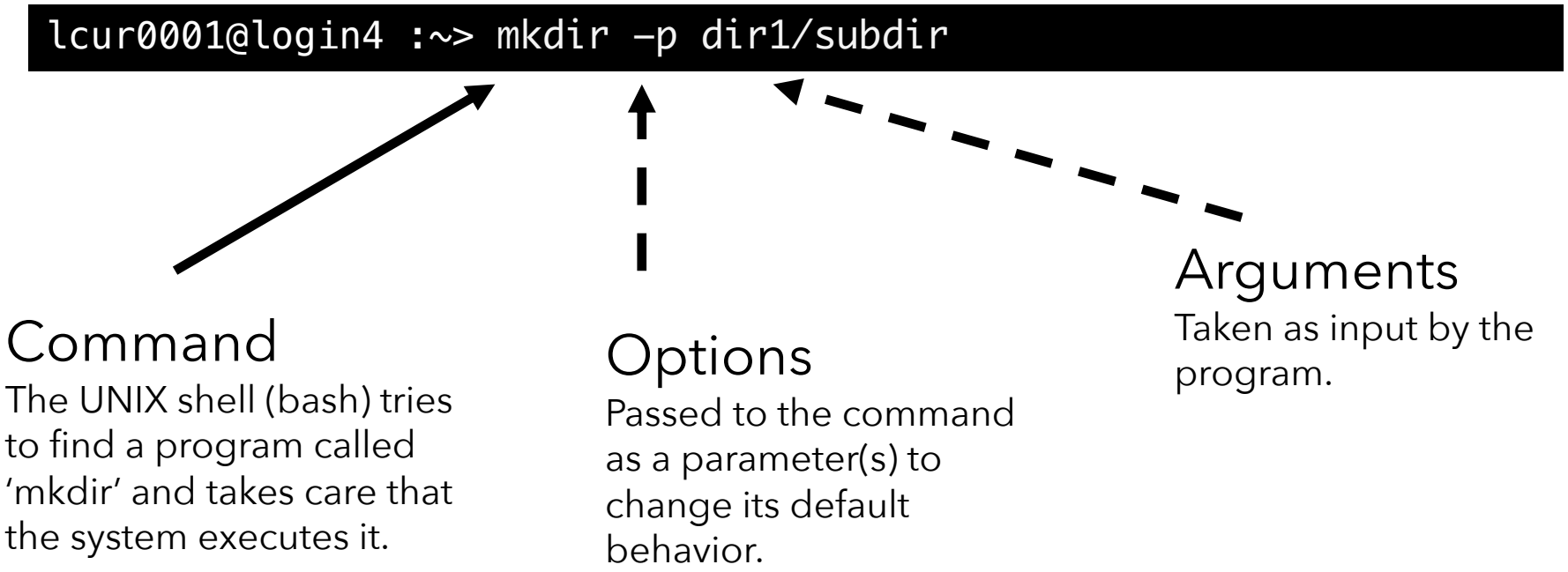
```
lcur0001@login4 :~> date
Thu Nov 14 11:00:00 CET 2019
lcur0001@login4 :~>
```

- A little bit more

```
lcur0001@login4 :~> uname -a
Linux login4.lisa.surfsara.nl 4.9.0-9-amd64 #1 SMP Debian 4.9.168-
1+deb9u5 (2019-08-11) x86_64 GNU/Linux
lcur0001@login4 :~>
```

Introduction to Linux

- Structure of a Linux command



- Case-sensitive (everything!)
- Spaces used to separate command, options and arguments

Introduction to Linux

- Where to find help?

"--help" flag

```
lcur0001@login4:~> uname --help
```

"man" built-in command

```
lcur0001@login4:~> man uname
```

"info" built-in command

```
lcur0001@login4:~> info uname
```

Introduction to Linux

- Where I am?

```
lcur0001@login4:~> pwd
/home/lcur0001/
```

- What files are there?

```
lcur0001@login4:~> ls
bin file1.txt file2.log
```

```
lcur0001@login4:~> ls -l
total 0
drwxr-xr-x 2 lcur0001 lcur0001 4096 May 5  2010  bin
-rw-r--r-- 1 lcur0001 lcur0001    0 Feb 13 01:17 file1.txt
-rw-r--r-- 1 lcur0001 lcur0001 1528 Feb 13 01:17 file2.log
```

Introduction to Linux

- Create directory

```
lcur0001@login4:~> mkdir dir
lcur0001@login4:~> mkdir –p dir2/subdir
```

- Remove directory

```
lcur0001@login4:~> rmdir dir
```

- Remove directory and its content (be careful!)

```
lcur0001@login4:~> rm –r dir2
```

Introduction to Linux

- Change directory

```
lcur0001@login4:~> cd dir/subdir
lcur0001@login4:~/dir/subdir>
```

- Going ”one level” up

```
lcur0001@login4:~/dir/subdir> cd ..
lcur0001@login4:~/dir/>
```

- Going back to home folder (~)

```
lcur0001@login4:~/dir/> cd
lcur0001@login4:~>
```

Introduction to Linux

- Relative path

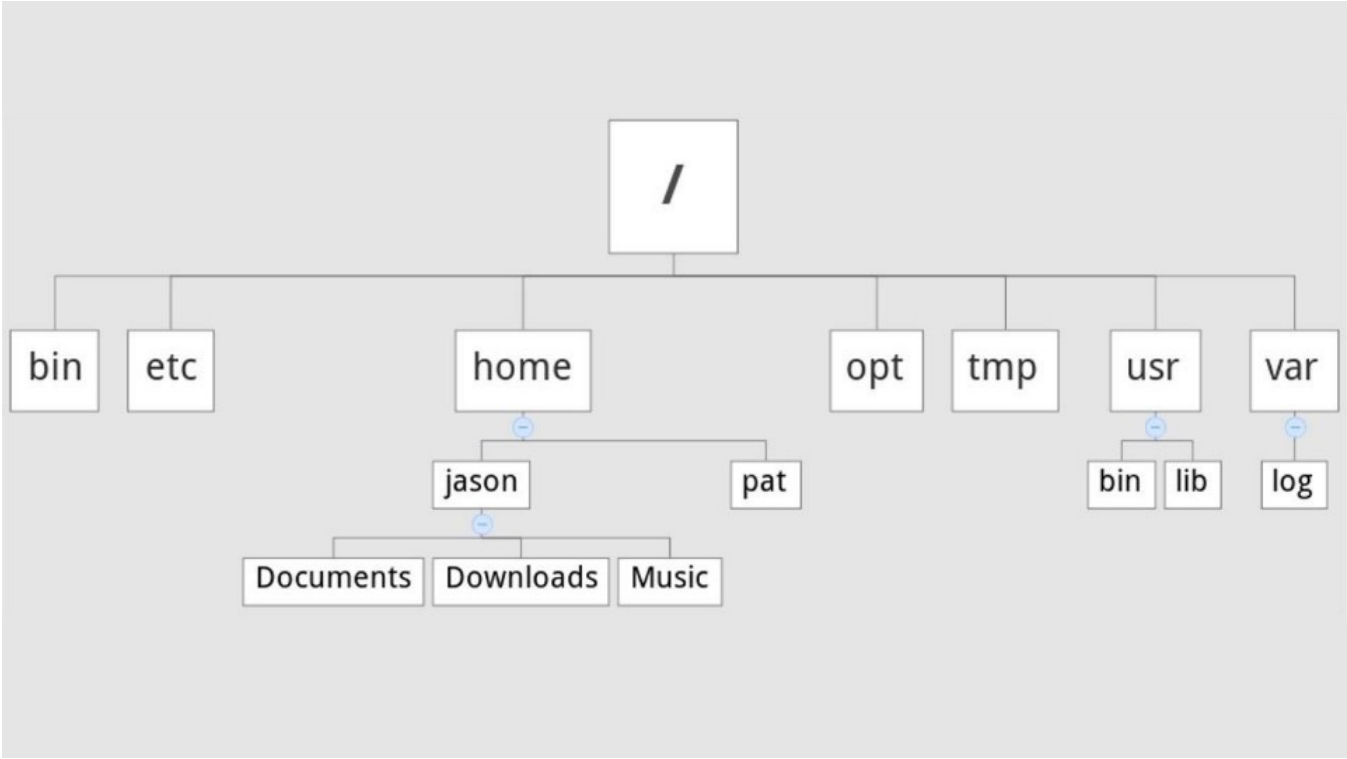
```
lcur0001@login4:~> ls dir/mydata.out
dir/mydata.out
```

- Absolute path

```
lcur0001@login4:~> ls ~/dir/mydata.out
/home/cur0001/dir/mydata.out
```

Introduction to Linux

- Directory Structure and Hierarchy



Source: www.linuxtrainingacademy.com

Introduction to Linux

- Copy files

```
lcur0001@login4:~> cp file1.txt file1.copy
```

- Copy files into directories

```
lcur0001@login4:~> cp file1.* dir/
lcur0001@login4:~> cp file1.txt dir/file1.copy2
```

- Move/Rename files

```
lcur0001@login4:~> mv file1.txt dir/file.txt.new
lcur0001@login4:~> mv file1.txt file.txt.old
```

Introduction to Linux

- Copy files to remote host

```
benjamic@local:~> scp file1.txt lcur0001@lisa.surfsara.nl:
```

- Copy files from remote host to local machine

```
benjamic@local:~> scp lcur0001@lisa.surfsara.nl:file1.txt .
```

- Copy folder from your local machine to a remote host

```
benjamic@local:~> scp –r Intro-to-HPC lcur0001@lisa.surfsara.nl:
```

Introduction to Linux - Exercise

- Download the material from the website:

  https://github.com/sara-nl/Intro-to-HPC

- Transfer the zip file to your account on Lisa:

```
~> scp main.zip lcur0001@lisa.surfsara.nl:
```

- Extract zip on the host:

```
~> ssh lcur0001@lisa.surfsara.nl
~> Password:
...
~> unzip main.zip
```

Introduction to Linux

- Extract zipped files

```
lcur0001@login4:~> unzip main.zip
lcur0001@login4:~> tar -zxvf main.tar.gz
```

- Open formatted files (e.g.: text files)

```
lcur0001@login4:~> nano Intro-to-HPC/README.md
lcur0001@login4:~> emacs Intro-to-HPC/README.md
lcur0001@login4:~> vim Intro-to-HPC/README.md
```

Introduction to Linux

Shell script programming

What if I want to run many bash commands?

…maybe in a workflow?

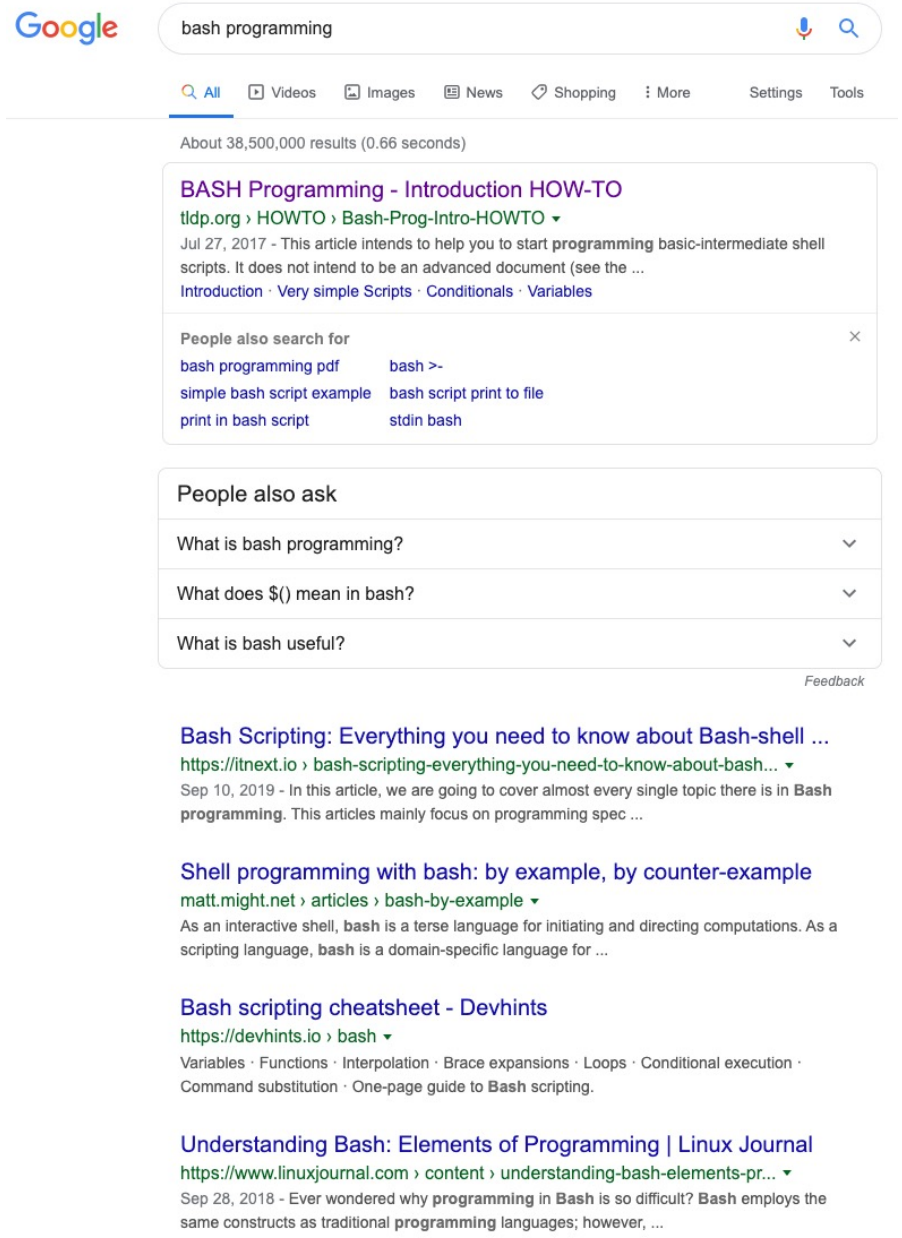
Bash scripts

- The “Shell” is the program which read commands and run other programs. Bash is a type of “Shell”.
- A *bash script* is a plain text file which contains a series of commands
- Any command you can run on the command line can be put into a script (v.v.)
- It will be executed like a normal program: ./script.sh

Introduction to Linux

Shell script programming

- Loops for, while, until
- Conditional statements: If, else, then
- Functions
- Variables
- and much more



Introduction to Linux

Shell script programming

```
lcur0001@login4:~> ls -l
total 0
drwxr-xr-x 2 lcur0001 lcur0001 4096 May 5  2010  bin
-rw-r--r-- 1 lcur0001 lcur0001   10 Feb 13 01:17 source.c
-rwxr-xr-x 1 lcur0001 lcur0001 1528 Feb 13 01:17 main.x
```

File permissions

Every file/directory has 9 permission bits associated (+ initial to diff):

- 3 user based permission groups: owner(2-4), group(5-7), all users(8-10)
- x3 permission types: read(r), write(w), execute(x)

Permission can be changed with the command “chmod”

Introduction to Linux - Exercise

- Move into the exercise folder:
  linux-cluster-computing/introlinux

- Inspect the “simple.sh” file

- Change permission of the script to allow execution

```
lcuur0001@login4:~> chmod +x simple.sh
```

- Run the script

```
lcuur0001@login4:~> ./simple.sh
```

Introduction to Linux - Exercise

- Move into the exercise folder:
  linux/example2

- Inspect the file “compute_factorial.sh”
  and the folder “src”

- Change permission of the script to allow execution

```
lcuur0001@login4:~> chmod +x compute_factorial.sh
```

- Run the script

```
lcur0001@login4:~> ./compute_factorial.sh
```

RUNNING JOBS ON THE BATCH SYSTEM

a. INTERACT WITH THE BATCH SYSTEM

b. RUN A REAL SCIENTIFIC WORK FLOW

Module management: useful commands

- module avail - available modules in the system
- module load <mod> - load <mod> in the shell environment
- module list - show a list of all loaded modules
- module unload <mod> - remove <mod> from the environment
- module purge - unload all modules
- module whatis <mod> - show information about <mod>

Running jobs on the HPC system

- Let’s try it the module command
- Get which version of Python is currently available

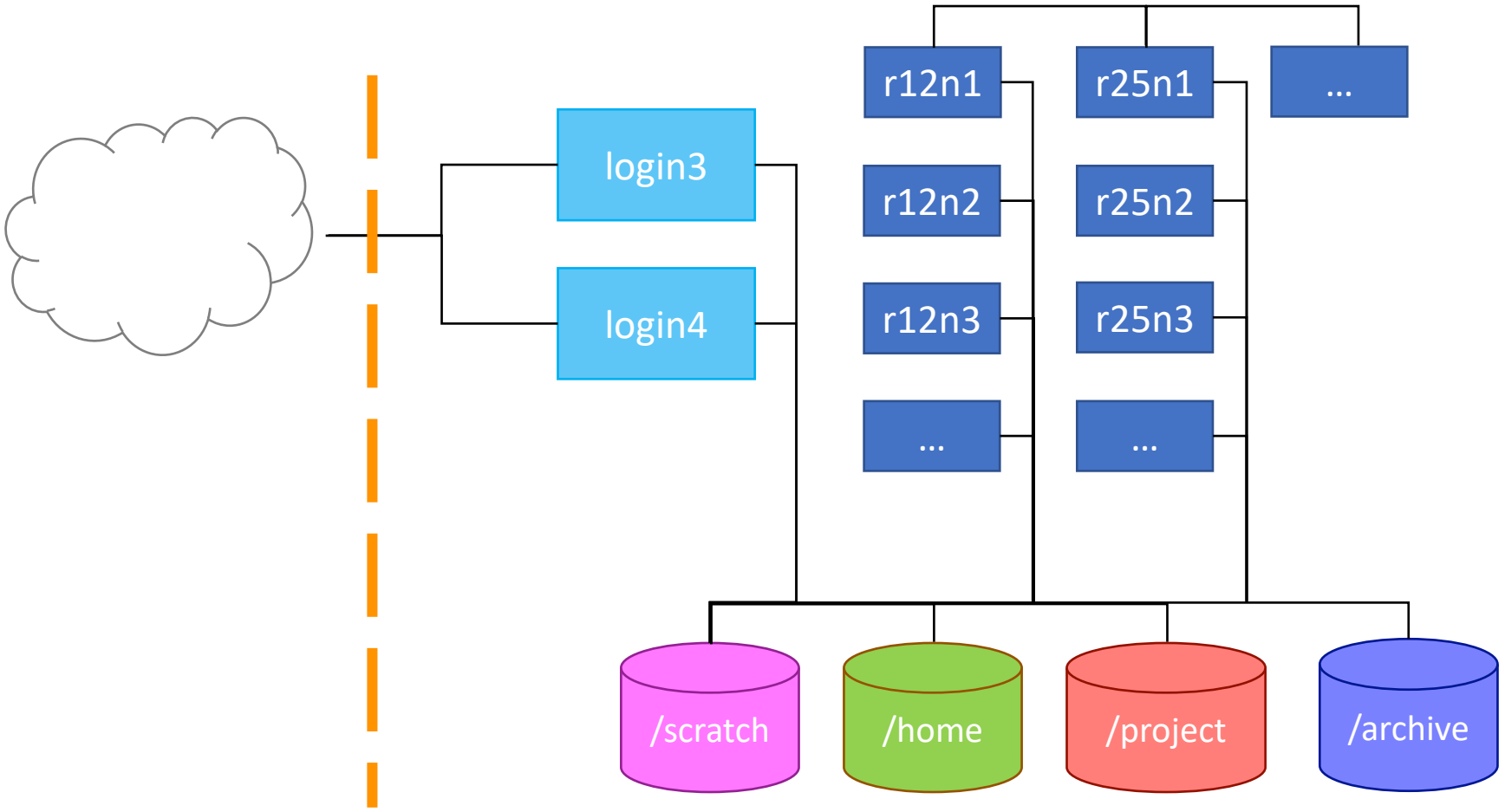
```
lcur0001@login4:~> python --version
lcur0001@login4:~> which python
```

- Try to load a different version of Python

```
lcur0001@login4:~> module load 2021
lcur0001@login4:~> module load Python/3.9.5-GCCcore-10.3.0
```

- Check again.

Specific example: Lisa architecture



Running jobs on the HPC system

The batch jobs scheduler

- Supercomputers use job schedulers to distribute computational tasks over the available nodes.
- Instead of executing commands interactively, you prepare a job script
  - Script containing the commands to execute
  - Resource characteristics (specific)
- The batch system is responsible for allocating cores, processors or nodes to a job.

Running jobs on the HPC system

The batch jobs scheduler

- It allows to run MANY jobs at the same time
    - The system takes care that they are run efficiently on the available resources.
- Multiusers, queue system
    - A batch system allows users to always submit jobs, even if a lot of people are using the system at the same time. In addition take care of budgeting and fair resource usage.
- System load balance
    - The system takes care of balancing the load across nodes and during time. In a batch system, most jobs may be submitted during office hours, but the scheduler will continue to start jobs at night as nodes become available.

Running jobs: useful commands of the SLURM scheduler

- sbatch <*jobscript*> - submit a job to the scheduler
- squeue -j <*job_id*> - inspect the status of job <*job_id*>
- squeue –u <*user_id*> - inspect all jobs of user <*user_id*>
- scancel <*job_id*> - cancel job <*job_id*> before it runs
- scontrol show job <*job_id*> - show estimated job start

Anatomy of a job script

- Job scripts consist of:
  - the “shebang” line: `#!/bin/bash`
  - scheduler directives
  - command(s) that load software modules and set the environment
  - command(s) to prepare the input
  - command(s) that run your main task(s)
  - command(s) to save your output

```
#!/bin/bash
```

```
#SBATCH --job-name="firsttest"
#SBATCH --nodes=1
#SBATCH --ntasks=10
#SBATCH --time=00:01:00
#SBATCH --partition=normal
```

```
module load 2021
module load foss/2021a
```

```
cp -r <my_folder> $TMPDIR
cd $TMPDIR
```

```
srun a.out
```

```
cp -r $TMDPDIR/* ~/results
```

Introduction to Linux

- Submit job to the queue:

```
lcur0001@login4:~> sbatch <job script>
```

- Show running and queued jobs:

```
lcur0001@login4:~> squeue –u $USER
```

- Remove a job from the queue or kill it if running:

```
lcur0001@login4:~> squeue –u $USER
```

Introduction to batch - Exercise

- Move into the exercise folder: batch/example1
- Inspect the file “slurm.sub”
- Run the script via bash

```
lcur0001@login4:~> bash slurm.sub
```

- submit the script to the batch scheduler

```
lcur0001@login4:~> sbatch slurm.sub
```

Running jobs on the HPC system - Ex

- Move into the exercise folder:
  batch/example2
- Inspect the file “pythonopenmp.sub”
- Submit the job to the queue

```
lcur0001@login4:~> sbatch pythonopenmp.sub
```

- Analyse the results.

Running jobs: best practices

- Give the scheduler a realistic *walltime* estimate
- Your home directory is slow. Use $TMPDIR.
- Load software modules as part of your job script – this improves reproducibility
- Run parallel versions of your programs (and use “srun” to ask SLURM to run multi-process applications)

Everything about jobs: service desk info pages

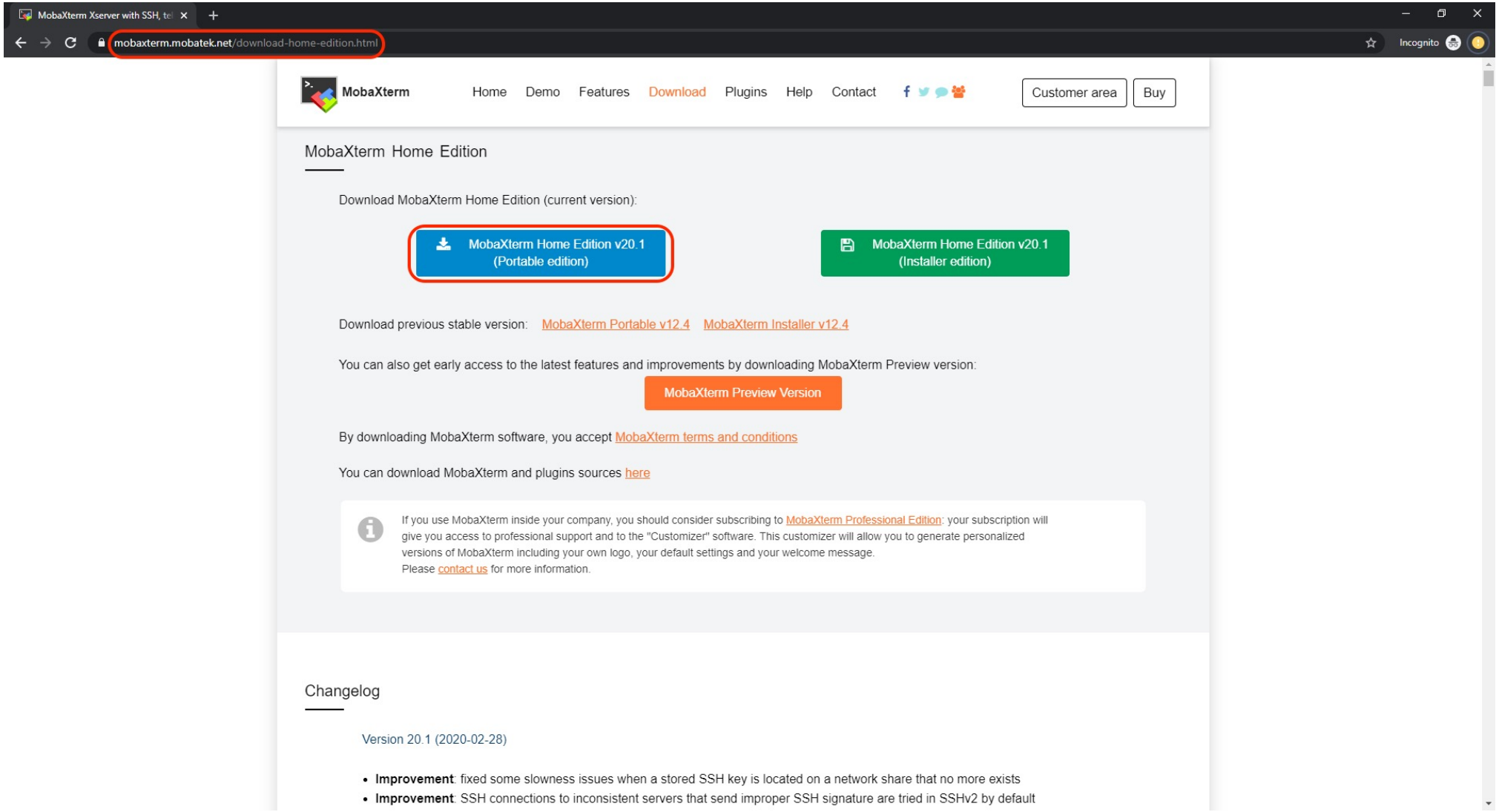
- **https://servicedesk.surfsara.nl/wiki/display/WIKI/Snellius+and+Lisa**

- More courses by SURF for research:
  - SURF Agenda for Research and ICT
    - https://www.surf.nl/en/agenda/research-and-ict
  - SURF course catalog and mailing list
    - https://www.surf.nl/en/training-courses-for-research

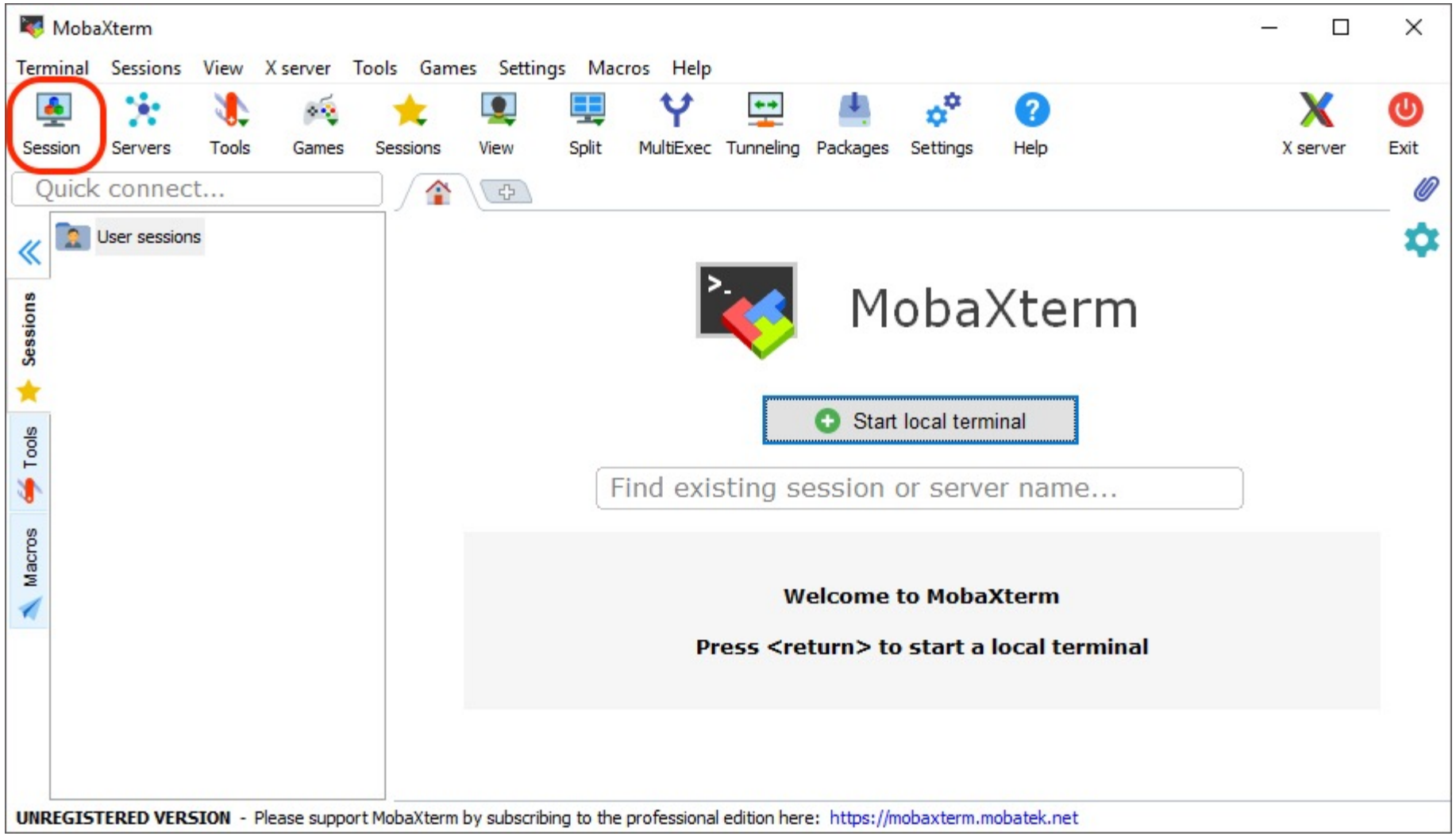
Thank you!

Benjamin Czaja, Marco Verdicchio
HPC Advisors, SURFsara

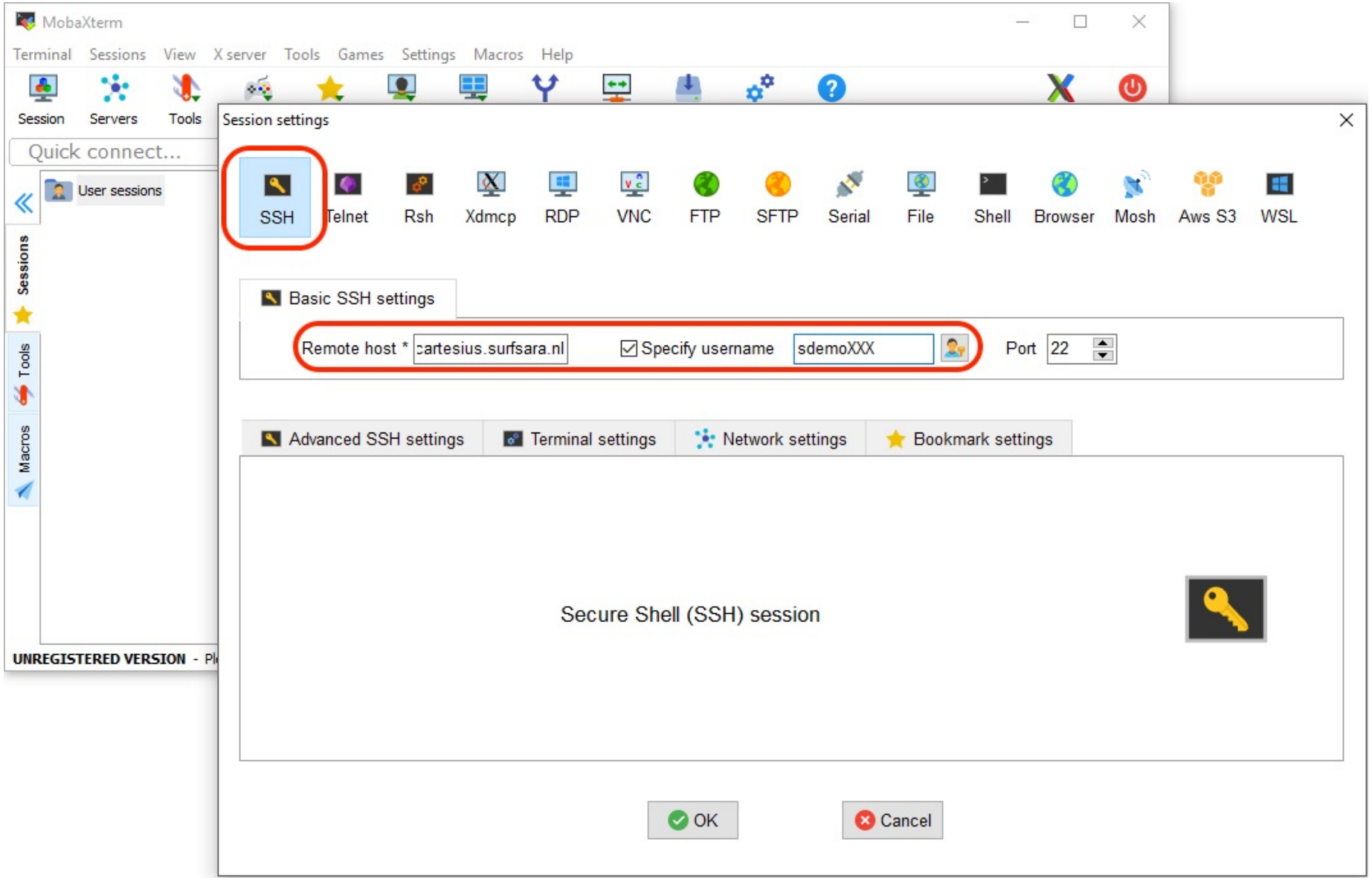
Download the portable edition of MobaXterm



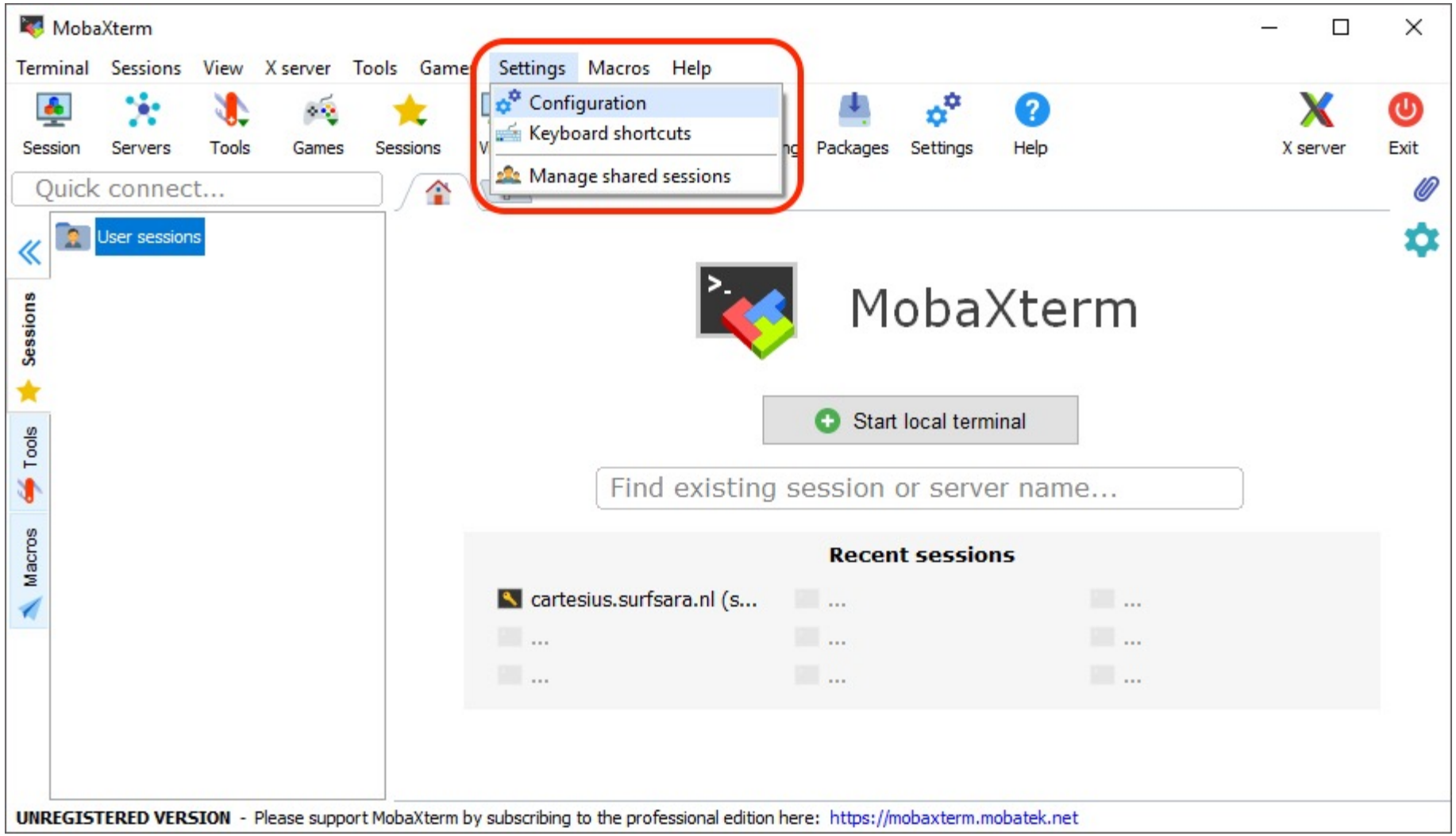
Open a new remote session



Open a new remote session



Change the root/home folders (via Settings->Configura



Change the root/home folders (via Settings->Configura