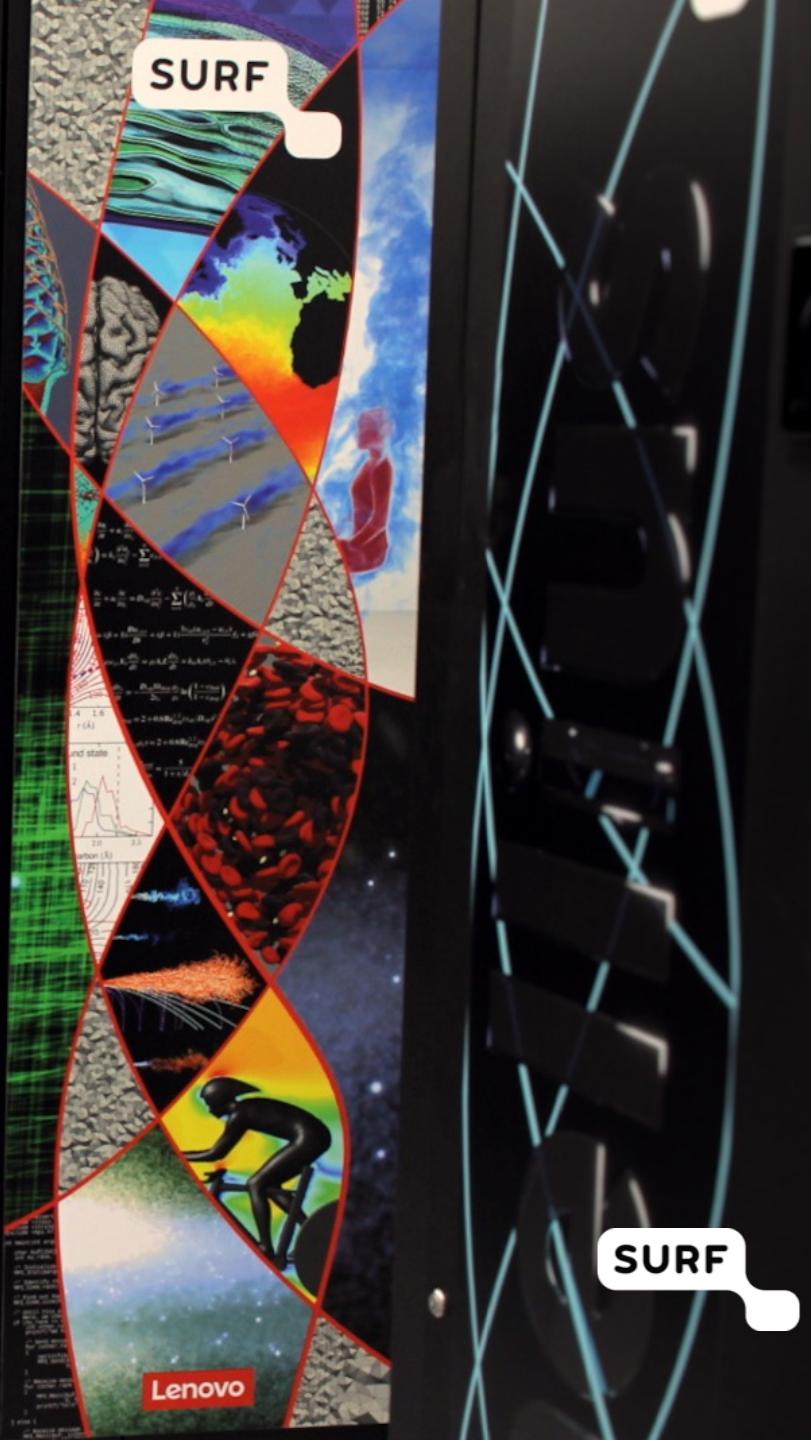
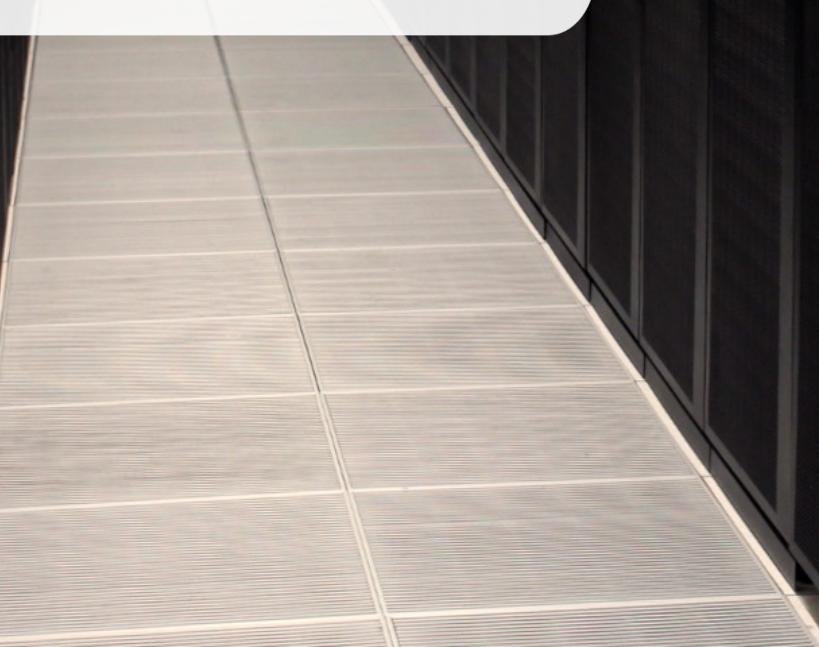
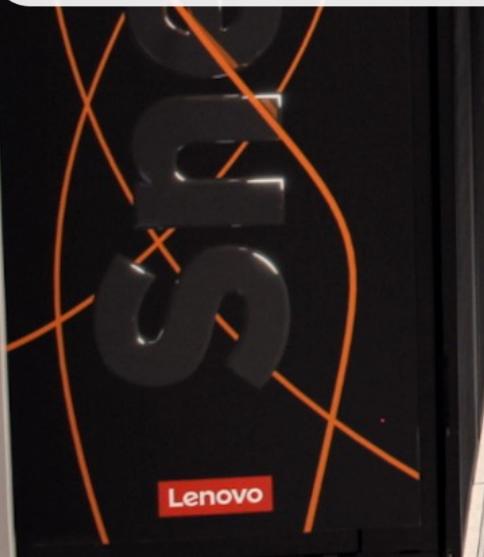


SURF

# Using a supercomputer

## Hands-on introduction

Benjamin Czaja, Marco Verdicchio  
HPC Advisors, SURFsara



# Linux and Cluster Computing

## 1) Introduction

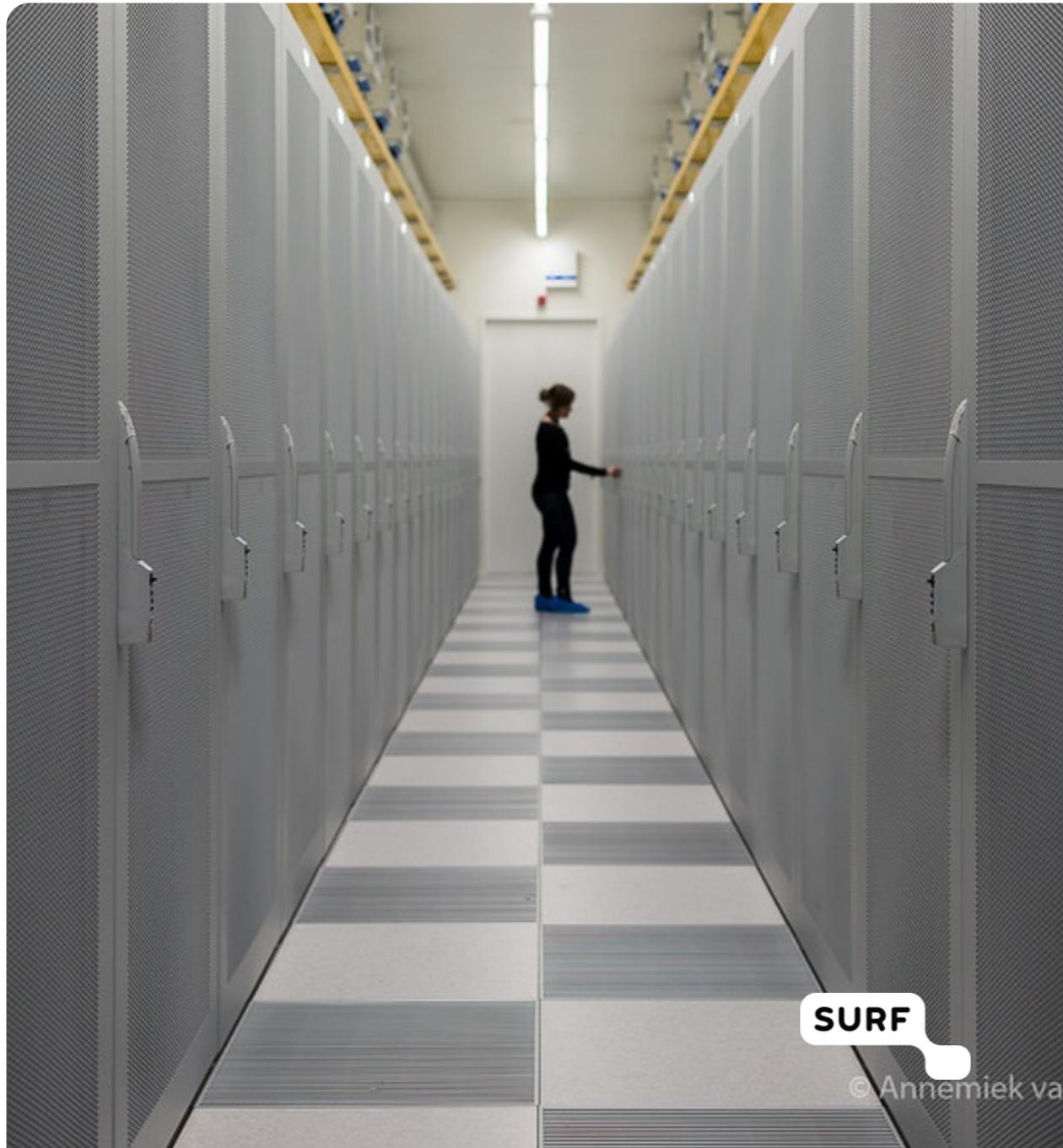
- a. What is a computer?
- b. What is a supercomputer?
- c. How is a supercomputer different from the cloud
- d. Access and usage

## 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

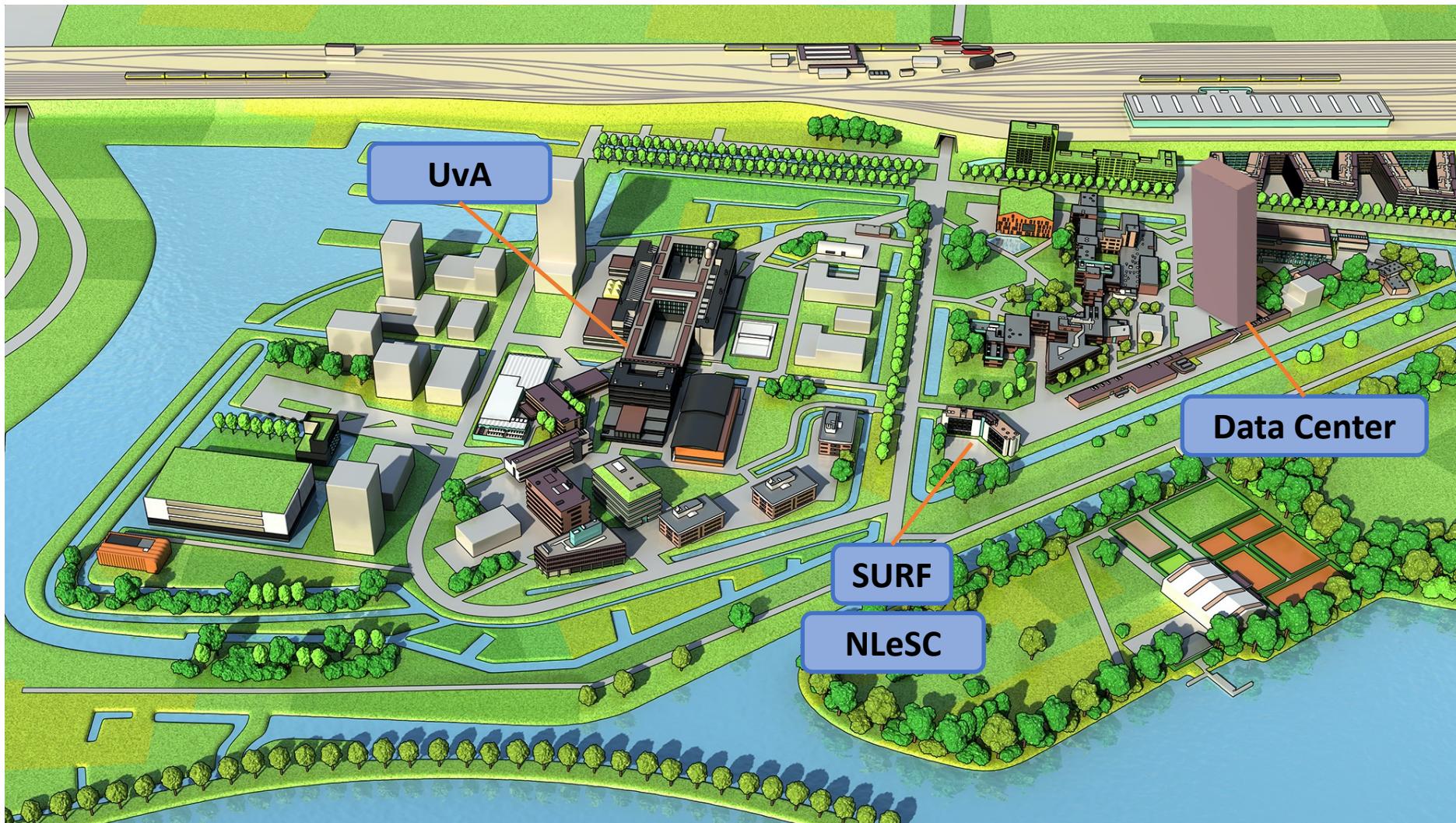
- Slides and exercises



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



# Location of SURF Amsterdam



**SURF**

# High-performance computing (HPC) is ...

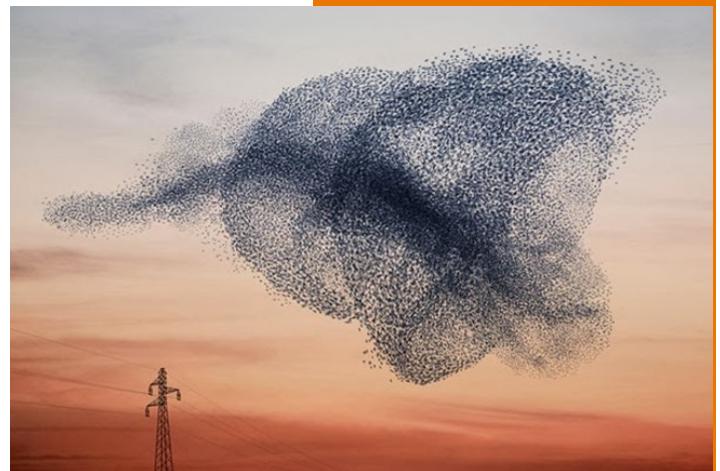
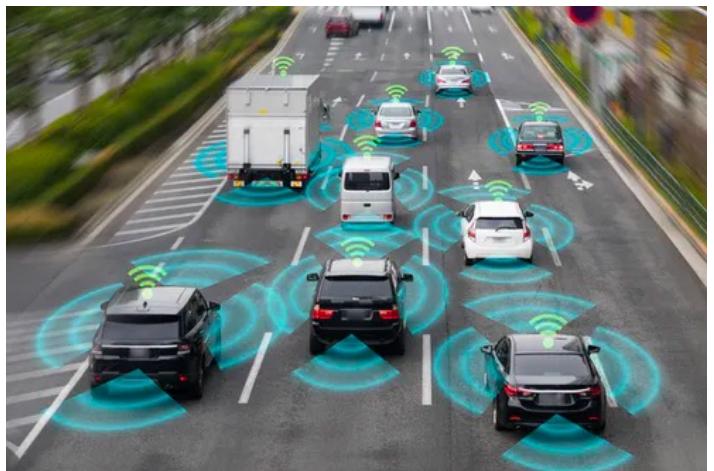
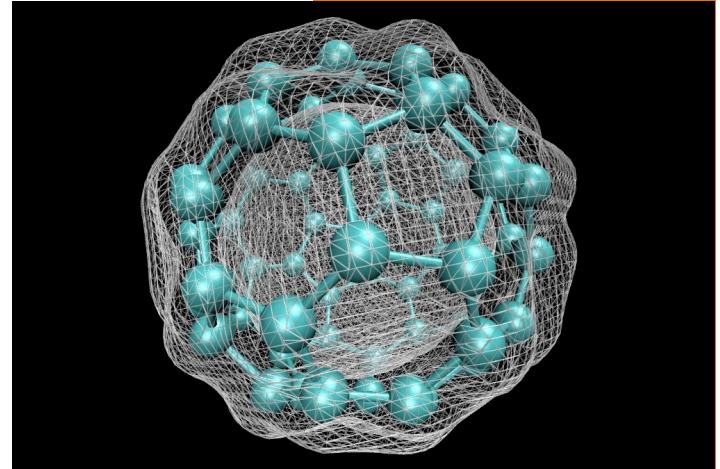


Image source: <https://www.trustedreviews.com/news/gran-turismo-ps5-will-complete-form-series-3895762>

Image source: <http://www.militarysystems-tech.com/articles/l-3-link-achieves-world-s-first-boeing-787-8-full-flight-simulator-level-d-certifications>

Image source: <https://www.zdnet.com/article/canberra-stands-up-au9-7m-transport-office-to-prep-for-autonomous-vehicles>

Image source: <https://spacenews.com/astranis-lands-anchor-customer-for-its-first-small-geo-satellite>

5 Image source: [https://medium.com/@info\\_89535/applications-of-fullerene-in-medicine-20942944e41d](https://medium.com/@info_89535/applications-of-fullerene-in-medicine-20942944e41d)

Image source: <https://thestrategybridge.org/the-bridge/2016/8/16/a-new-plan-using-complexity-in-the-modern-world>

# High-performance computing (HPC) ...

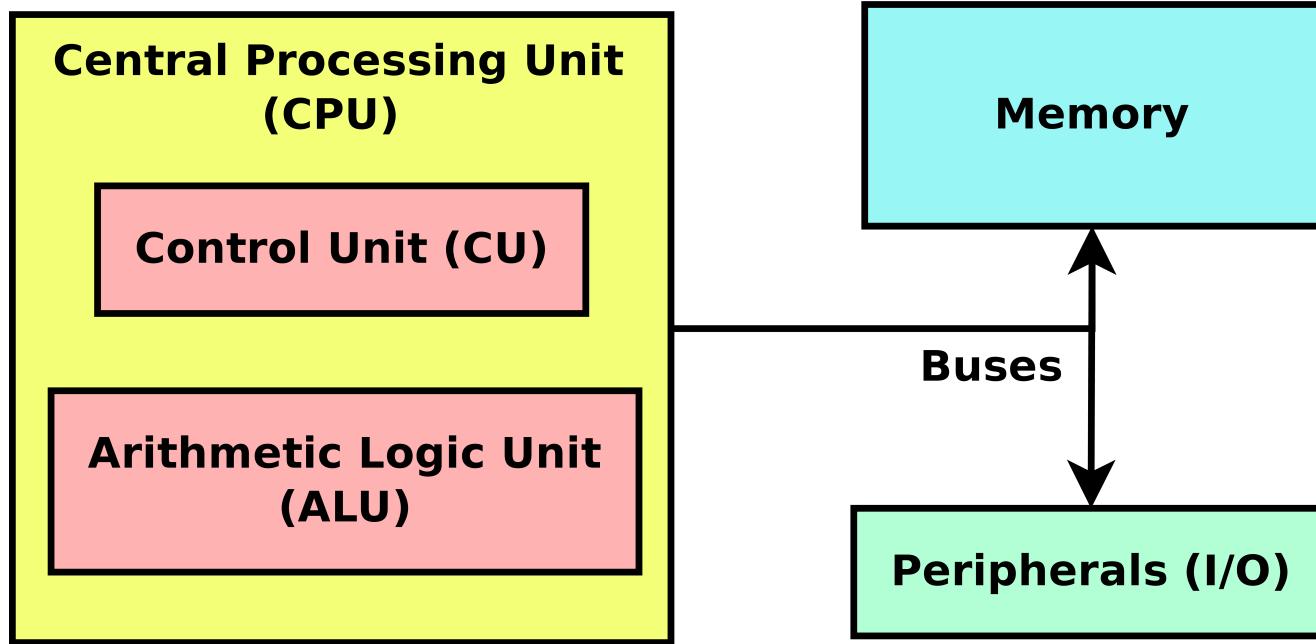
- ... *is an area of computer-based computation. It includes all computing work that requires a high computing capacity or storage capacity.*
- ... *is the use of parallel processing for running advanced application programs efficiently, reliably and fast.*
- ... *refers to the practice of aggregating 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 ...

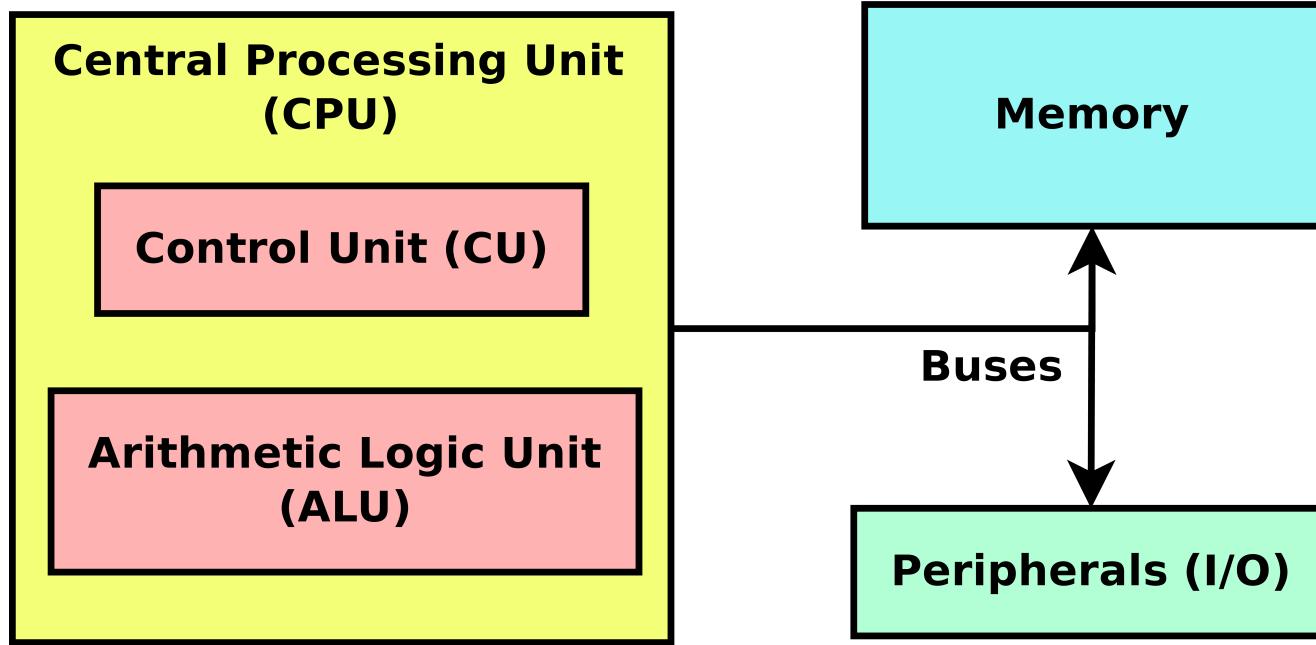


*Image source: [https://media.sciencephoto.com/image/t4150120/800wm/T4150120-Piles\\_of\\_discarded,\\_redundant\\_computer\\_keyboards.jpg](https://media.sciencephoto.com/image/t4150120/800wm/T4150120-Piles_of_discarded,_redundant_computer_keyboards.jpg)*

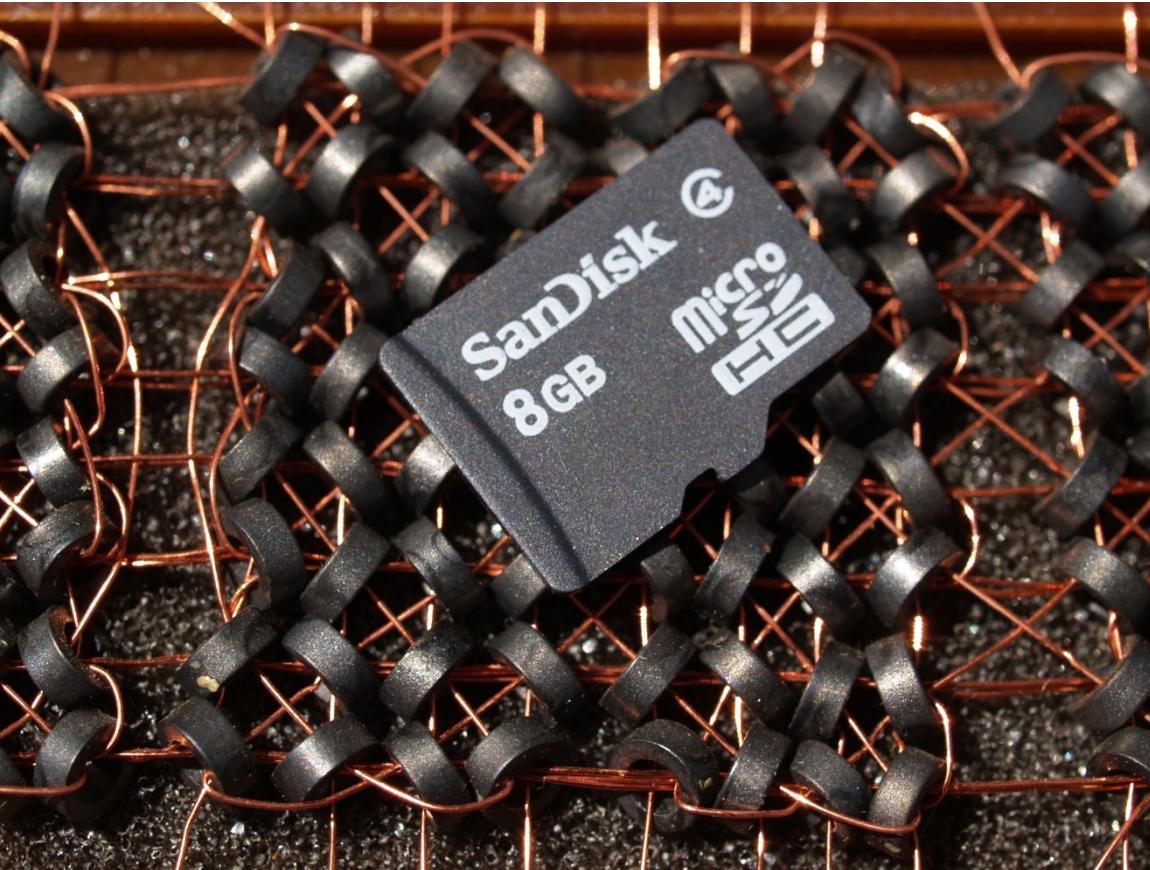
*Image source: <https://static.guim.co.uk/sys-images/Guardian/Pix/pictures/2014/2/10/1392028631237/Pile-of-computer-monitors-008.jpg>*

SURF

# A computer is ...

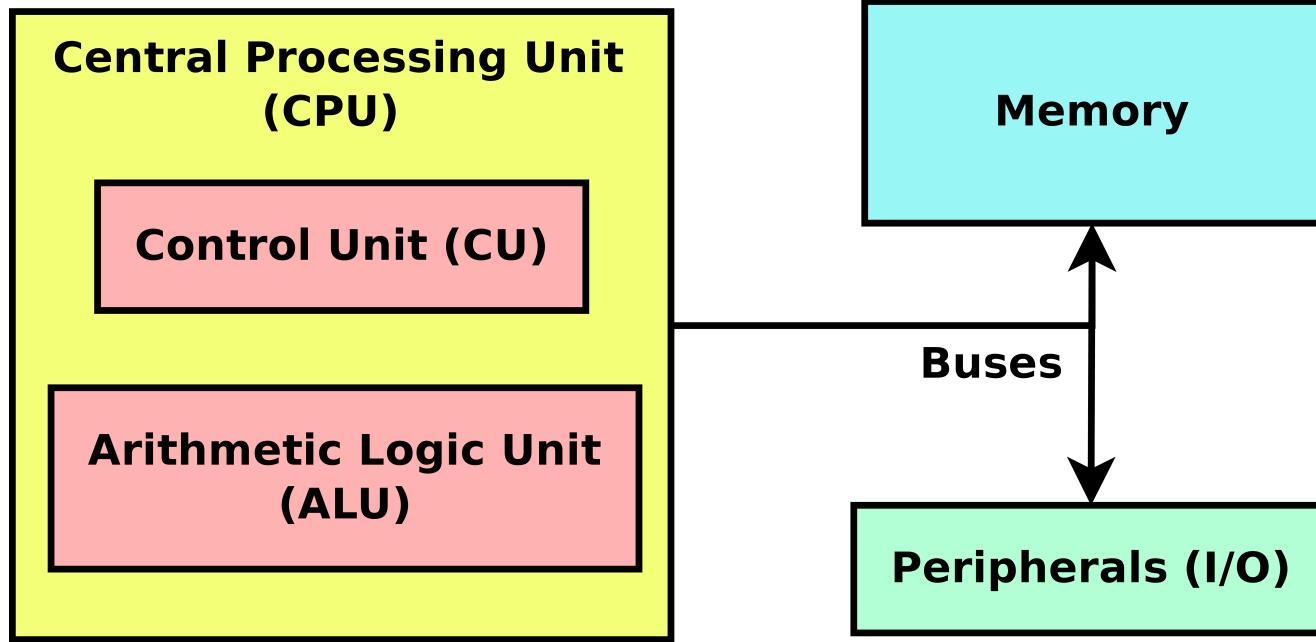


# A memory is ...

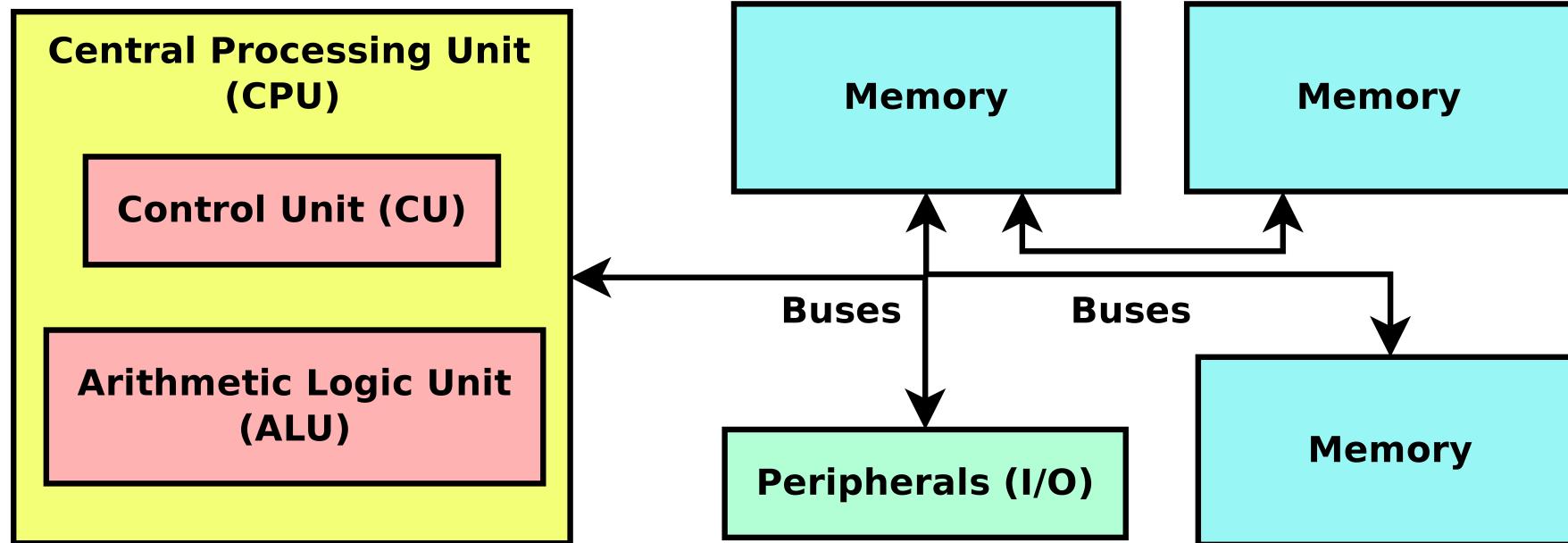


*Image source: [https://upload.wikimedia.org/wikipedia/commons/c/c0/8 bytes vs. 8Gbytes.jpg](https://upload.wikimedia.org/wikipedia/commons/c/c0/8%20bytes%20vs.%208Gbytes.jpg)*

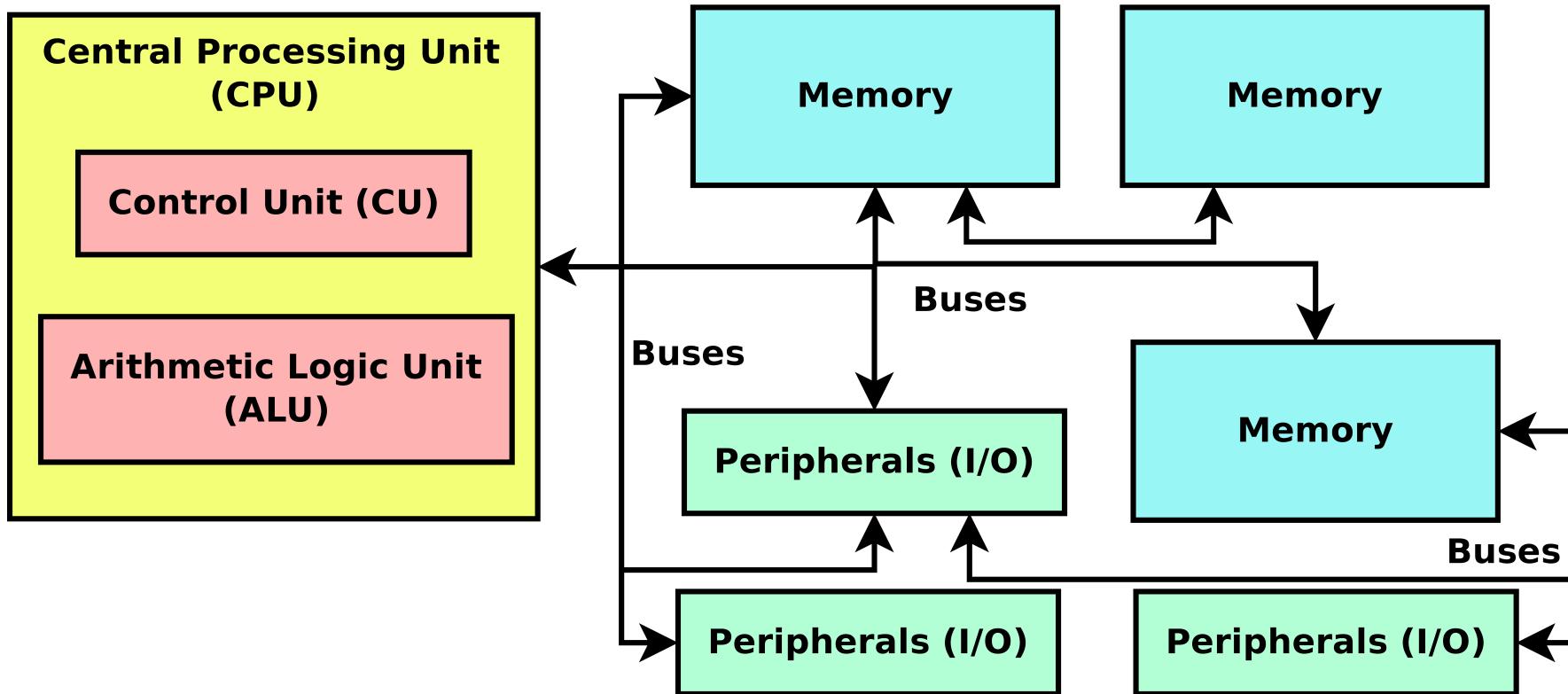
# A computer is ...



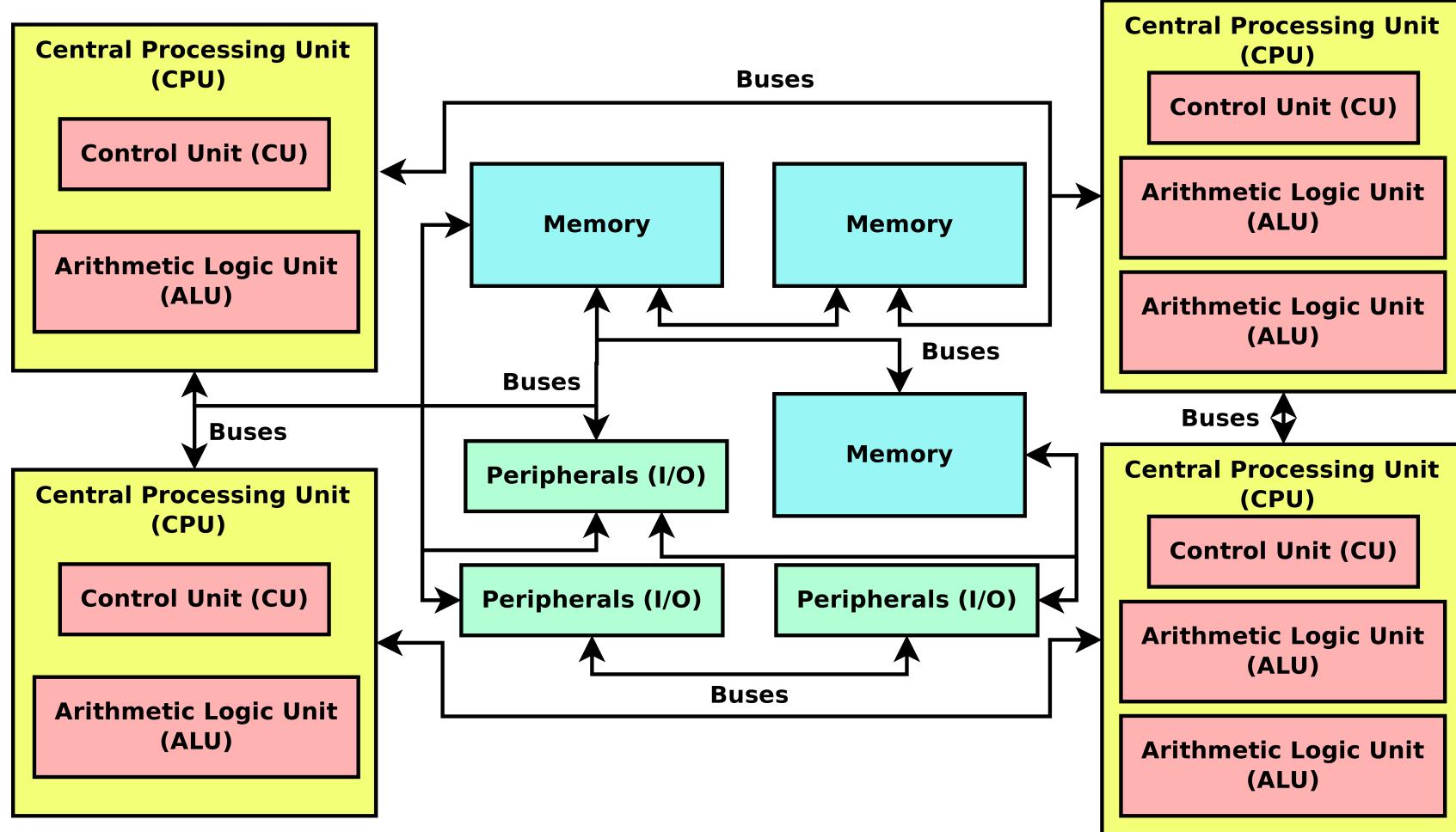
# A larger computer could be ...



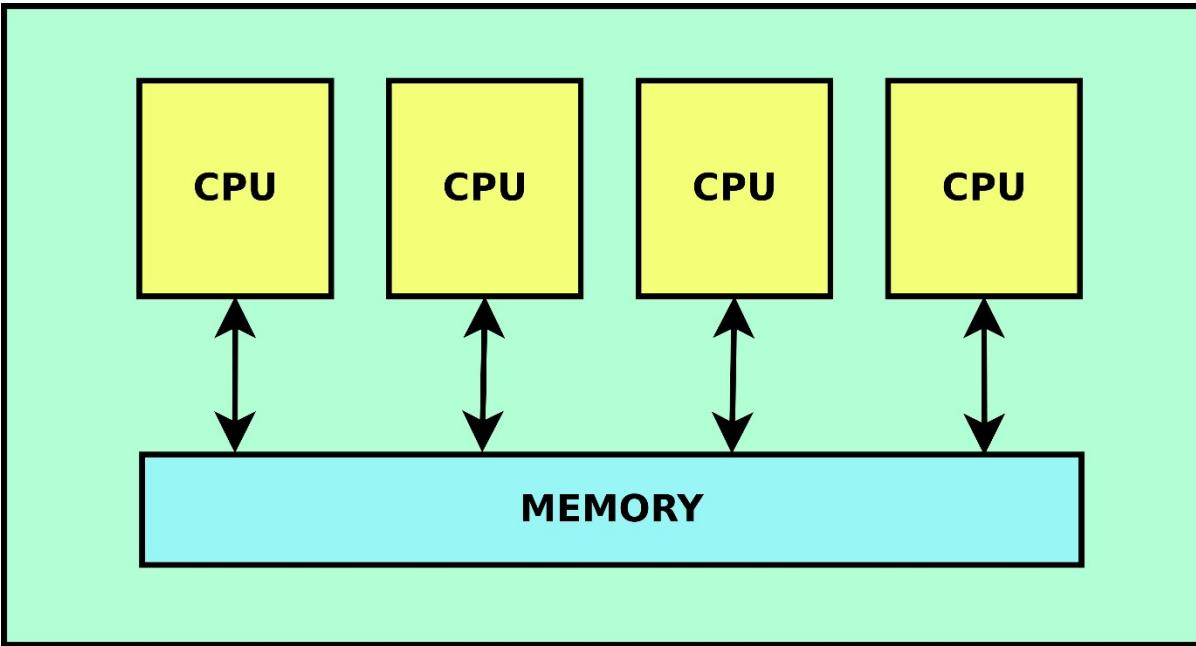
# A larger computer could be ...



# A larger computer could be ...

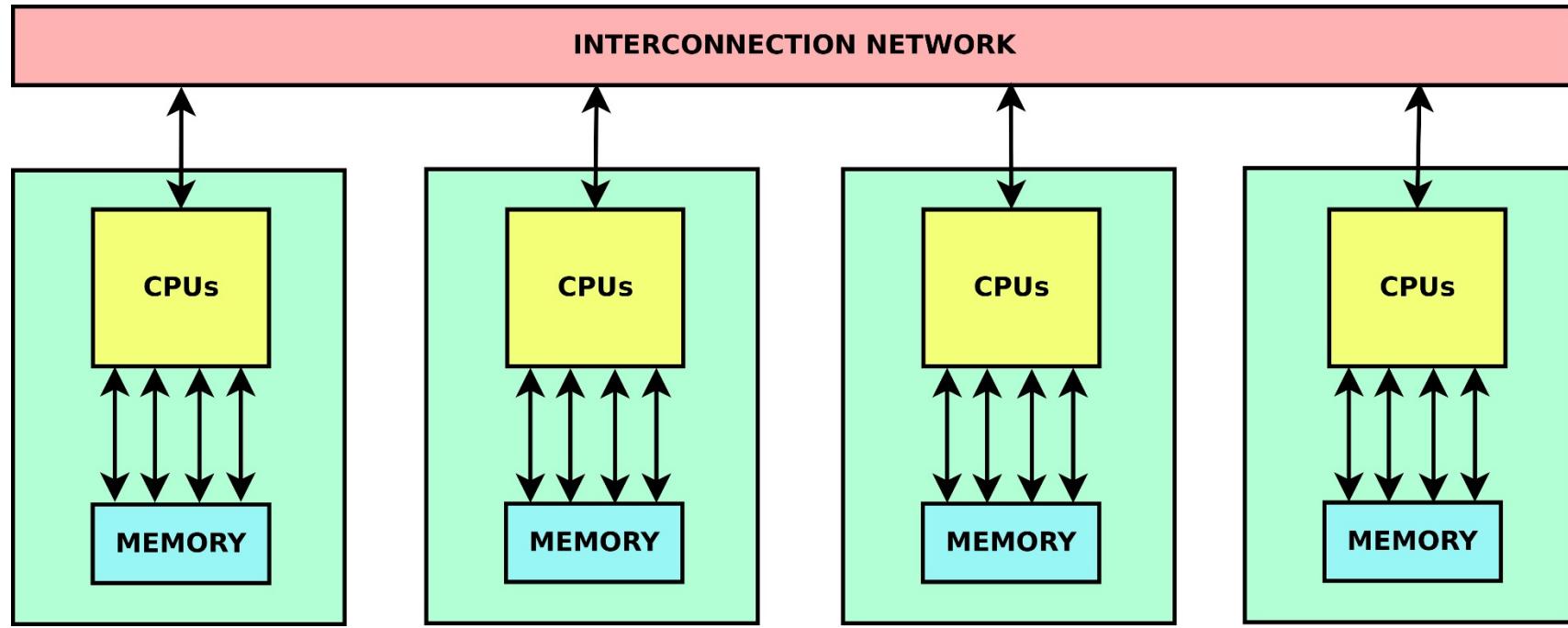


# A larger computer actually is ...



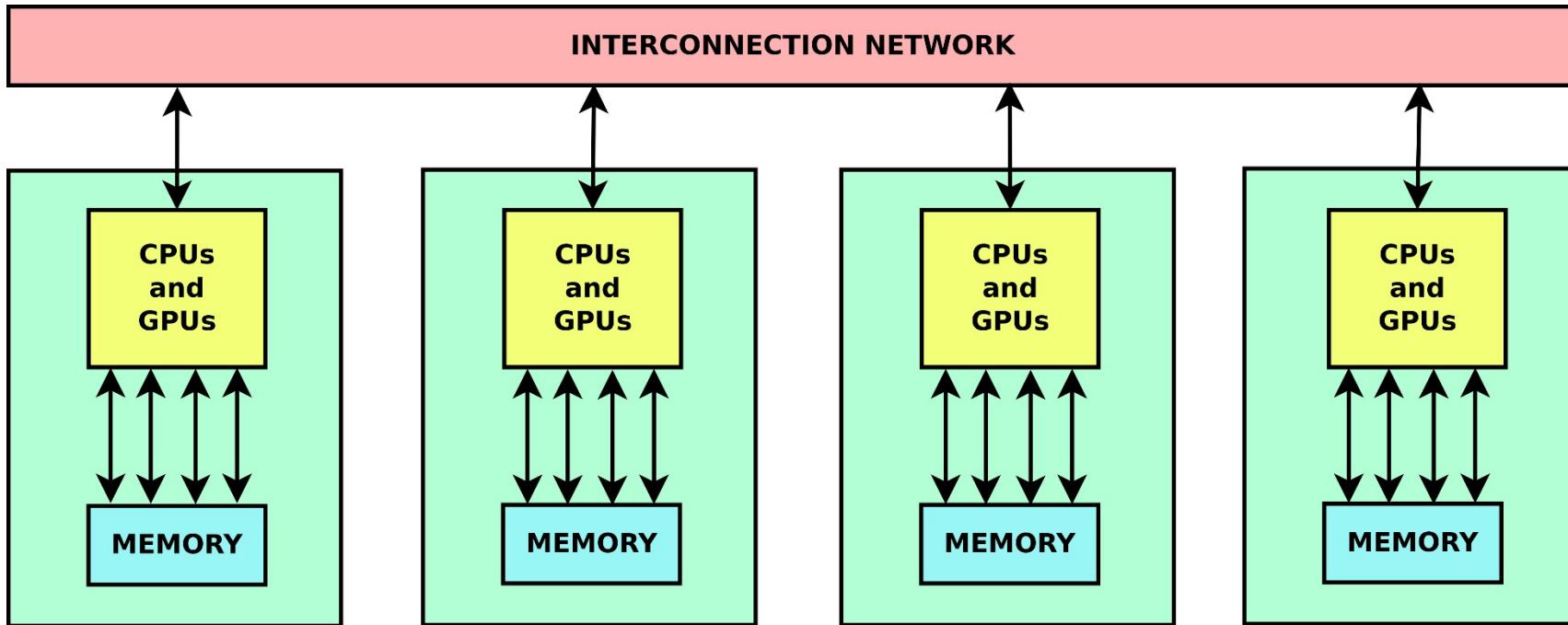
SURF

# A larger computer actually is ...



SURF

# A larger computer actually is ...



# Schematic overview of a supercomputer

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

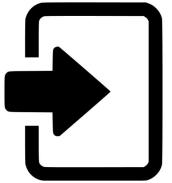


# Dutch national supercomputers: performance increase

Year	Machine	R <sub>peak</sub> (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 (1 <sup>st</sup> phase)	~ 6,100,000	610	10000
2016	Raspberry PI 3 (35 euro)	0.44	0.004	110

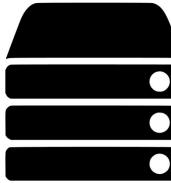


# Working with a Supercomputer



## 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

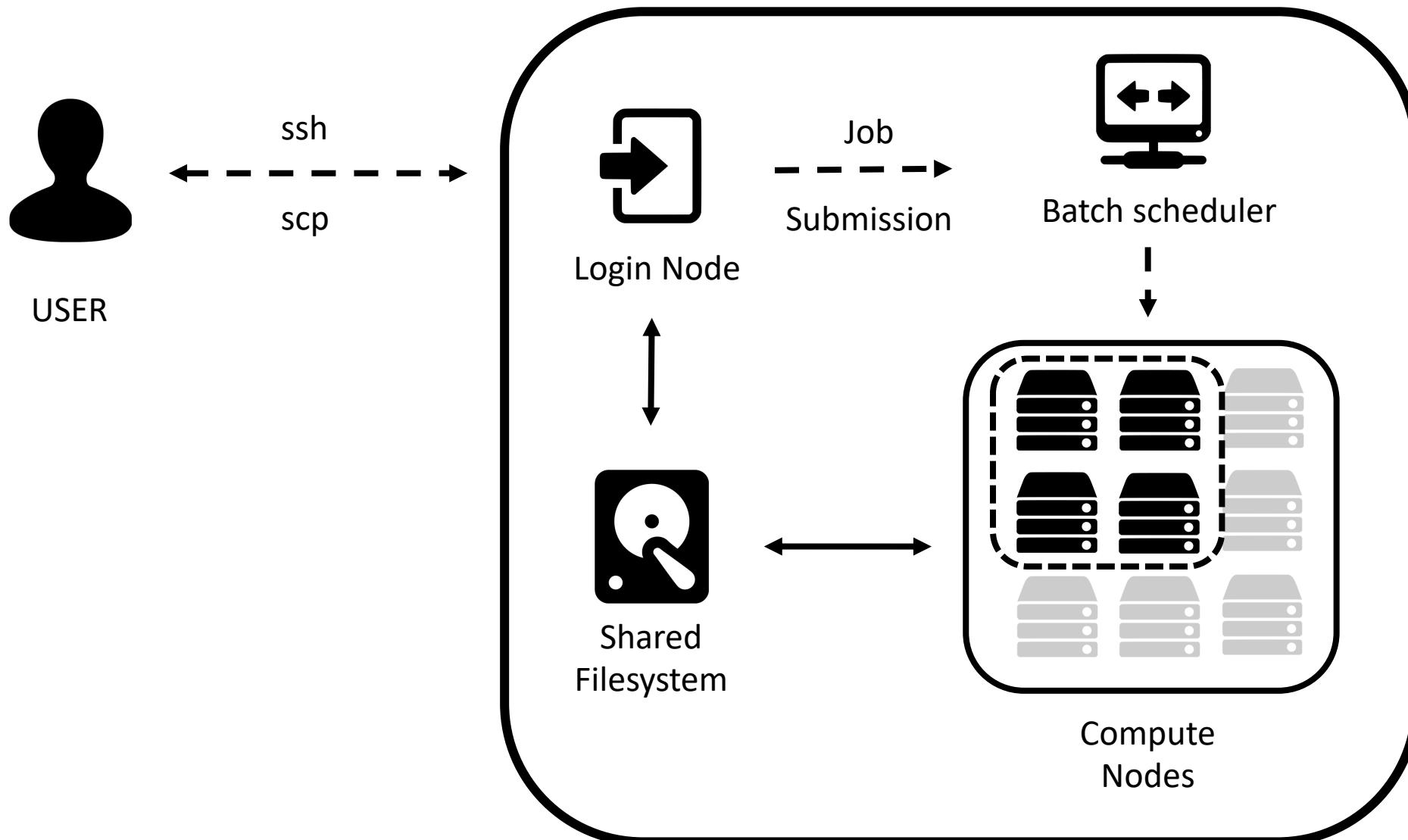


## File system

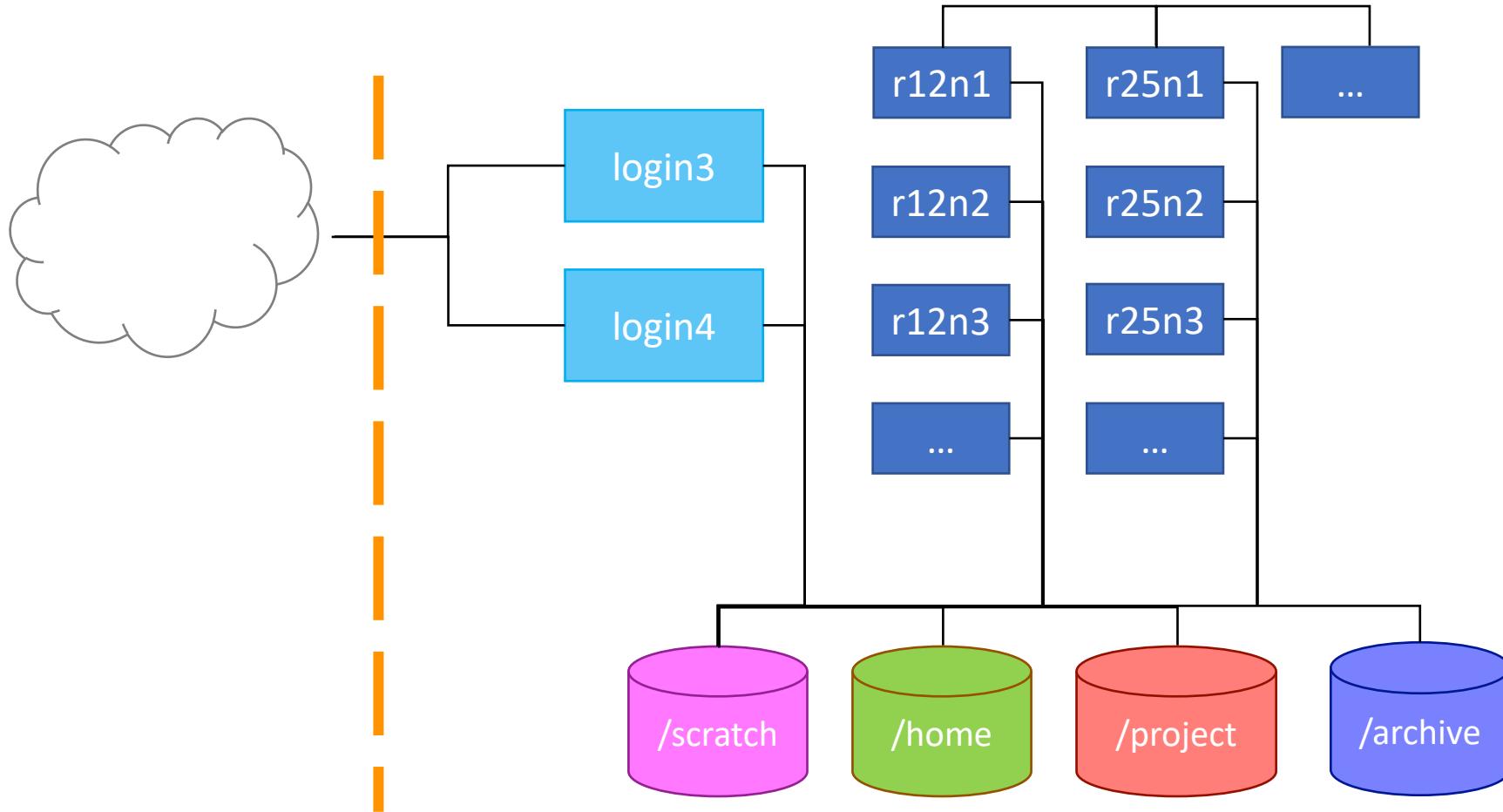
- Parallel FS
- Efficient I/O
- Node local disks



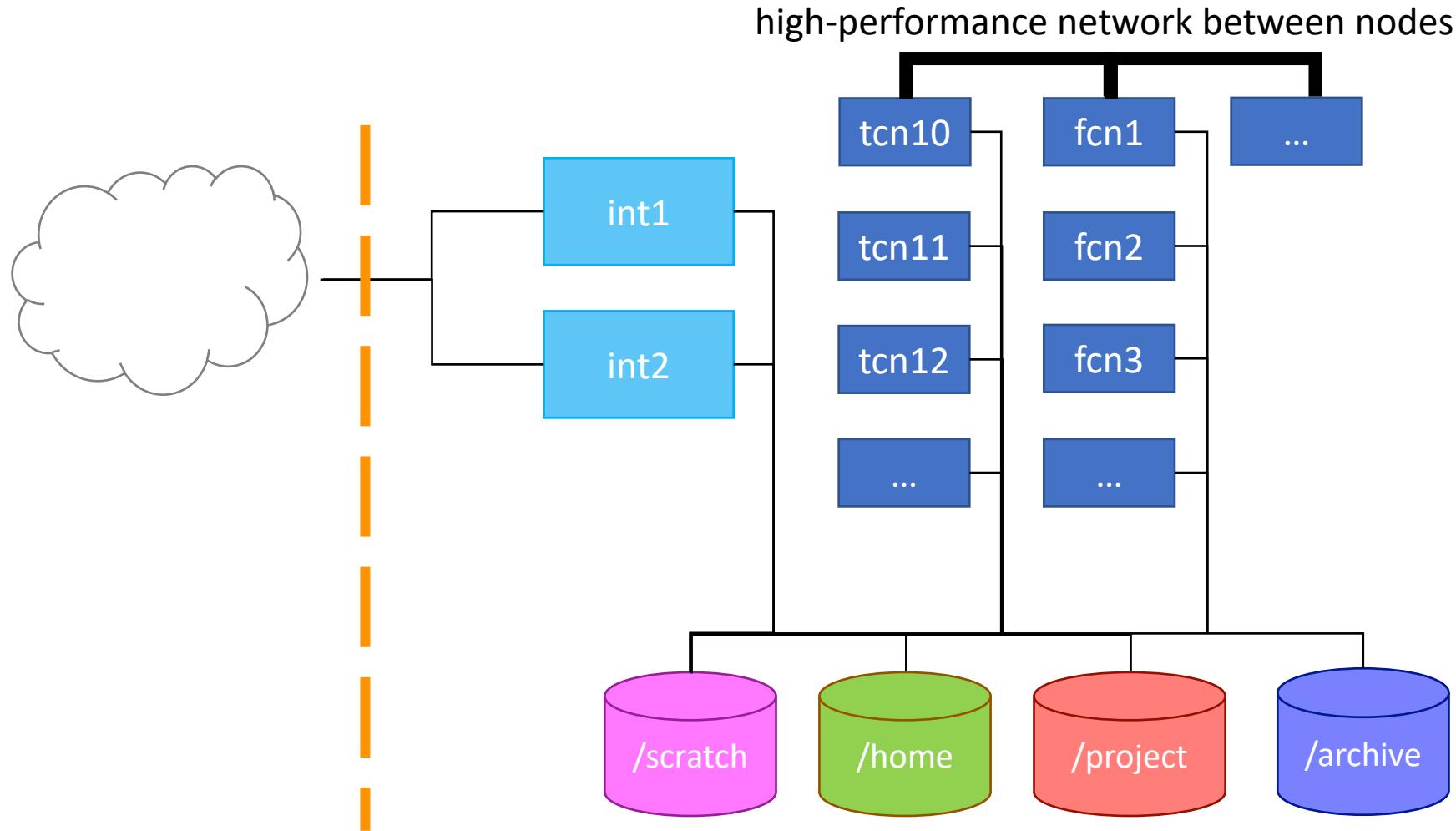
# Working with a Supercomputer



# 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....



SURF

# Working with a Supercomputer

```
Terminal — ssh sdemo050@lisa.surfsara.nl — 139x56
SURFsara

Welcome to SURFsara

** Please accept Usage Agreement at https://portal.surfsara.nl before using LISA services **

This is a private computer facility. Access for any reason must be
specifically authorized by the owner. Unless you are so authorized,
your continued access and any other use may expose you to criminal
and/or civil proceedings.

Information: http://www.surfsara.nl

[Password:
*****
*   *
* Information and documentation: https://userinfo.surfsara.nl/systems/lisa *
*   *
* Project space is now reachable at /project/[<username>|<projectname>] *
* Archive ( /archive ) is reachable on hosts lisa.surfsara.nl. *
*   *
***** - Please use /scratch as scratch (output) space for jobs *
* - Processes on the login nodes that consume more than 15 minutes cputime *
* or 1GB resident memory will be automatically killed. Certain system and *
* login programs are excluded from this, such as ssh and scp. *
***** MAINTENANCE on November 20th 2019 from 08:00 till 17:00 hrs. *
*   *
* - batch will be drained *
* - interactive nodes and batch nodes not available *
*   *
***** As of October 4th, the new module environment (previously 'surf-devel') is *
* now the default. For more information, please check the user mailing send *
* out on October 4th or: *
* - https://edu.nl/43x3m *
***** last modified: 07/11/19,07:57 ***

Budget information
Account      Budget      Used      Avail      Expires
lisademo (NRC)  50000:00  27637:14  22362:45  2019-12-31

You have 45% budget left!

Budget numbers are specified in hours. For detailed information
use command accinfo
Accounting information:
Your account is about to expire in 48 day(s)

Filesystem      Quota      Used      Avail      Use%  Server
/home/sdemo050    200.0 GB    12 KB    200.0 GB    0%    fs12

sdemo050@login3:~$ ]
```



# 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](mailto:helpdesk@surfsara.nl)



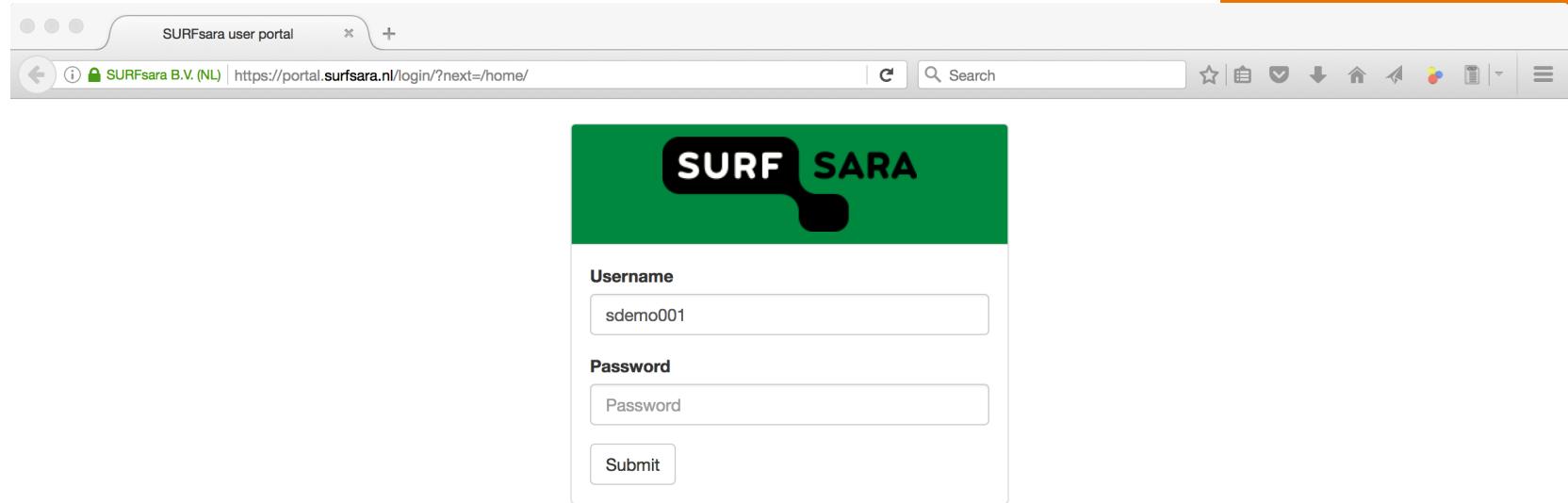
# **INTRODUCTION TO LINUX**

- 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



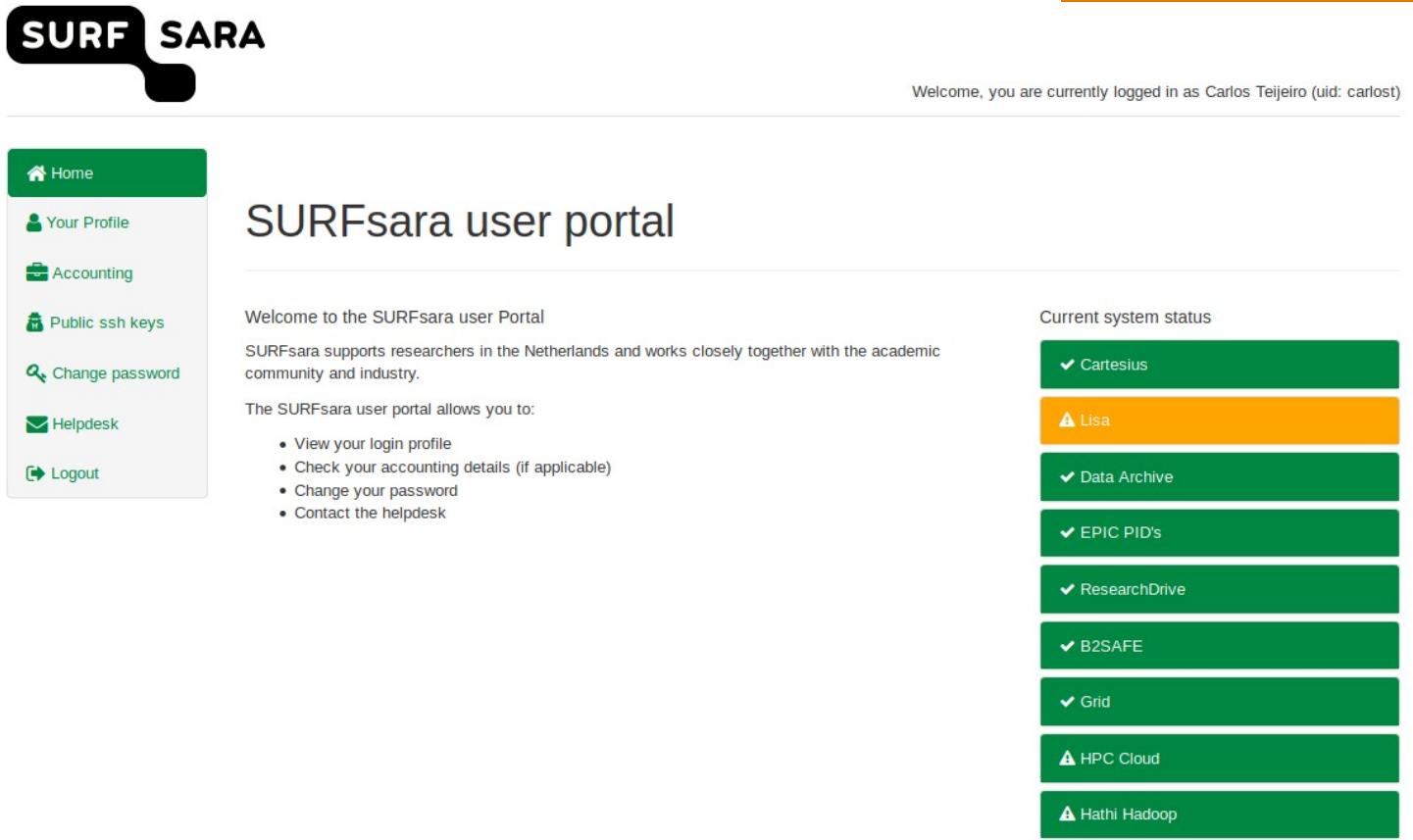
The screenshot shows a web browser window titled "SURFsara user portal". The address bar displays "SURFsara B.V. (NL) https://portal.surfsara.nl/login/?next=/home/". The main content is a login form with a green header containing the "SURF SARA" logo. The form has fields for "Username" (sdemo001) and "Password", and a "Submit" button.

<https://portal.surfsara.nl>

# Working with a Supercomputer

## Login to LISA system

- Email from [helpdesk@surfsara.nl](mailto:helpdesk@surfsara.nl) with credentials (sdemoXXX)
- Login to SURFsara portal
- Accept usage agreement
- Change password
- Check systems status

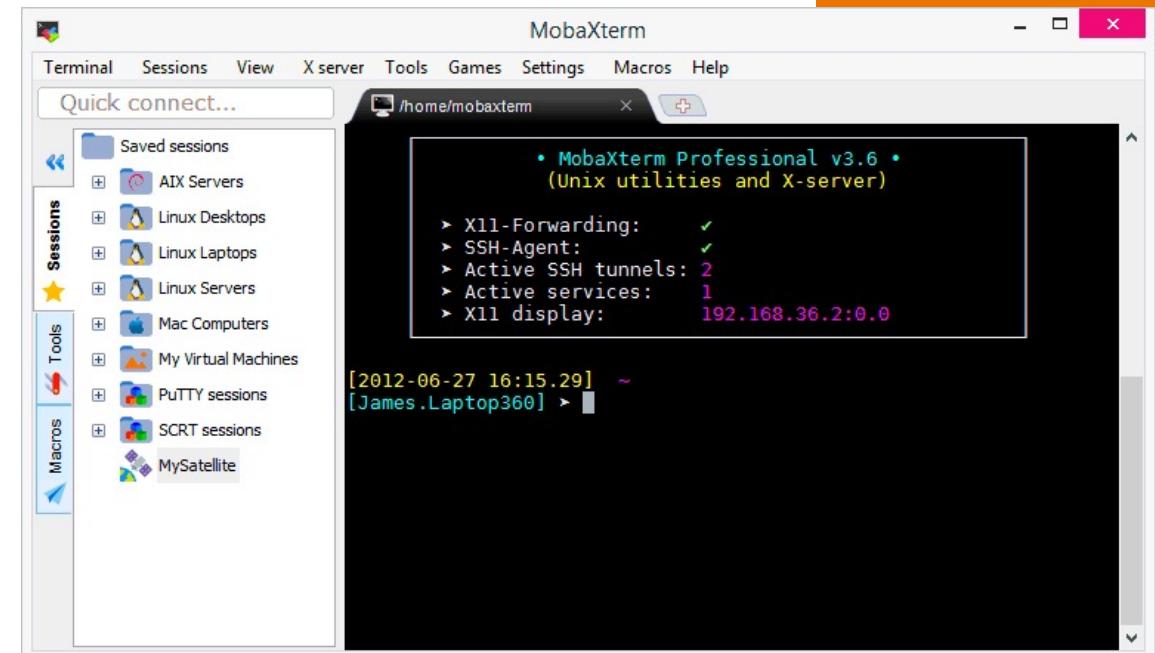


The screenshot shows the SURFsara user portal homepage. At the top, there is a logo with the words "SURF SARA". Below it, a welcome message says "Welcome, you are currently logged in as Carlos Teijeiro (uid: carlost)". On the left, there is a sidebar with a green header containing links: "Home", "Your Profile", "Accounting", "Public ssh keys", "Change password", "Helpdesk", and "Logout". The main content area has a title "SURFsara user portal" and a welcome message: "Welcome to the SURFsara user Portal. SURFsara supports researchers in the Netherlands and works closely together with the academic community and industry." It lists what the portal allows: "View your login profile", "Check your accounting details (if applicable)", "Change your password", and "Contact the helpdesk". To the right, there is a section titled "Current system status" with a list of systems: Cartesius (green bar with checkmark), Lisa (orange bar with warning icon), Data Archive (green bar with checkmark), EPIC PIDs (green bar with checkmark), ResearchDrive (green bar with checkmark), B2SAFE (green bar with checkmark), Grid (green bar with checkmark), HPC Cloud (green bar with warning icon), and Hathi Hadoop (green bar with warning icon).

# Working with a Supercomputer

## Install UNIX tools on your local machine

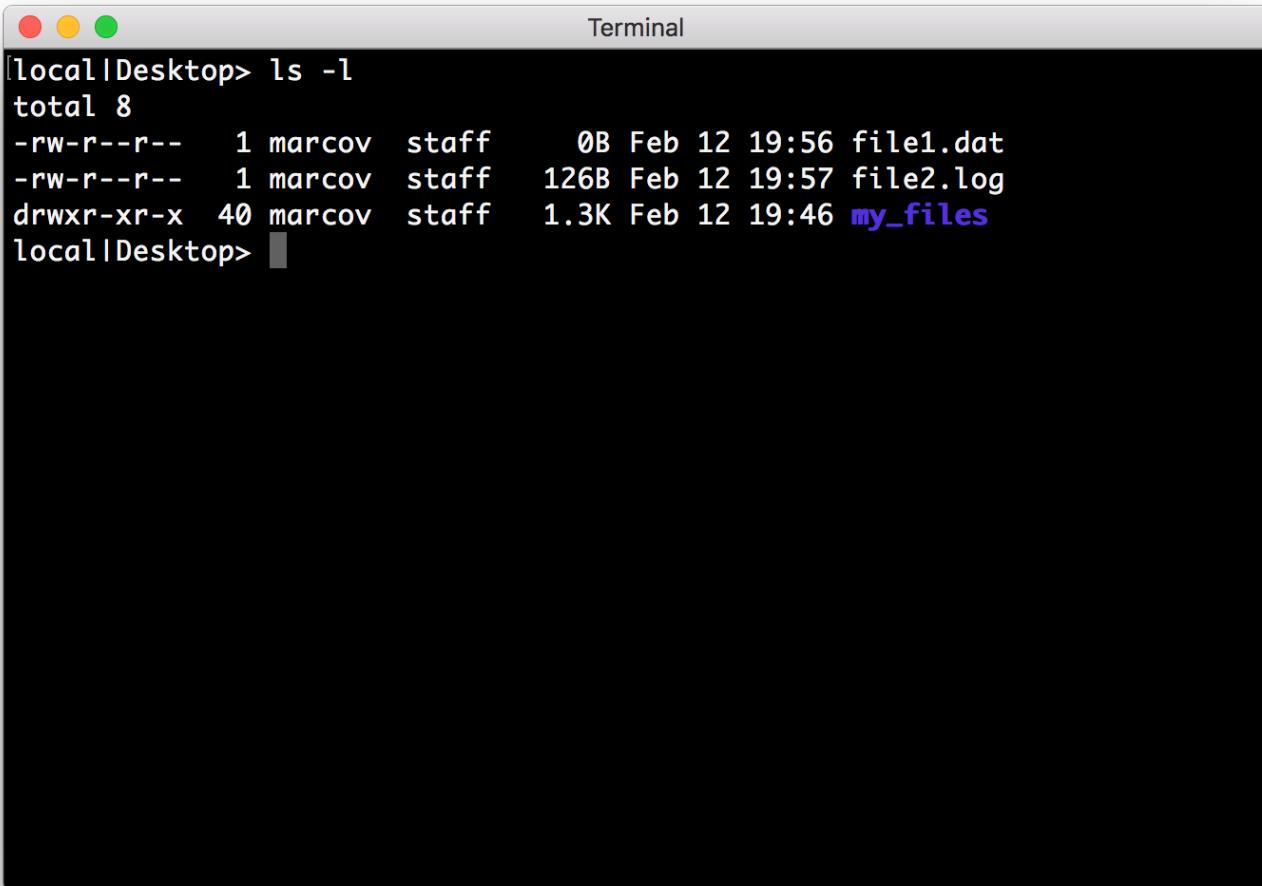
- Windows
  - Putty (<https://www.putty.org/>)
  - MobaXterm (<http://mobaxterm.mobatek.net>)
- Mac OSX
  - Terminal (pre-installed)
  - iTerm2 (<https://iterm2.com>)
- Linux
  - You are already well equipped!



MobaXterm interface

# Working with a Supercomputer

## The Terminal and the command line



```
[local|Desktop> ls -l
total 8
-rw-r--r--  1 marcov  staff      0B Feb 12 19:56 file1.dat
-rw-r--r--  1 marcov  staff   126B Feb 12 19:57 file2.log
drwxr-xr-x  40 marcov  staff  1.3K Feb 12 19:46 my_files
local|Desktop> ]
```

# 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 lcur001@lisa.surfsara.nl  
Password:
```

The SURF logo consists of the word "SURF" in a bold, black, sans-serif font, positioned within a white speech bubble shape with a black outline.

# Working with a Supercomputer

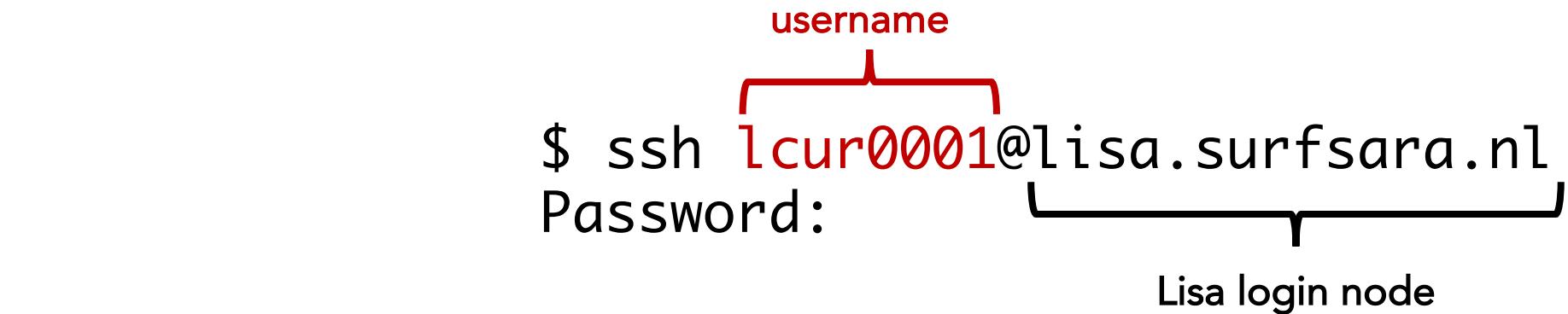
## SSH, or Secure SHell

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

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

username

Lisa login node



# Working with a Supercomputer

You are logged in!!!

```
Default (ssh)
Welcome to SURFsara

** Please accept Usage Agreement at https://portal.surfsara.nl before using LISA services **

This is a private computer facility. Access for any reason must be
specifically authorized by the owner. Unless you are so authorized,
your continued access and any other use may expose you to criminal
and/or civil proceedings.

Information: http://www.surfsara.nl

Password:
Last login: Wed Nov 13 09:55:04 2019 from 145.100.1.88
*****
*   *
*   * Information and documentation: https://userinfo.surfsara.nl/systems/lisa *
*   *
*   * Project space is now reachable at /project/[<username>|<projectname>] *
*   * Archive ( /archive ) is reachable on hosts lisa.surfsara.nl. *
*   *
***** - Please use /scratch as scratch (output) space for jobs *
*   - Processes on the login nodes that consume more than 15 minutes cputime *
*   or 1GB resident memory will be automatically killed. Certain system and *
*   login programs are excluded from this, such as ssh and scp. *
***** MAINTENANCE on November 20th 2019 from 08:00 till 17:00 hrs. *
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*   out on October 4th or: *
*   - https://edu.nl/43x3m
***** last modified: 07/11/19,07:57 ***

Budget information
Account          Budget      Used      Avail      Expires
lisademo (NRC)  50000:00  27637:14  22362:45  2019-12-31

You have 45% budget left!

Budget numbers are specified in hours. For detailed information
use command accinfo
Accounting information:
Your account is about to expire in 48 day(s)

Filesystem        Quota      Used      Avail      Use%    Server
/home/sdemo050   200.0 GB   2.09 GB   197.91 GB  1%     fs12

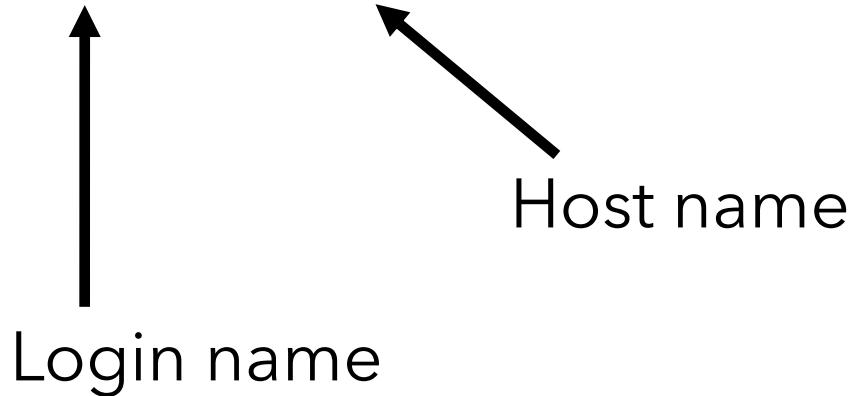
sdemo050@login4:~$
```

# Introduction to Linux



- After successful login

```
lcur001@login4:~>
```



- Now the system is ready to accept commands



# Introduction to Linux - Exercise

- Explore the file system

- ls, cd, pwd

cd VU\_HPC-master

:~> ls  
bin file1.txt file2.log

- Create and edit files and directories

- mkdir, touch, cp, mv, nano, less, vi

nano README.md

- Use variable (env. variables)

- \$USER, \$HOME

:~> echo \$USER

- System tools

- history, find, zip, tar

:~> echo \$USER



# 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

```
lcur0001@login4 :~> mkdir -p dir1/subdir
```

### Command

The UNIX shell (bash) tries to find a program called 'mkdir' and takes care that the system executes it.

### Options

Passed to the command as a parameter(s) to change its default behavior.

### Arguments

Taken as input by the program.

- 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
```

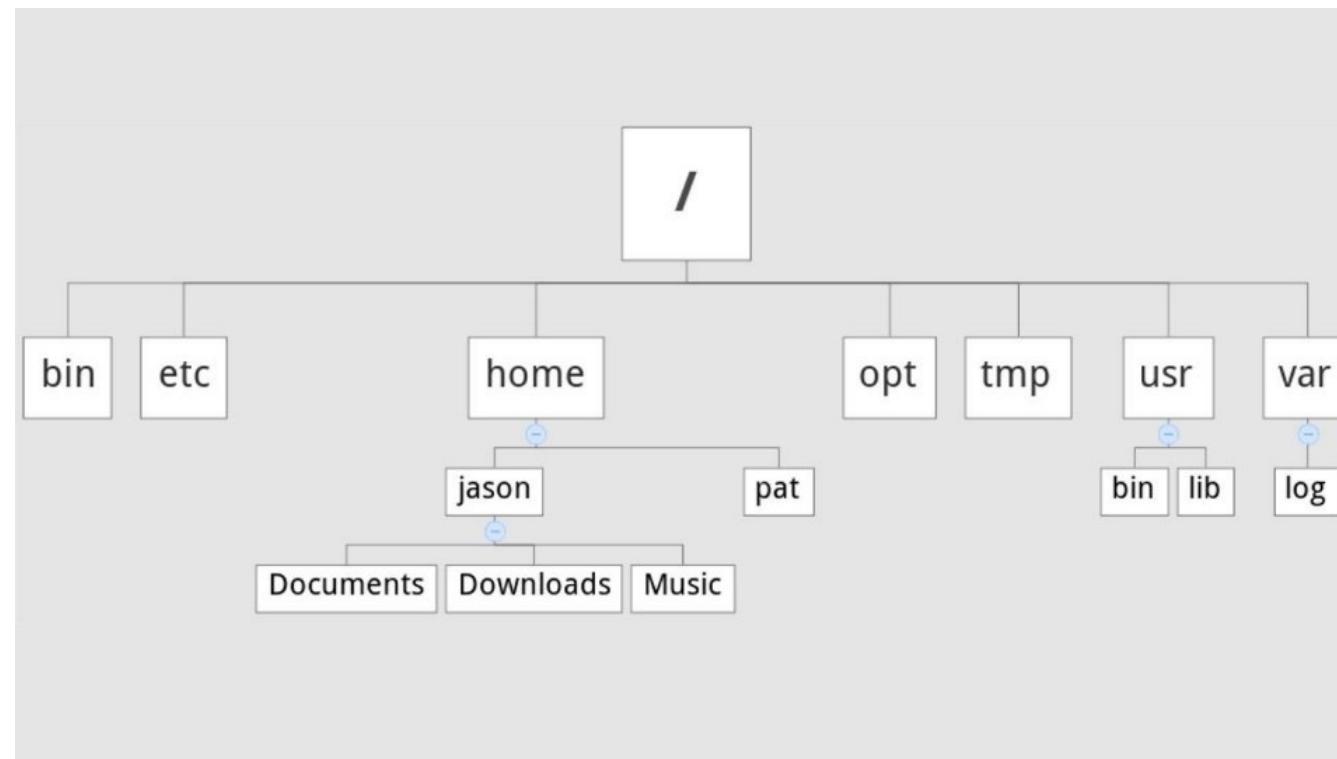
- Absolute path

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

# Introduction to Linux



- Directory Structure and Hierarchy



# 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

A screenshot of a Google search results page for the query "bash programming". The search bar at the top contains "bash programming". Below it, a navigation bar includes "All", "Videos", "Images", "News", "Shopping", "More", "Settings", and "Tools". A message indicates "About 38,500,000 results (0.66 seconds)". The top result is a link to "BASH Programming - Introduction HOW-TO" from tldp.org, dated Jul 27, 2017. The snippet describes it as an introduction to basic-intermediate shell scripts. Below the result is a "People also search for" box containing links like "bash programming pdf", "simple bash script example", and "print in bash script". To the right is a "People also ask" box with three expandable questions: "What is bash programming?", "What does \$() mean in bash?", and "What is bash useful?".

[Bash Scripting: Everything you need to know about Bash-shell ...](#)  
https://itnext.io › bash-scripting-everything-you-need-to-know-about-bash... ▾  
Sep 10, 2019 - In this article, we are going to cover almost every single topic there is in Bash programming. This articles mainly focus on programming spec ...

[Shell programming with bash: by example, by counter-example](#)  
matt.might.net › articles › bash-by-example ▾  
As an interactive shell, bash is a terse language for initiating and directing computations. As a scripting language, bash is a domain-specific language for ...

[Bash scripting cheatsheet - Devhints](#)  
https://devhints.io › bash ▾  
Variables · Functions · Interpolation · Brace expansions · Loops · Conditional execution · Command substitution · One-page guide to Bash scripting.

[Understanding Bash: Elements of Programming | Linux Journal](#)  
https://www.linuxjournal.com › content › understanding-bash-elements-pr... ▾  
Sep 28, 2018 - Ever wondered why programming in Bash is so difficult? Bash employs the same constructs as traditional programming languages; however, ...

# 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

```
lcur001@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

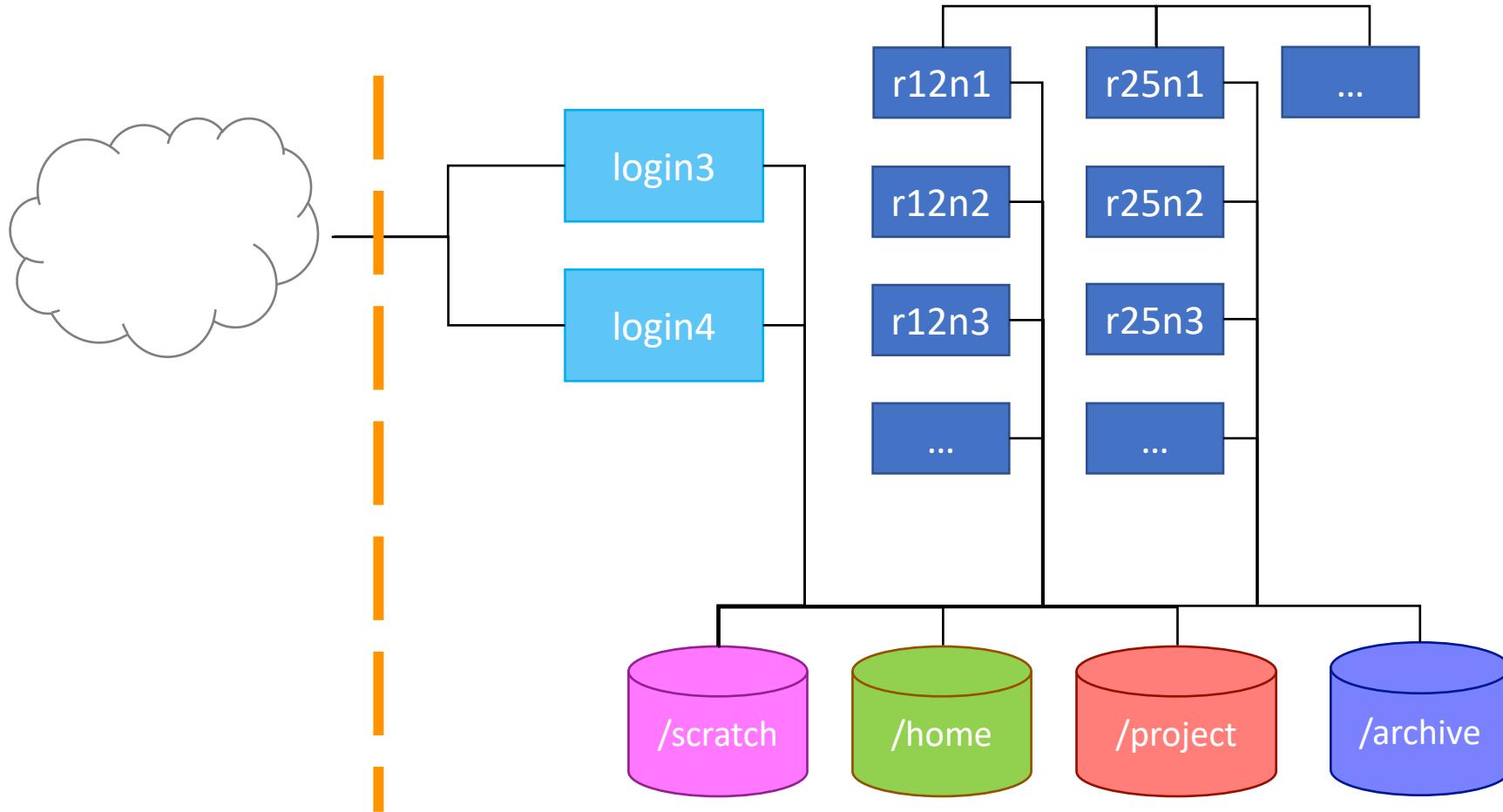
```
lcur0001@login4:~> python --version  
lcur0001@login4:~> which python
```

- 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 $TMPDIR/* ~/results
```

SURF

# 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
```

SURF

# 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/Snellijs+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>

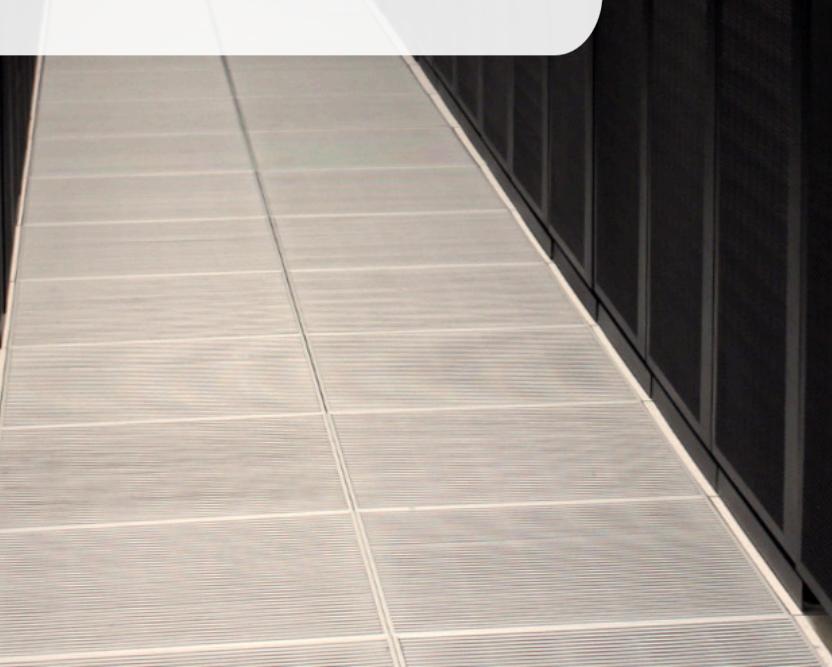
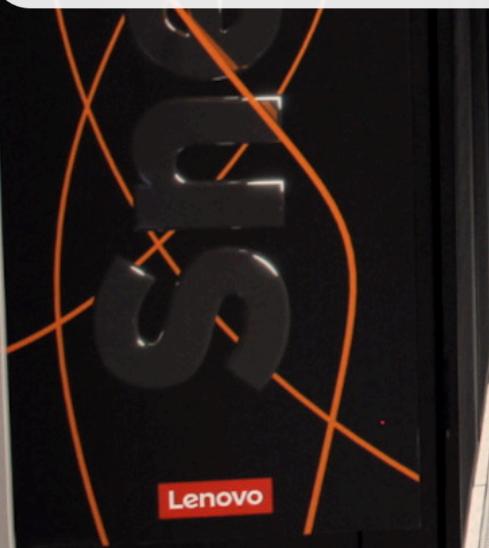




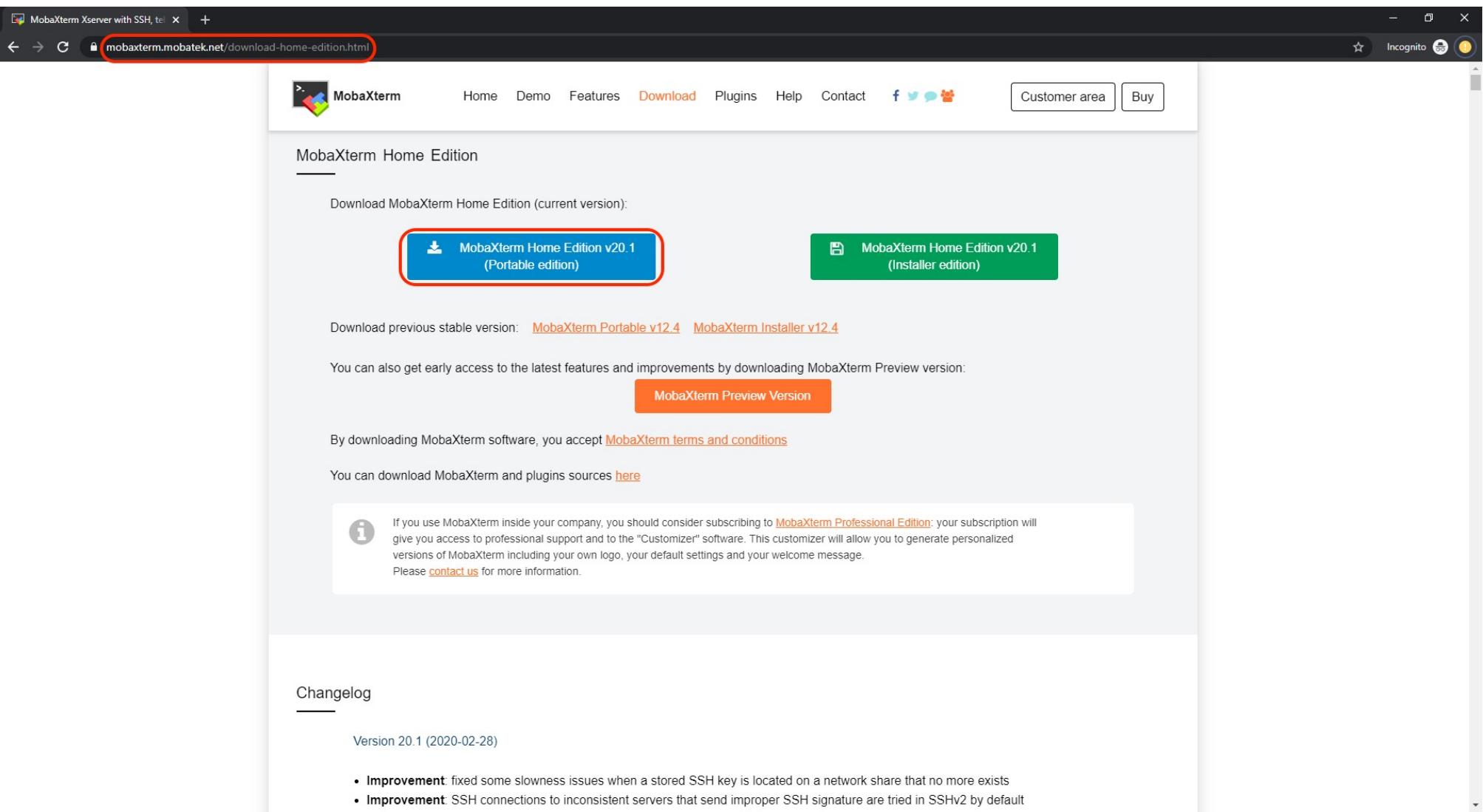
SURF

# Thank you!

Benjamin Czaja, Marco Verdicchio  
HPC Advisors, SURFsara



# Download the portable edition of MobaXterm



The screenshot shows a web browser window with the URL [mobaxterm.mobatek.net/download-home-edition.html](http://mobaxterm.mobatek.net/download-home-edition.html) highlighted with a red box. The page content is as follows:

MobaXterm Home Edition

Download MobaXterm Home Edition (current version):

[MobaXterm Home Edition v20.1 \(Portable edition\)](#) (button highlighted with a red box)

[MobaXterm Home Edition v20.1 \(Installer edition\)](#)

Download previous stable version: [MobaXterm Portable v12.4](#) [MobaXterm Installer v12.4](#)

You can also get early access to the latest features and improvements by downloading MobaXterm Preview version:

[MobaXterm Preview Version](#)

By downloading MobaXterm software, you accept [MobaXterm terms and conditions](#)

You can download MobaXterm and plugins sources [here](#)

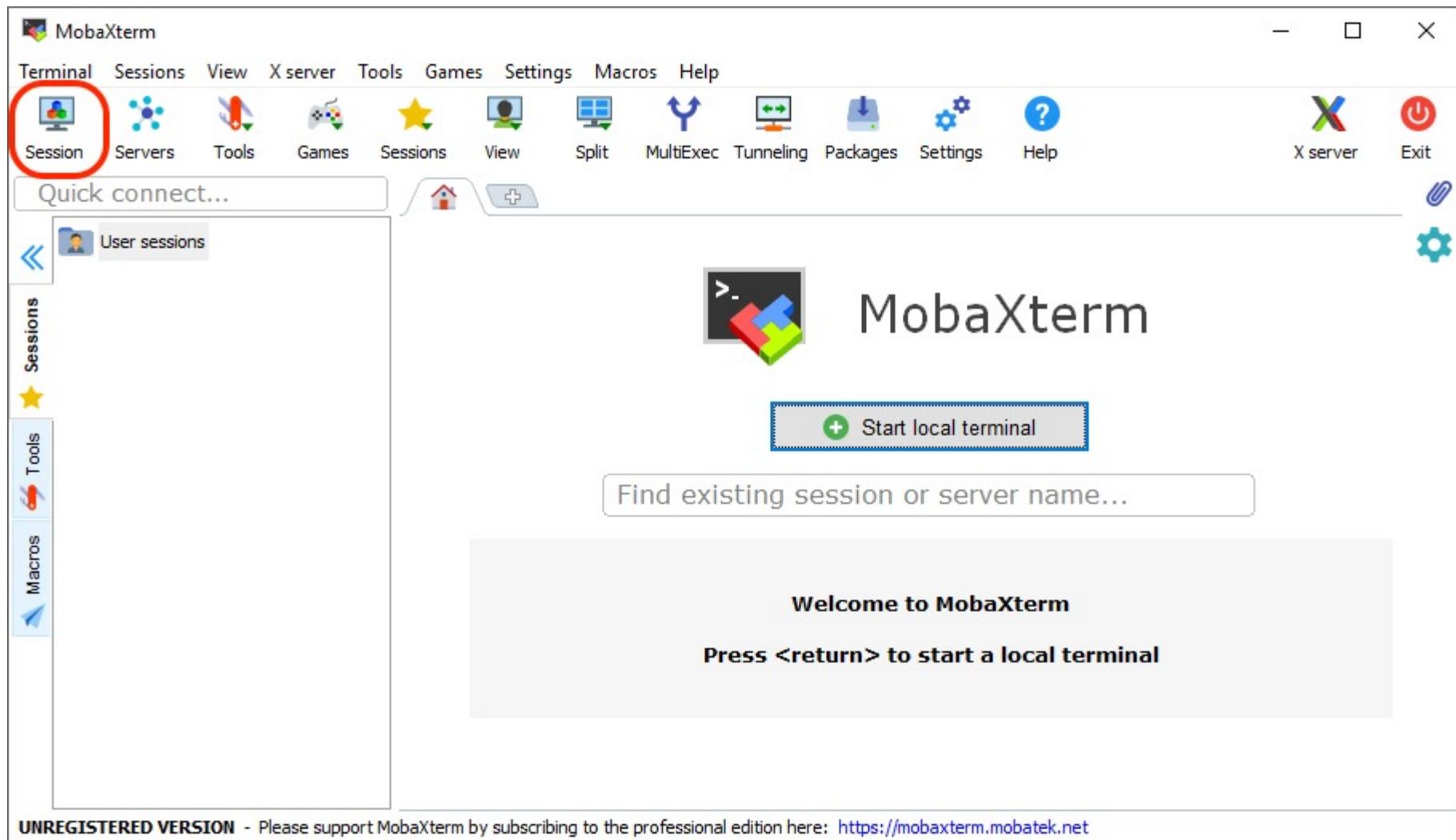
**i** If you use MobaXterm inside your company, you should consider subscribing to [MobaXterm Professional Edition](#): your subscription will give you access to professional support and to the "Customizer" software. This customizer will allow you to generate personalized versions of MobaXterm including your own logo, your default settings and your welcome message.  
Please [contact us](#) for more information.

Changelog

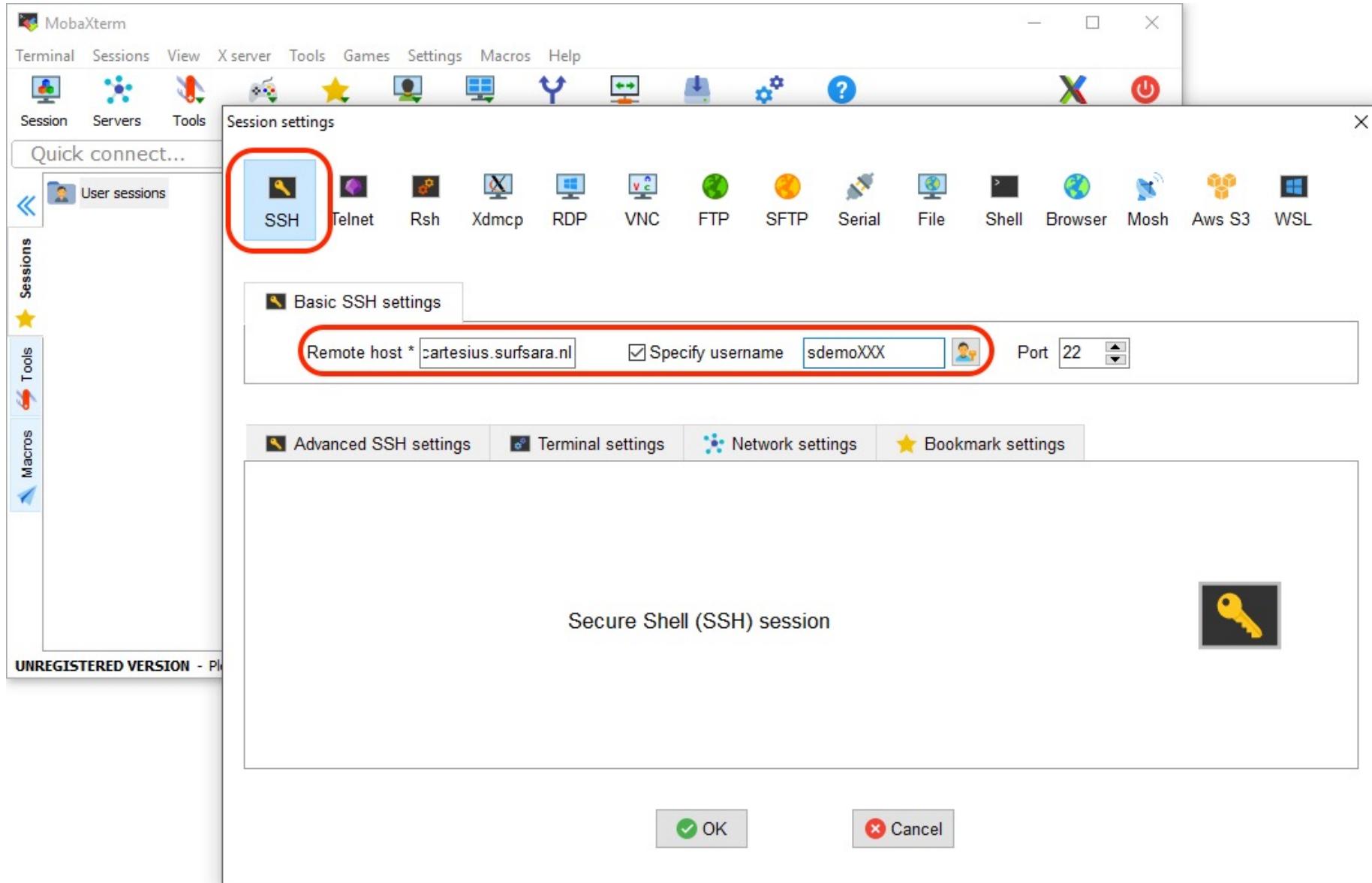
Version 20.1 (2020-02-28)

- **Improvement:** fixed some slowness issues when a stored SSH key is located on a network share that no more exists
- **Improvement:** SSH connections to inconsistent servers that send improper SSH signature are tried in SSHv2 by default

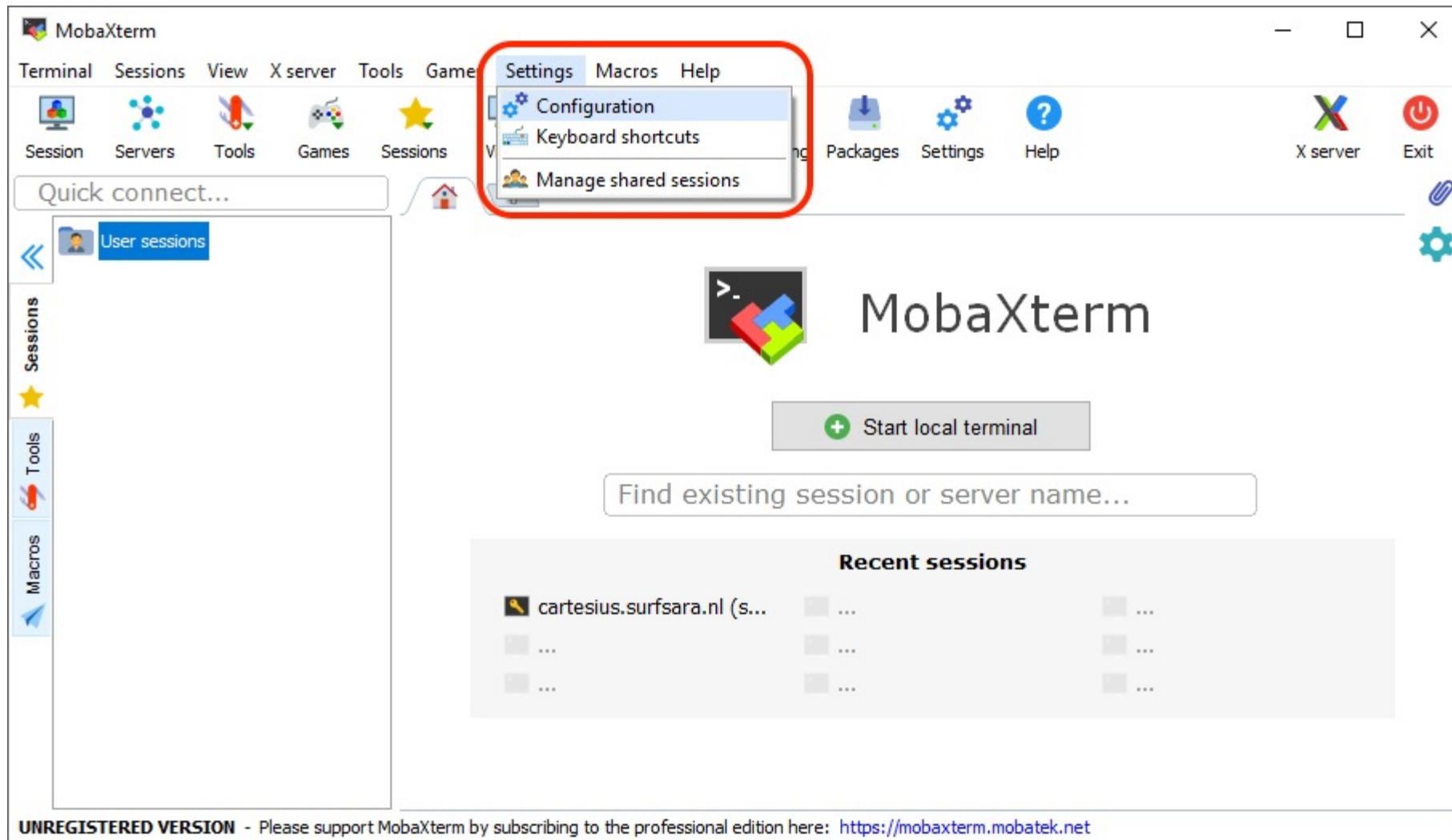
# Open a new remote session



# Open a new remote session



# Change the root/home folders (via Settings->Configuration)



# Change the root/home folders (via Settings->Configuration)

