

<https://hpcleuven.github.io/Linux-for-HPC/>



Linux for HPC



Overview

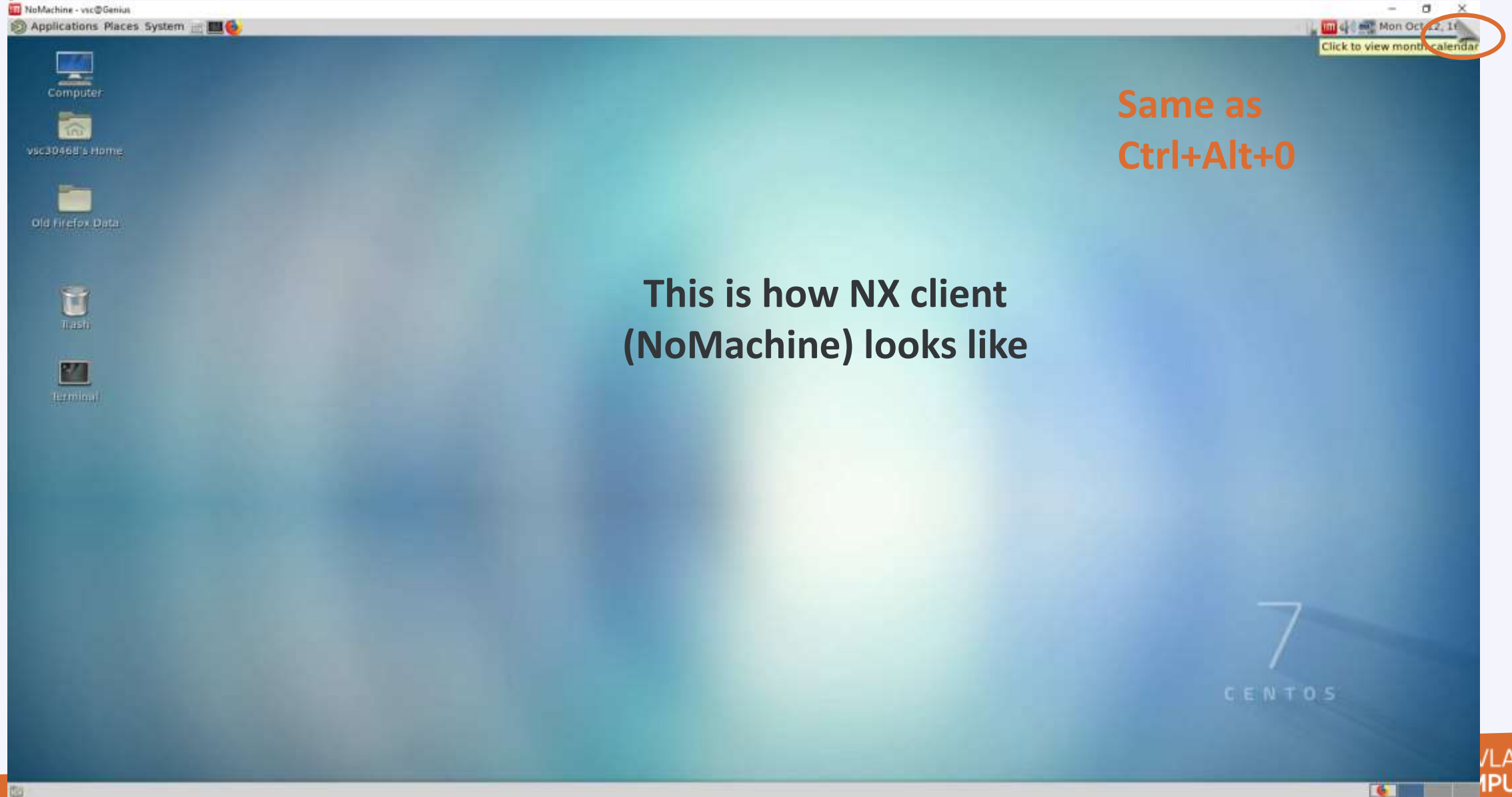
- Who is this course for?
 - You know Linux basics
 - You use HPC platforms
 - Need a generic overview of Linux tools

Outline

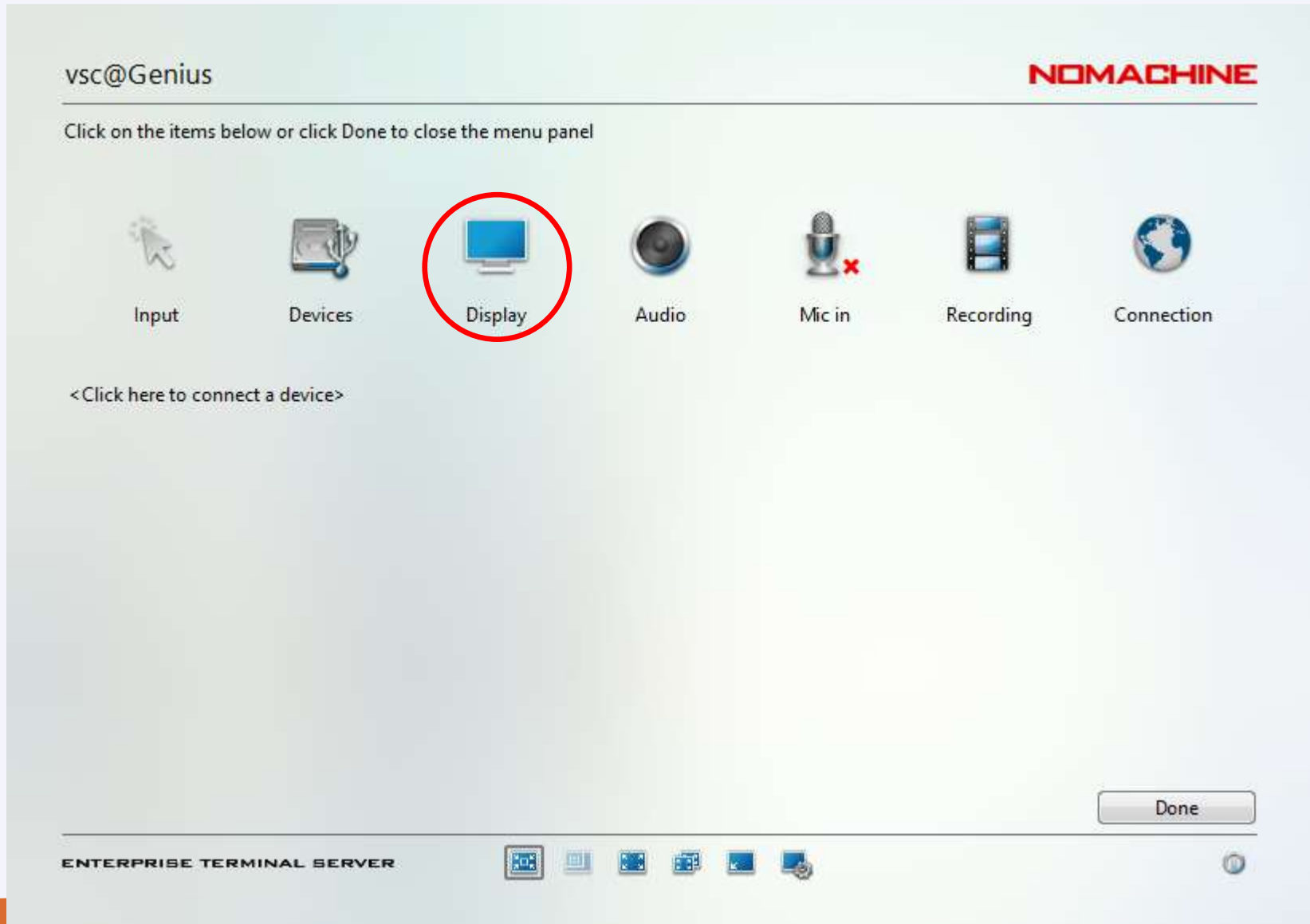
- Using NX
- More Linux commands
- Key Concepts, Redirection & Pipes
- Shell, Bash and Job Scripts
- Installing & Compiling Code

Customizing GUI (NX)

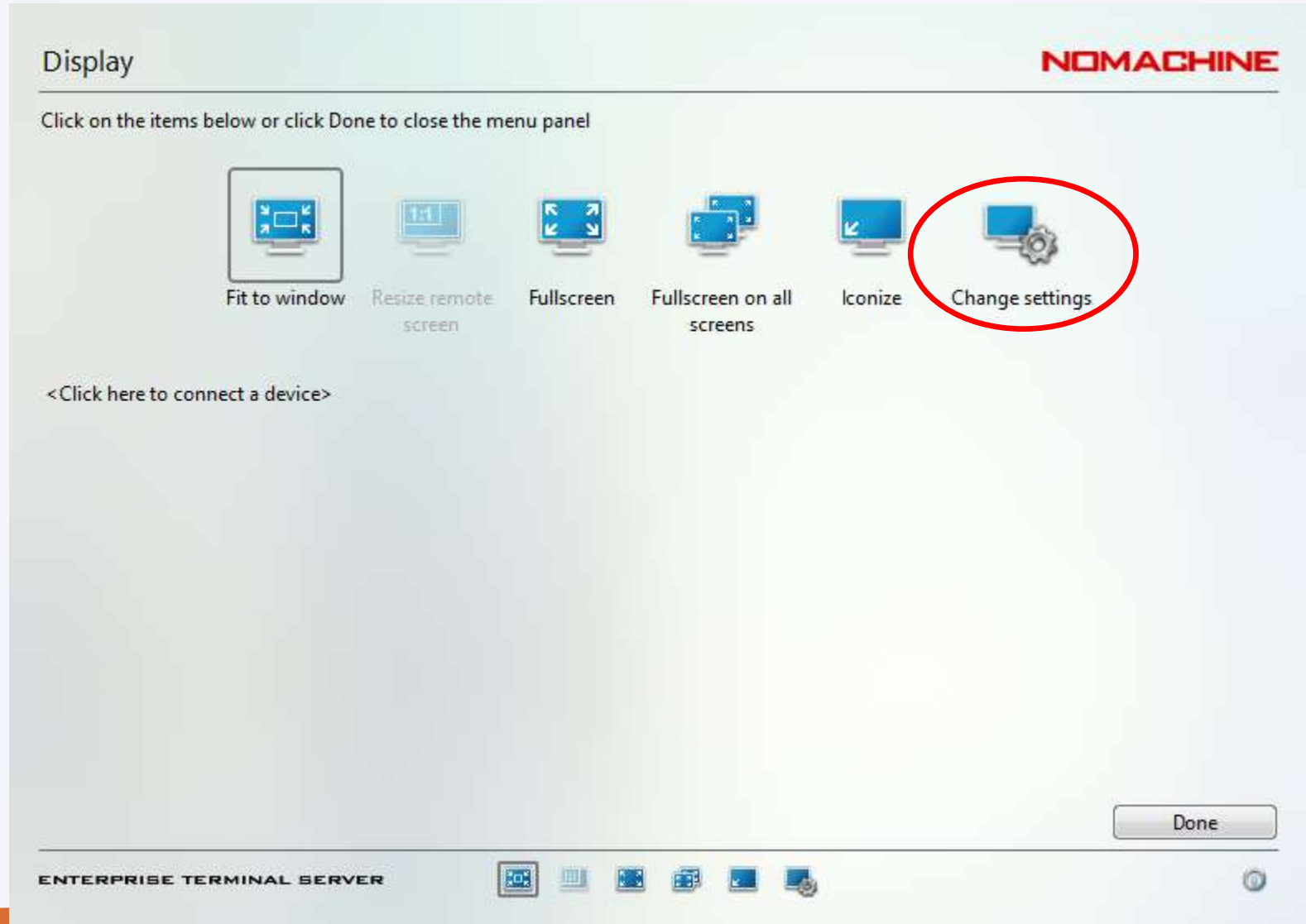
System tools



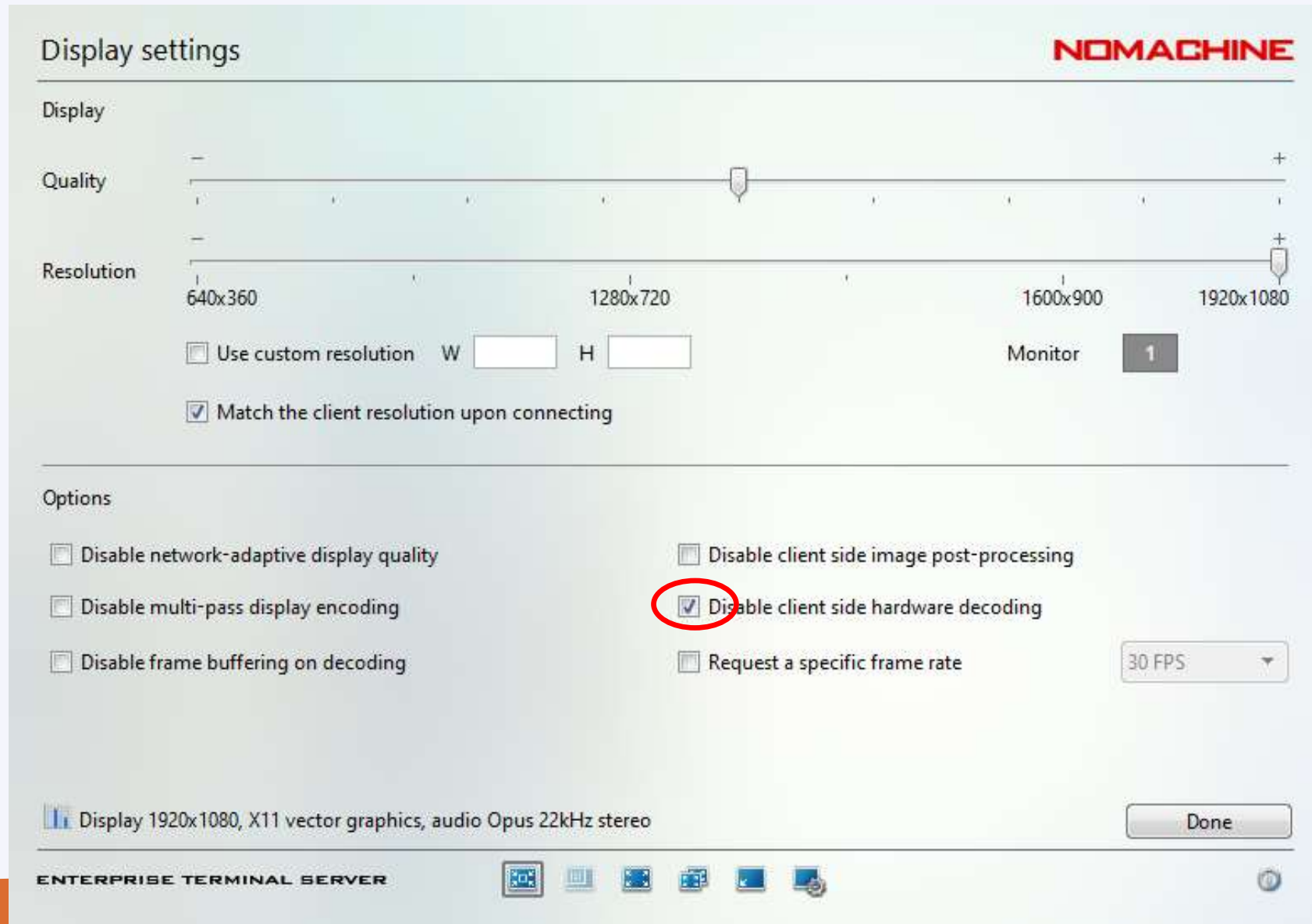
System tools – proper display



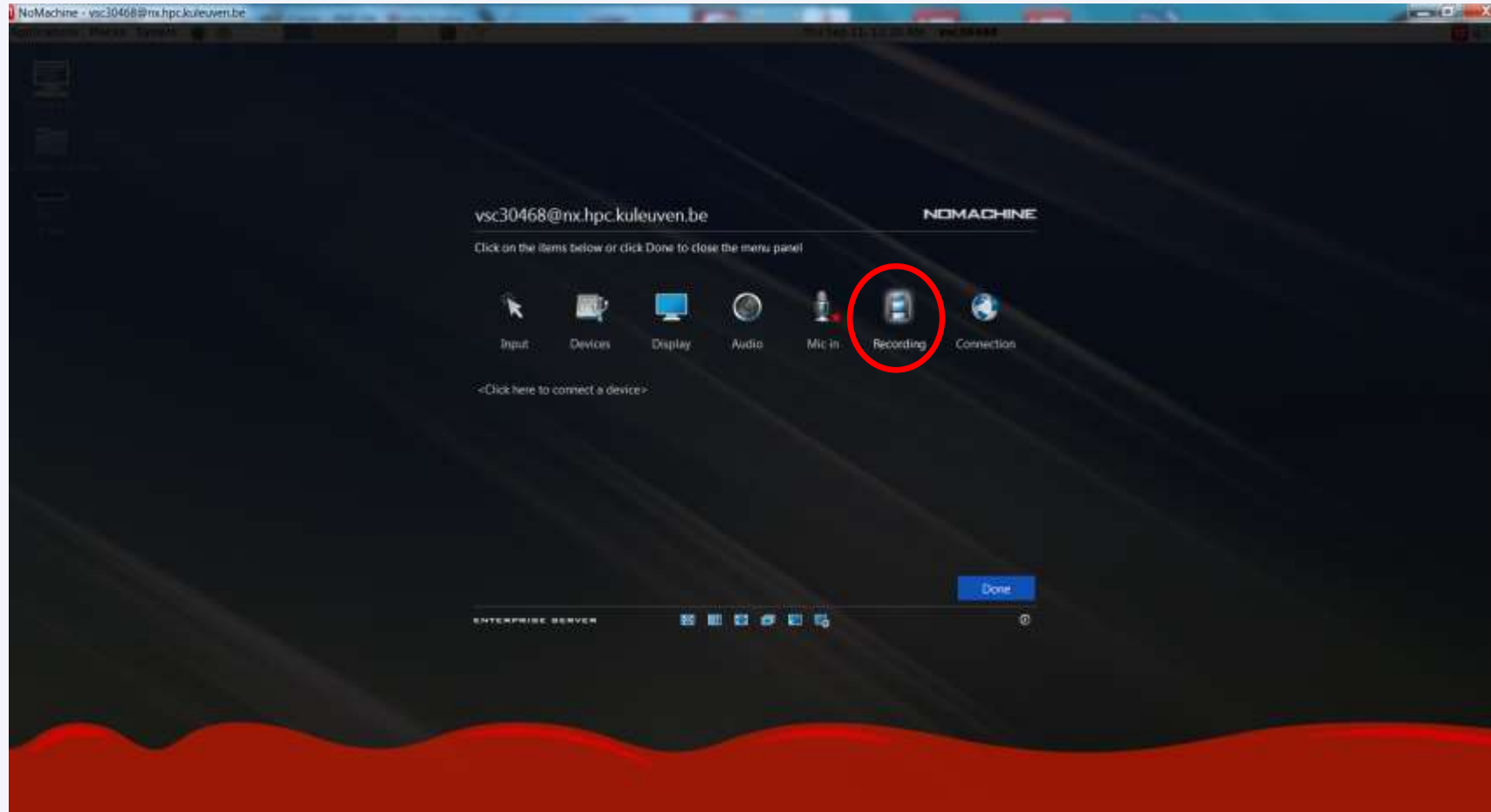
System tools – proper display



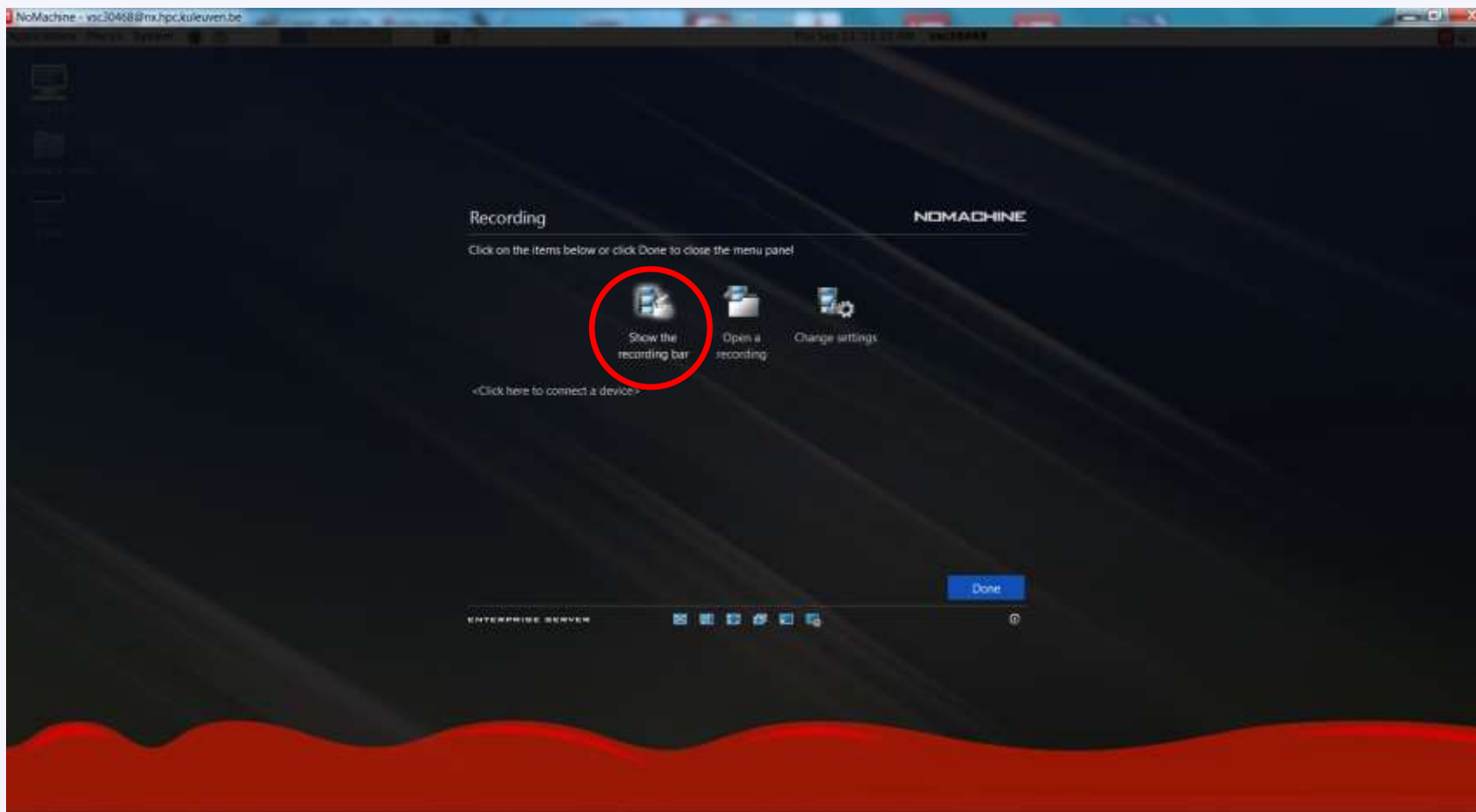
System tools – proper display



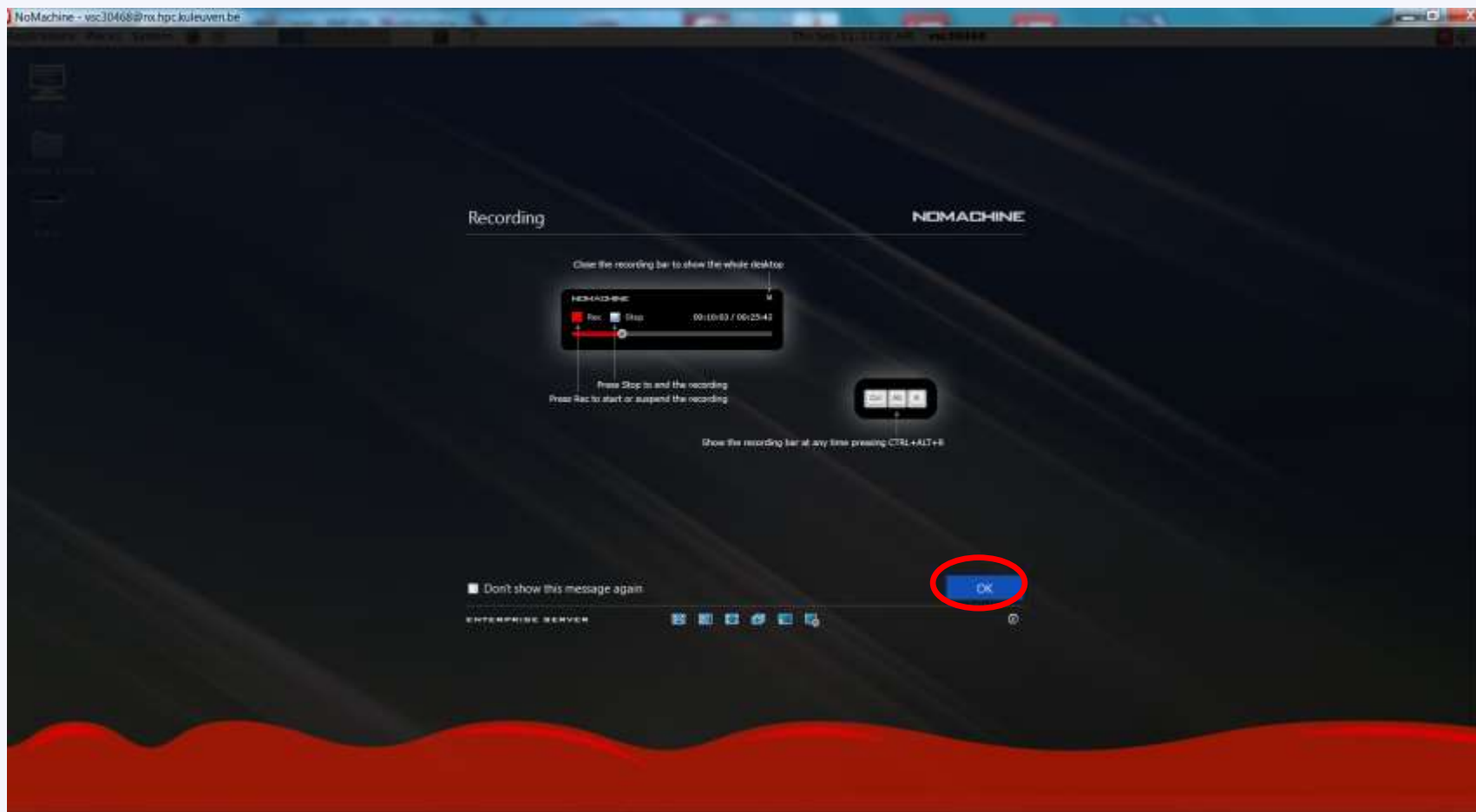
System tools - recording



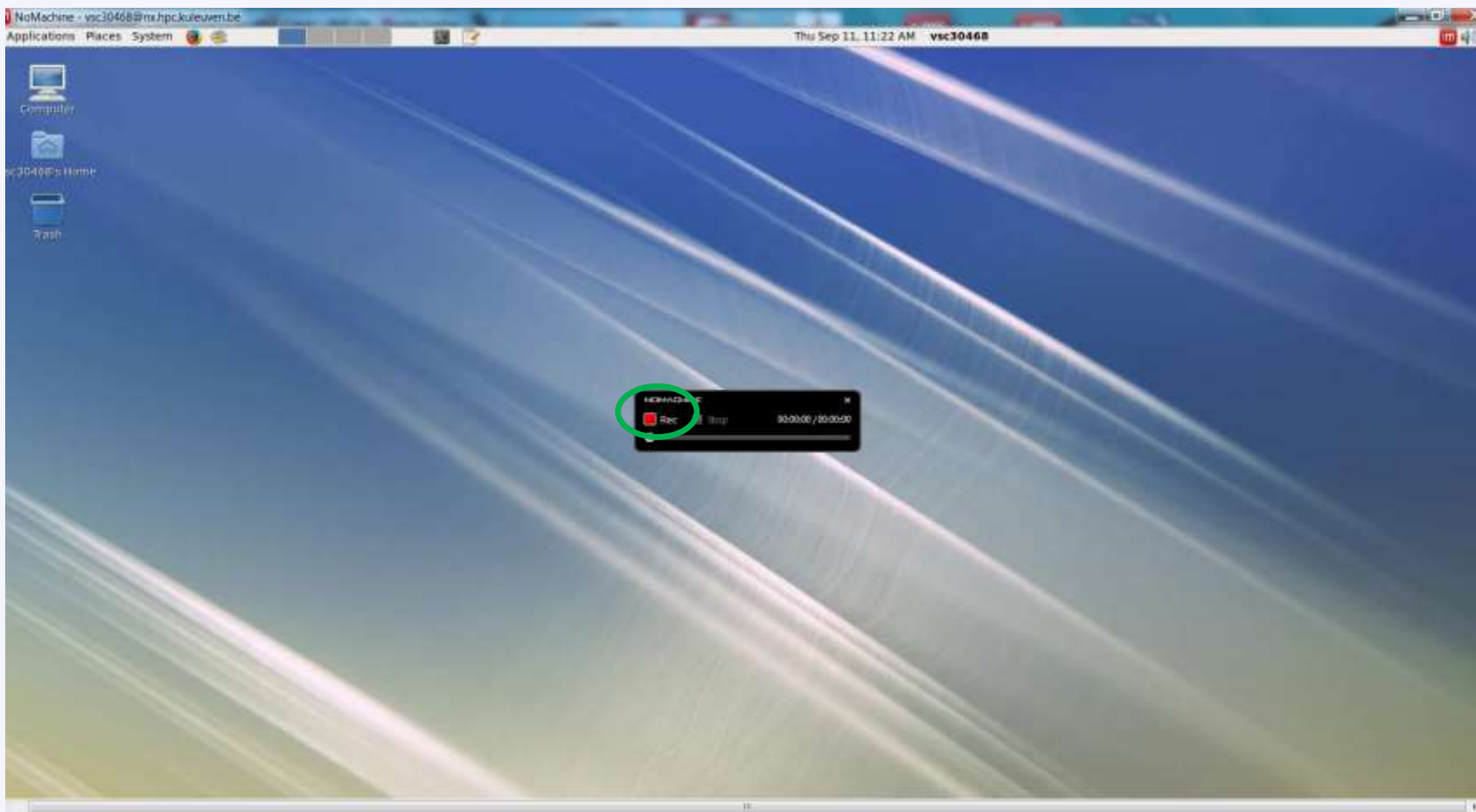
System tools - recording



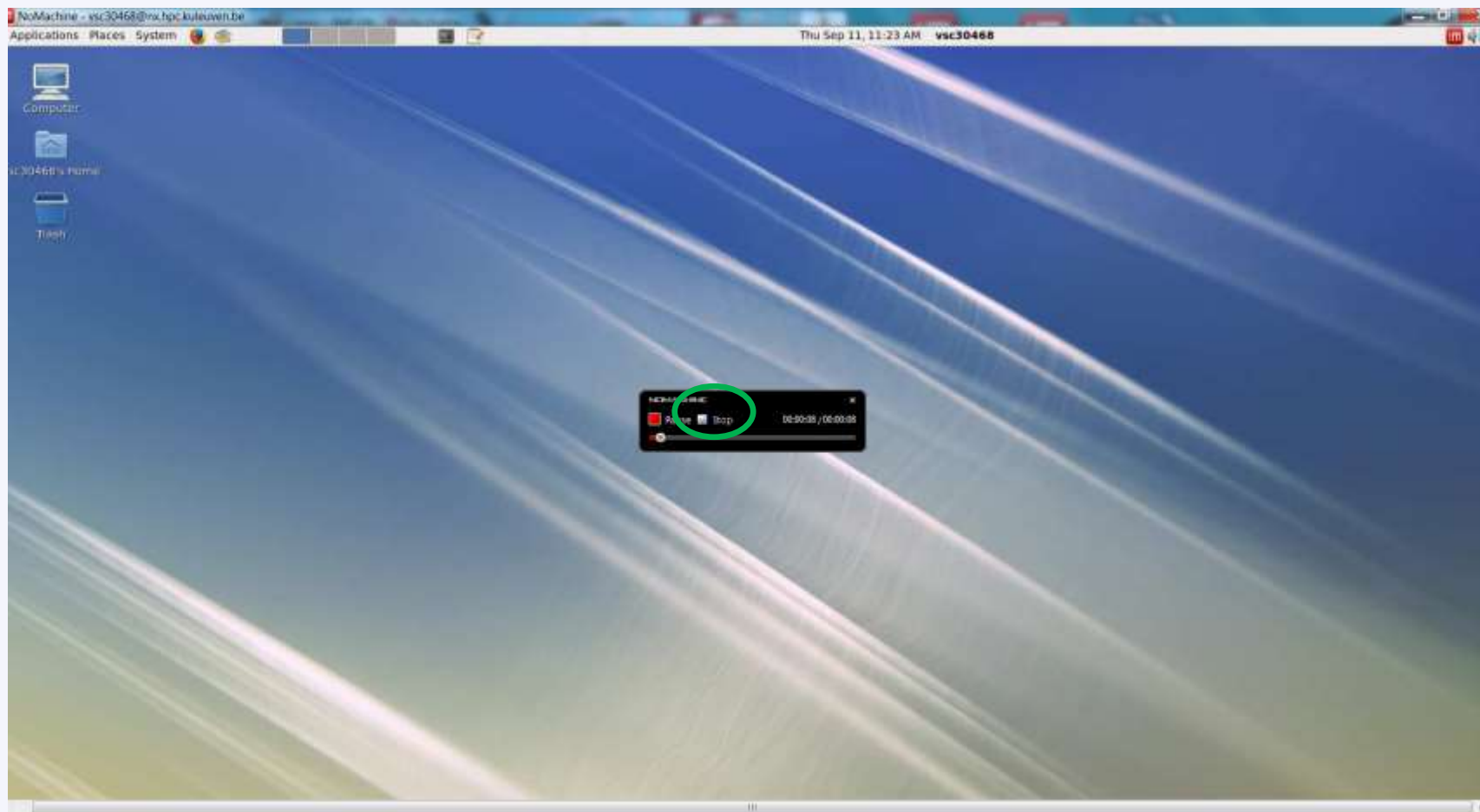
System tools - recording



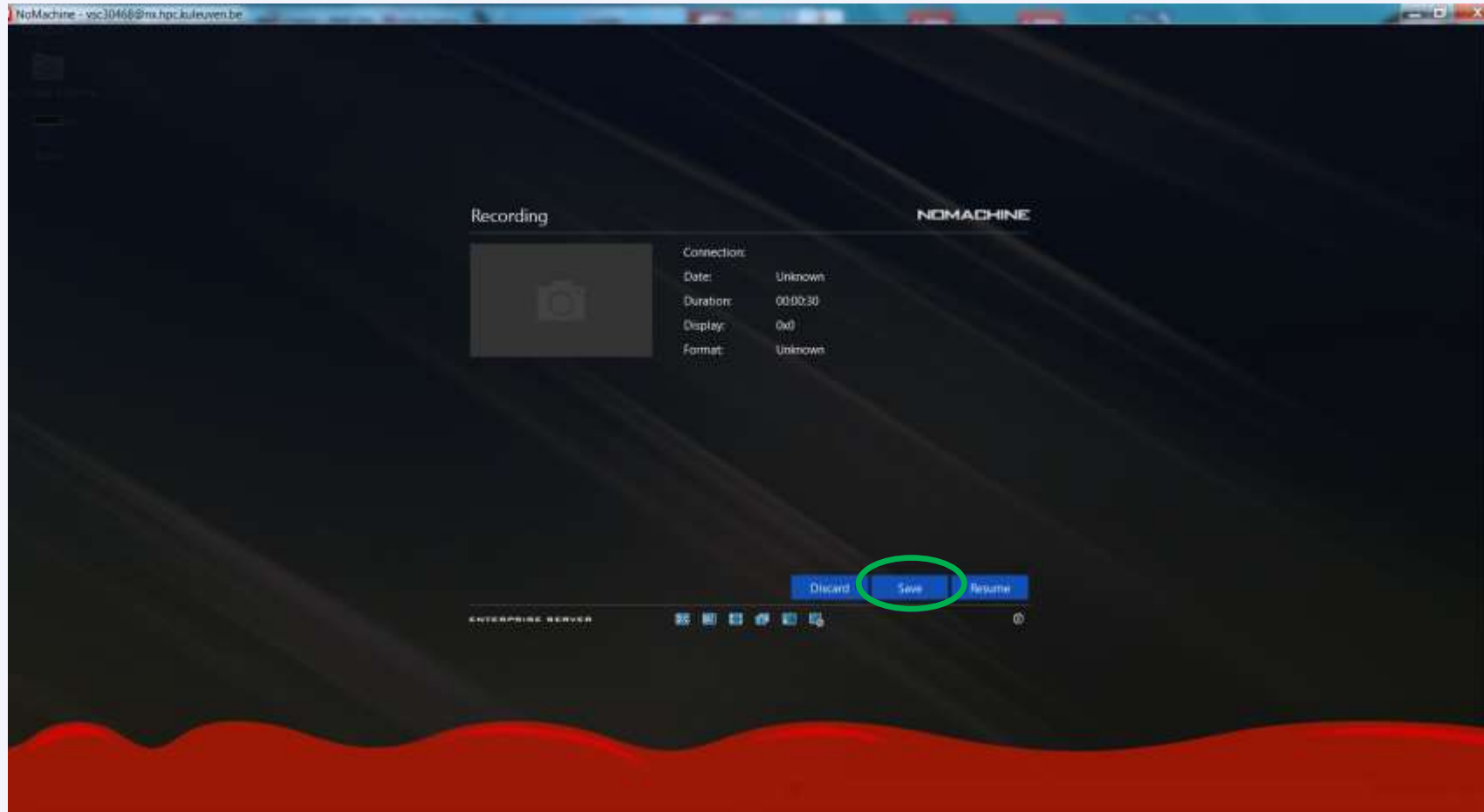
System tools - recording



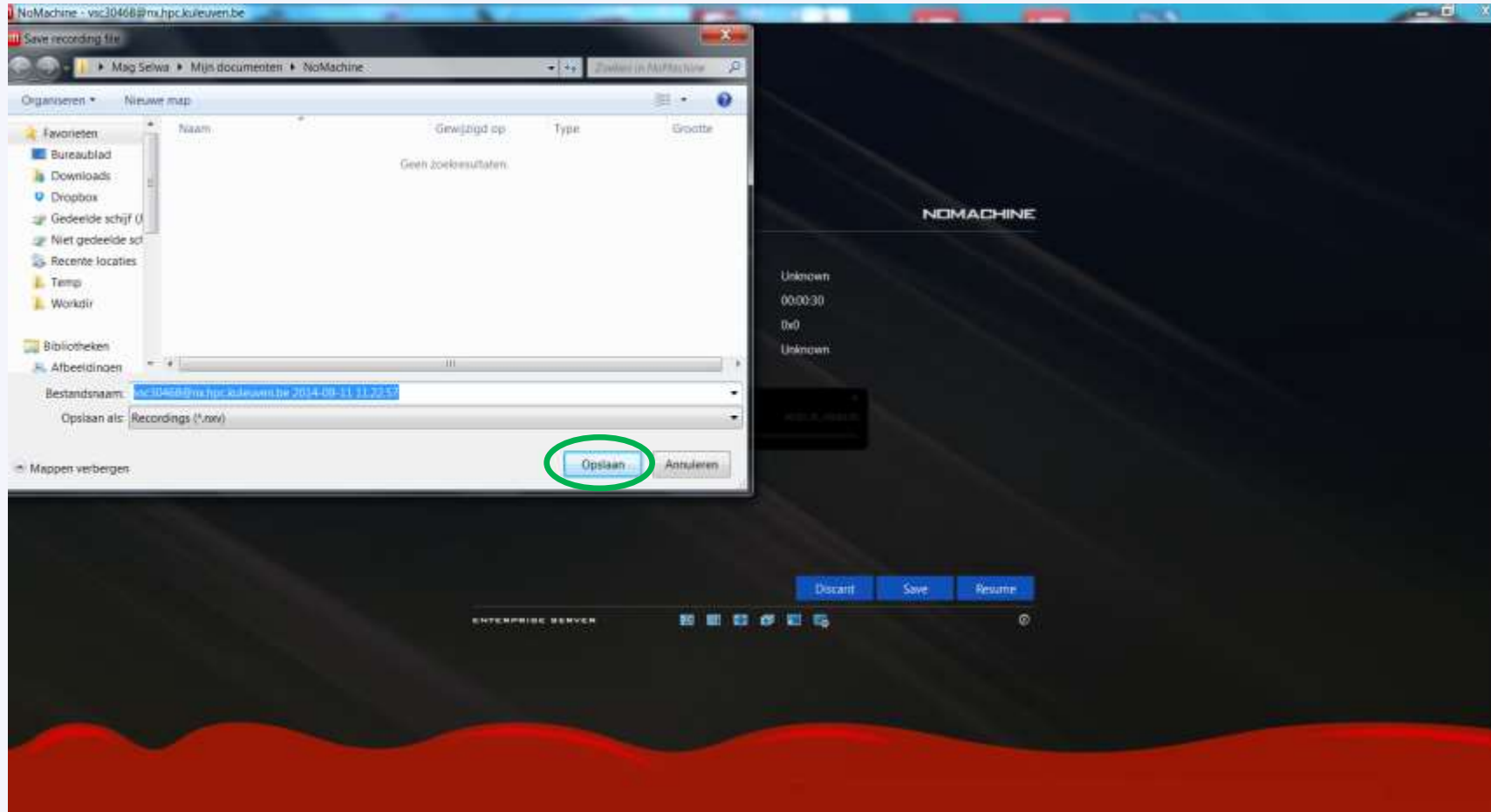
System tools - recording



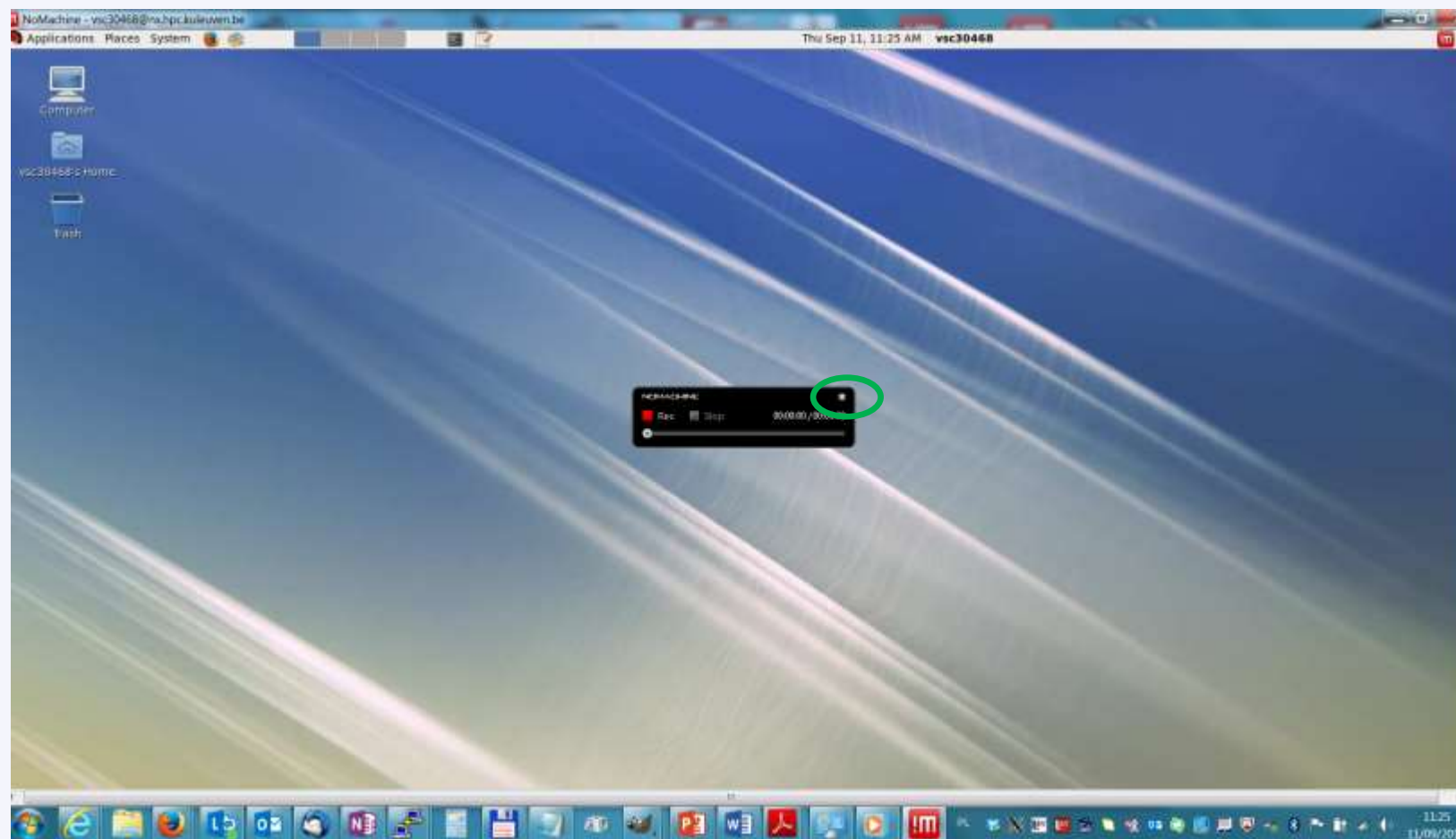
System tools - recording



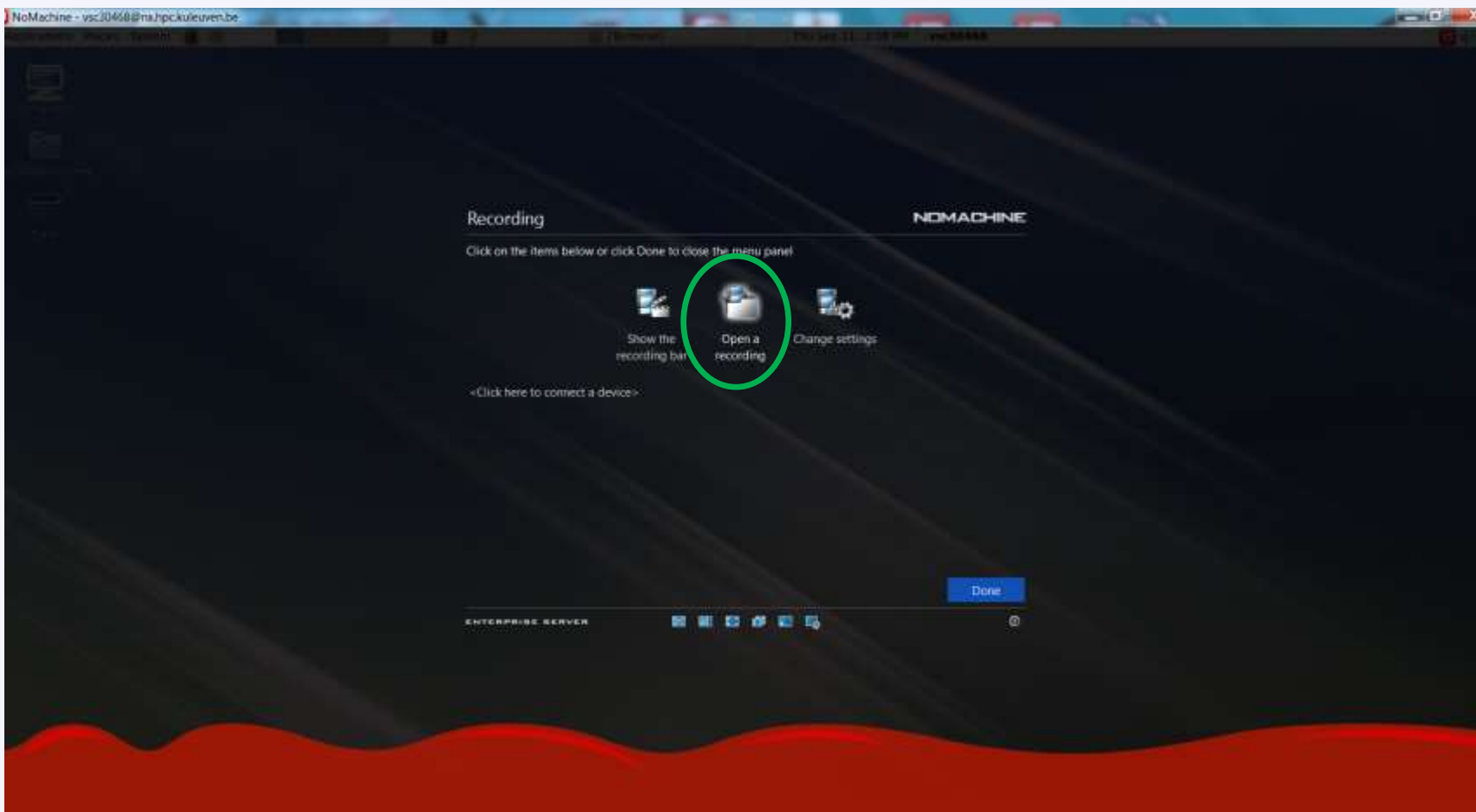
System tools - recording



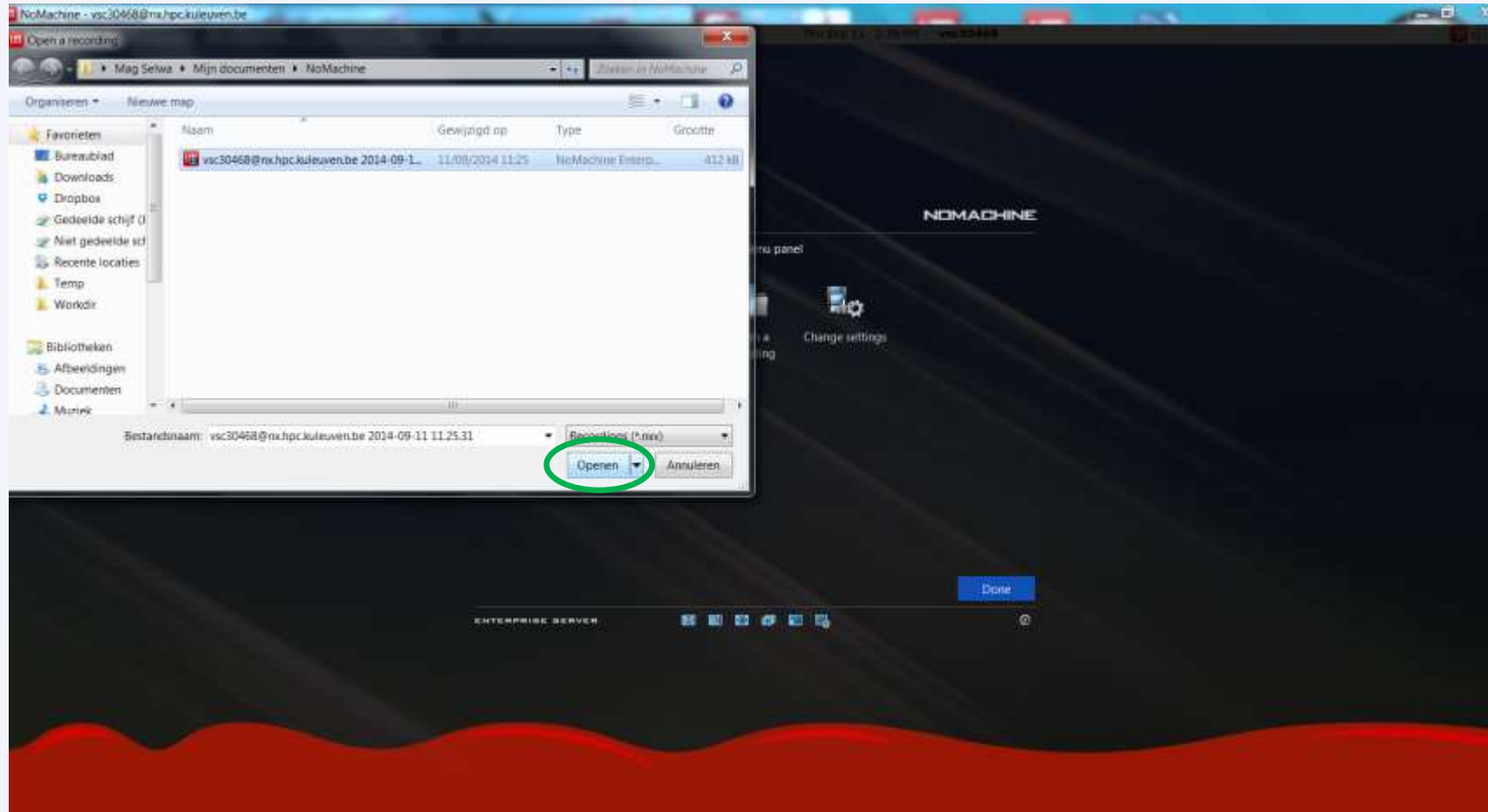
System tools - recording



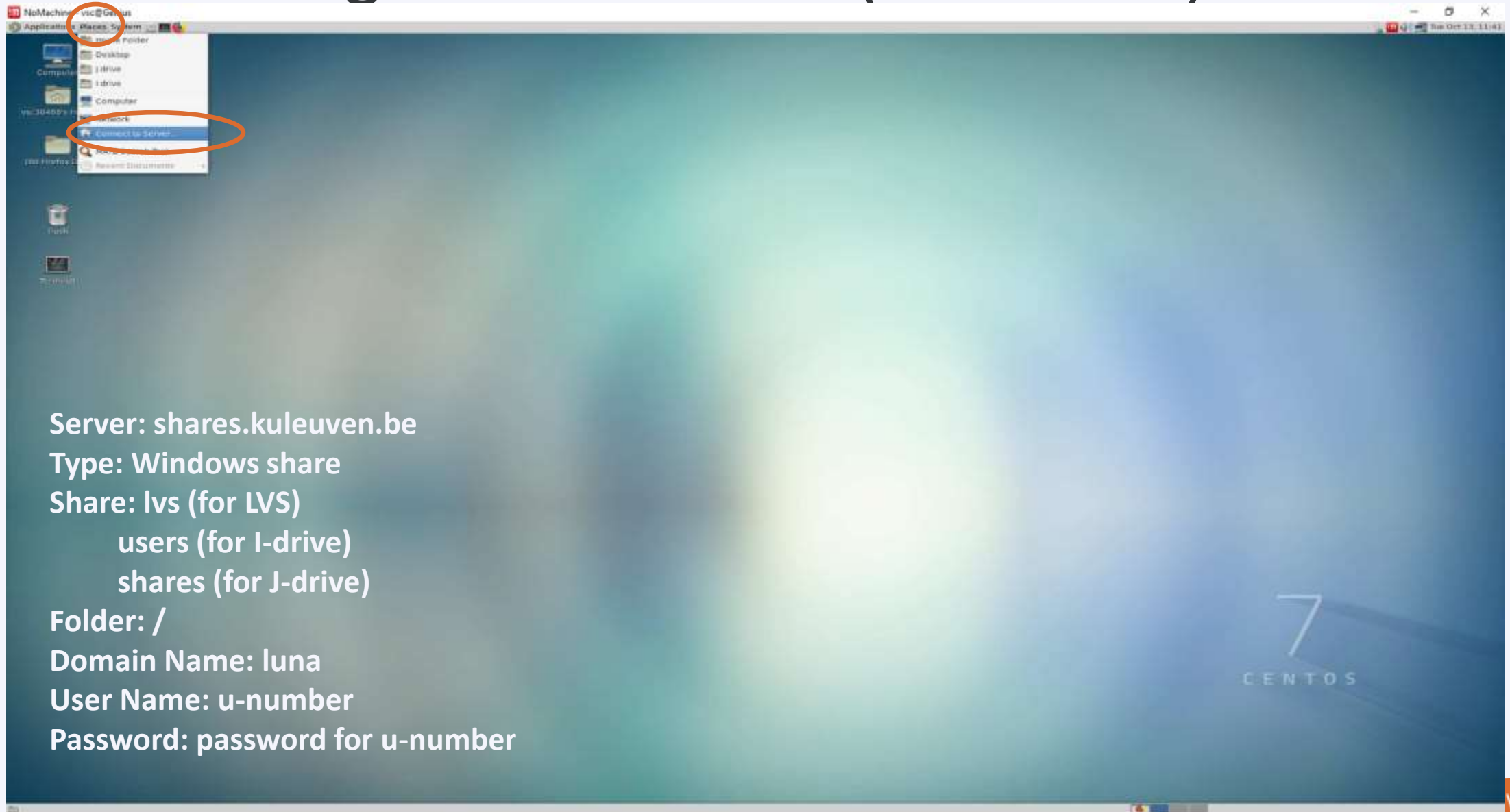
System tools



System tools - recording



Connecting shared drives (Windows)



Server: shares.kuleuven.be

Type: Windows share

Share: lvs (for LVS)

users (for I-drive)

shares (for J-drive)

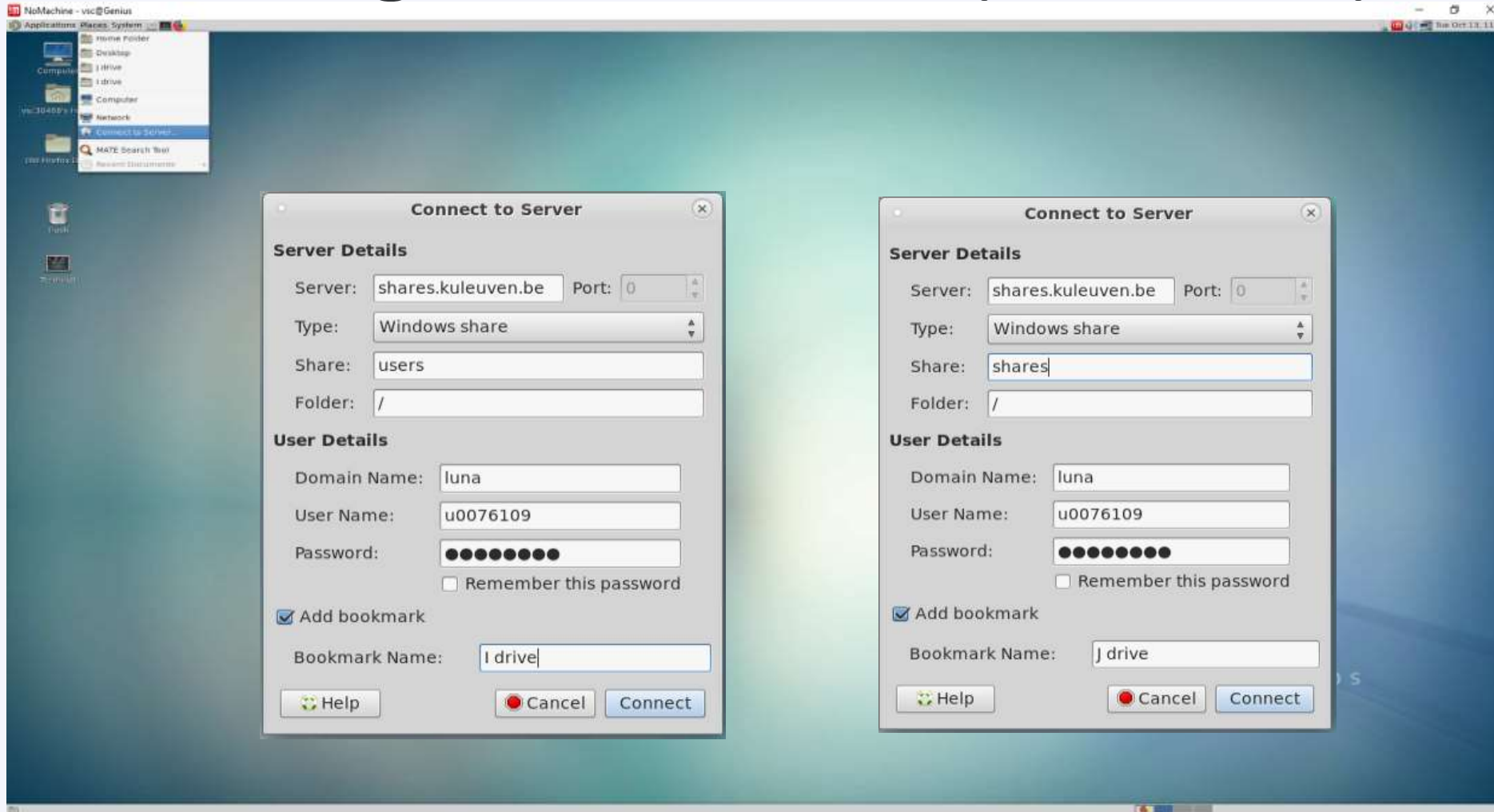
Folder: /

Domain Name: luna

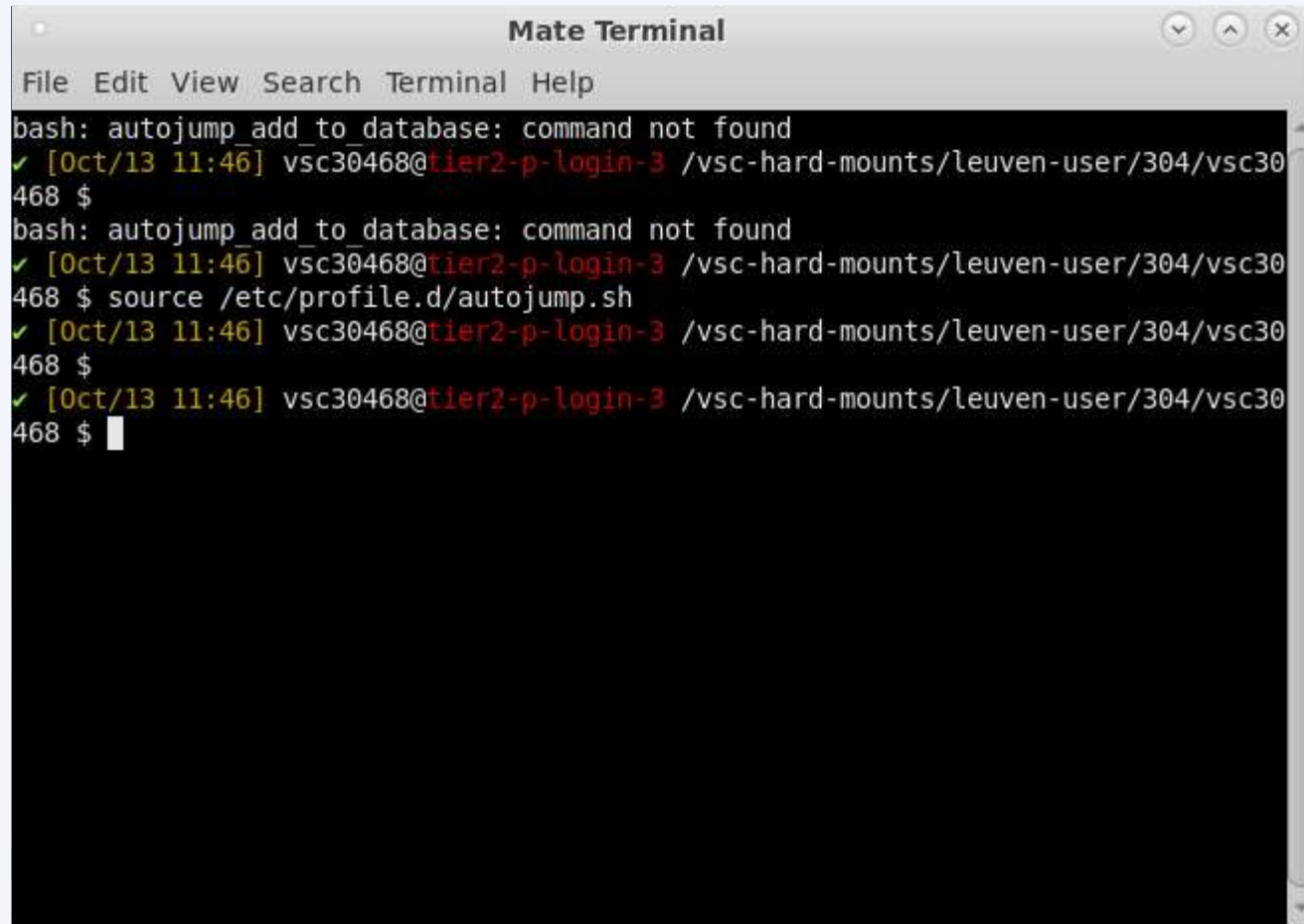
User Name: u-number

Password: password for u-number

Connecting shared drives (Windows)



NX – adjusting terminal



```
Mate Terminal
File Edit View Search Terminal Help
bash: autojump_add_to_database: command not found
✓ [Oct/13 11:46] vsc30468@tier2-p-login-3 /vsc-hard-mounts/leuven-user/304/vsc30468 $
bash: autojump_add_to_database: command not found
✓ [Oct/13 11:46] vsc30468@tier2-p-login-3 /vsc-hard-mounts/leuven-user/304/vsc30468 $ source /etc/profile.d/autojump.sh
✓ [Oct/13 11:46] vsc30468@tier2-p-login-3 /vsc-hard-mounts/leuven-user/304/vsc30468 $
✓ [Oct/13 11:46] vsc30468@tier2-p-login-3 /vsc-hard-mounts/leuven-user/304/vsc30468 $
```

To remove the autojump line
type in the terminal

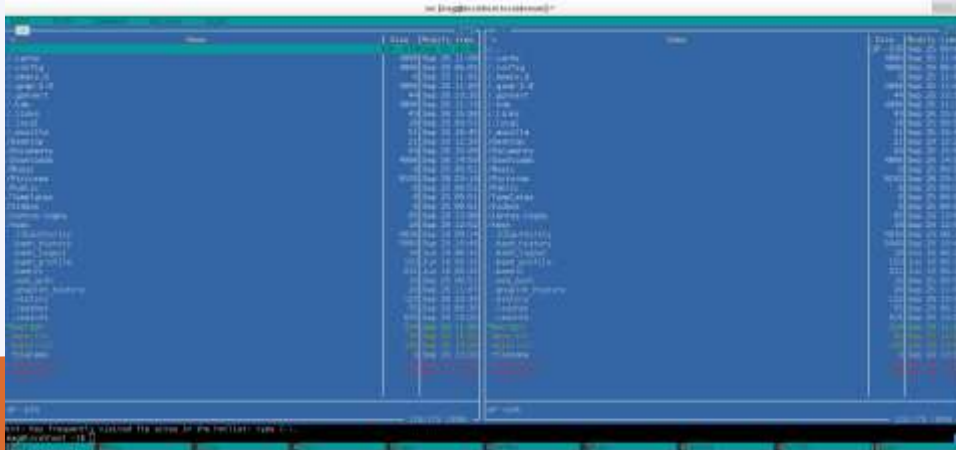
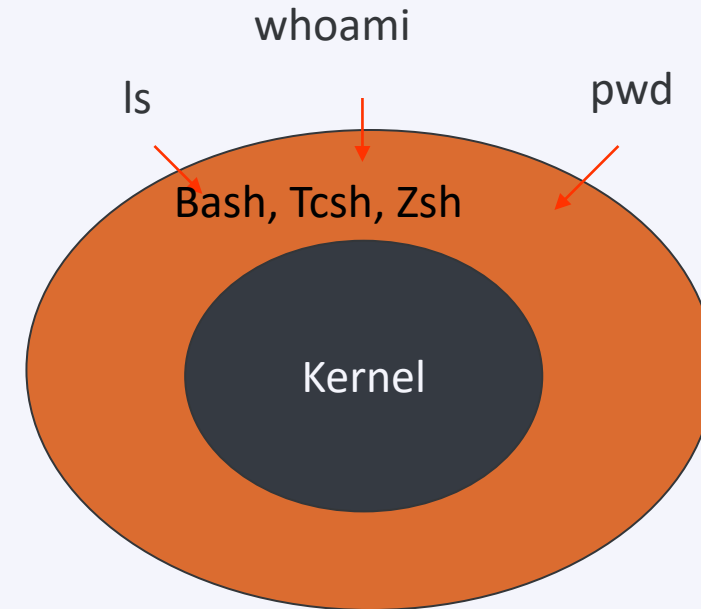
```
$ source  
/etc/profile.d/autojump.sh
```

Or add into .bashrc file in your home directory

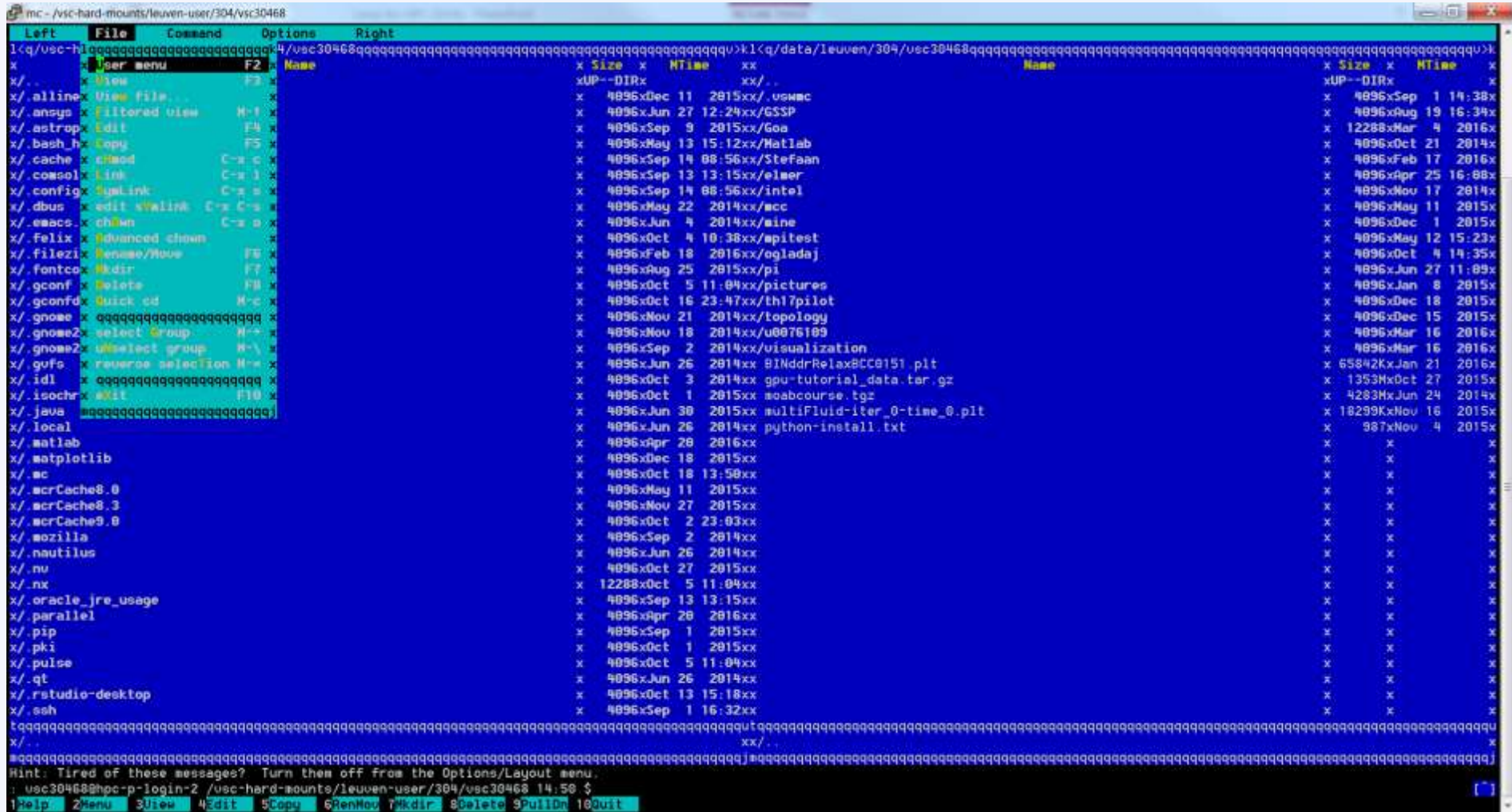
```
source /etc/profile.d/autojump.sh
```

Linux shell

- Shell interprets the command and request service from kernel
- Similar to DOS but DOS has only one set of interface while Linux can select different shell
- Bourne Again shell (Bash), TC shell (Tcsh), Z shell (Zsh)
- Different shell has similar but different functionality
- Bash is the default for Linux
- Graphical user interface of Linux is in fact an application program work on the shell
- Special (visual) type of shell is mc (midnight commander) – easy to process files



Midnight commander



Midnight commander

- **Keyboard Shortcuts**
- In normal browsing mode:
 - F1 - help. More readable than the 2000-line man page, although difficult to browse.
 - F2 - user menu (offers option to gzip files, etc.)
 - F3 - view (handy to check the contents of an rpm or tgz file, or read contents of files)
 - F4 - edit with internal editor, mcedit
 - F5 - copy
 - F6 - rename or move
 - F7 - create a directory
 - F8 - delete
 - F9 - pull-down - accesses the menu bar at the top.
 - F10 - quit. Closes mc, as well as mcedit and any unwanted open menu.

Midnight commander

Selecting files

- Insert (Ctrl + t alternatively) - select files (for example, for copying, moving or deleting).
- + - select files based on a pattern.
- \ -unselect files based on a pattern.
- * - reverse selection. If nothing was selected, all files will get selected.

Accessing the shell

- There's a shell awaiting your command at the bottom of the screen - just start typing (when no other command dialog is open, of course).
- Since Tab is bound to switching panels (or moving the focus in dialogs), you have to use Esc Tab to use autocompletion. Hit it twice to get all the possible completions (just like in a shell). This works in dialogs too.
- If you want inspect the output of the command, do some input or just prefer a bigger console, no need to quit mc. Just hit **Ctrl + o** - the effect will be similar to putting mc in the background. Your current working directory from mc will be passed on to the shell... and vice versa! Hit Ctrl + o again to return to mc.

Midnight commander

Panels

- Alt + , - switch mc's layout from left-right to top-bottom. Useful for operating on files with long names.
- Alt + t - switch the panel's listing mode in a loop: default, brief, long, user-defined. "long" is especially useful, because it maximizes one panel so that it takes full width of the window and longer filenames fit on screen.
- Alt + i - synchronize the active panel with the other panel. That is, show the current directory in the other panel.
- Ctrl + u - swap panels.
- Alt + o - if the currently selected file is a directory, load that directory on the other panel and move the selection to the next file. If the currently selected file is not a directory, load the parent directory on the other panel and moves the selection to the next file. Ctrl + PgUp (or just left arrow, if you've enabled Lynx-like motion, see later) - move to the parent directory.
- Alt + Shift + h - show the directory history. Might be easier to navigate than going back one entry at a time.
- Alt + y - move to the previous directory in history.
- Alt + u - move to the next directory in history.

Midnight commander

Searching files

- Alt + ? - shows the full Find dialog.
- Alt + s or Ctrl + s - quick search mode. Start typing and the selection will move to the first matching file. Press the shortcut again to jump to another match. Use wildcards (*, ?) for easier matching.

Common actions

- Ctrl + Space - calculate the size of the selected directories. Press this shortcut when the selection is on .. to calculate the size of all the directories in the current directory.
- Ctrl + x s (that is press Ctrl + x, let it go and then press s) - create a symbolic link (change s to l for a hardlink). I find it very useful and intuitive - the link will, of course, be created in the other panel. You can change it's destination and name, like with any other file operation.
- Ctrl + x c - open the chmod dialog.
- Ctrl + x o - open the chown dialog.

Hands-on 1

VSC-related commands

Information about users and processes

- `who`
Lists all the users logged on the system.
- `groups`
Tells which groups I belong to – important to check if already assigned to credits
- `top`
Displays all processes (change with `<` or `>` for different parameters).
- `ps tree`
Displays process tree (`ps tree -u $USER`).
- `tree`
Lists contents of directories in a tree-like format (`tree $VSC_HOME`).

Available space

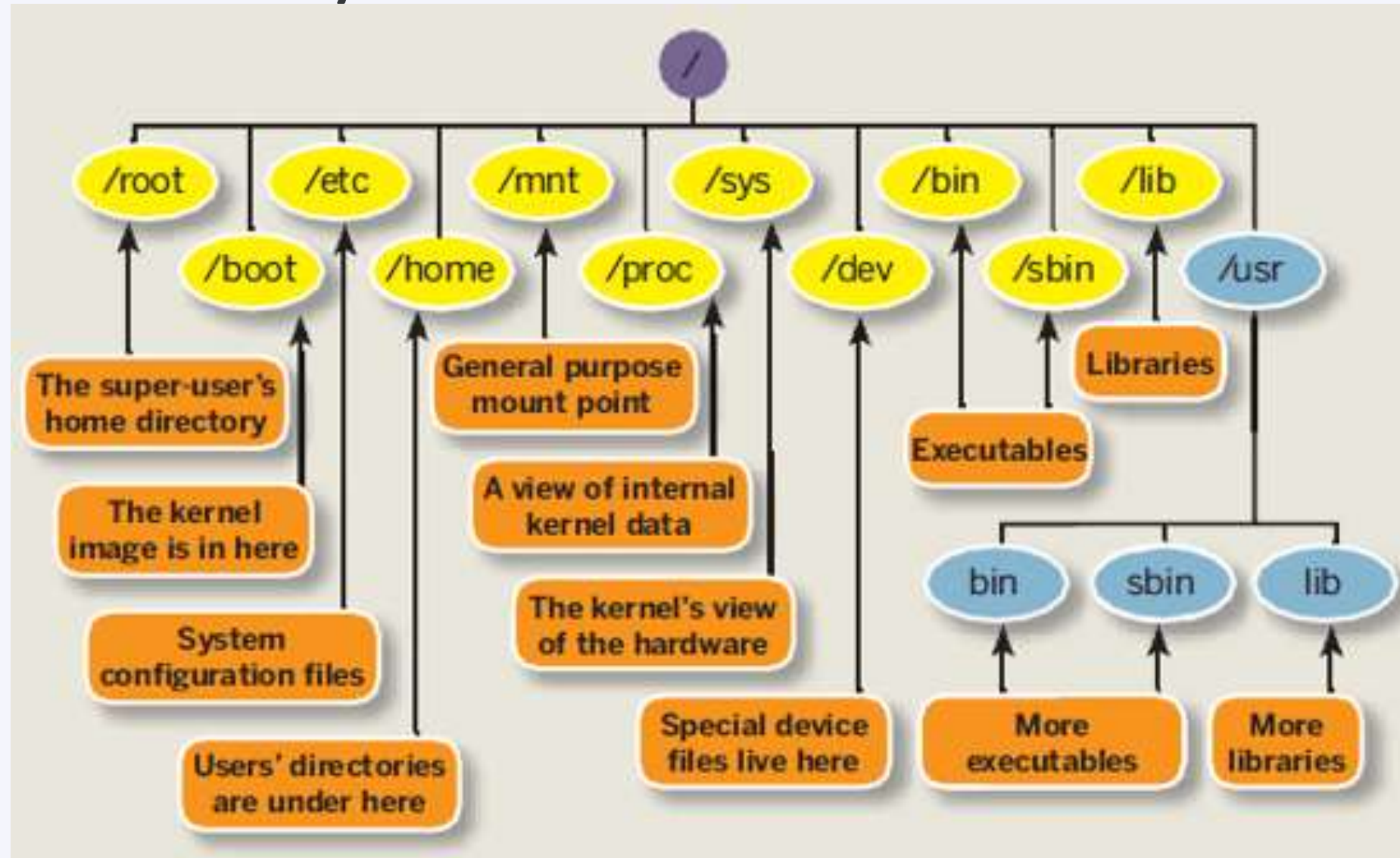
- How much space do I have?
 - `$ myquota`
 - `$ quota -s ($VSC_HOME and $VSC_DATA)`
- How much space am I taking up?
 - `$ du -kah $VSC_HOME` (or `du -ksh` without listing all the files)
 - command to find out how much space a folder or directory uses
 - `$ df -kah`
 - display space information for the entire system

- Bit – either a 1 or 0
- Byte – 8 bits “0000 1111”, or “x0F”, or 16
- KB, Kilobyte – 1024 Bytes
- MB, Megabyte – 1024KB
- GB, Gigabyte – 1024MB
- TB, Terabyte – 1024 GB

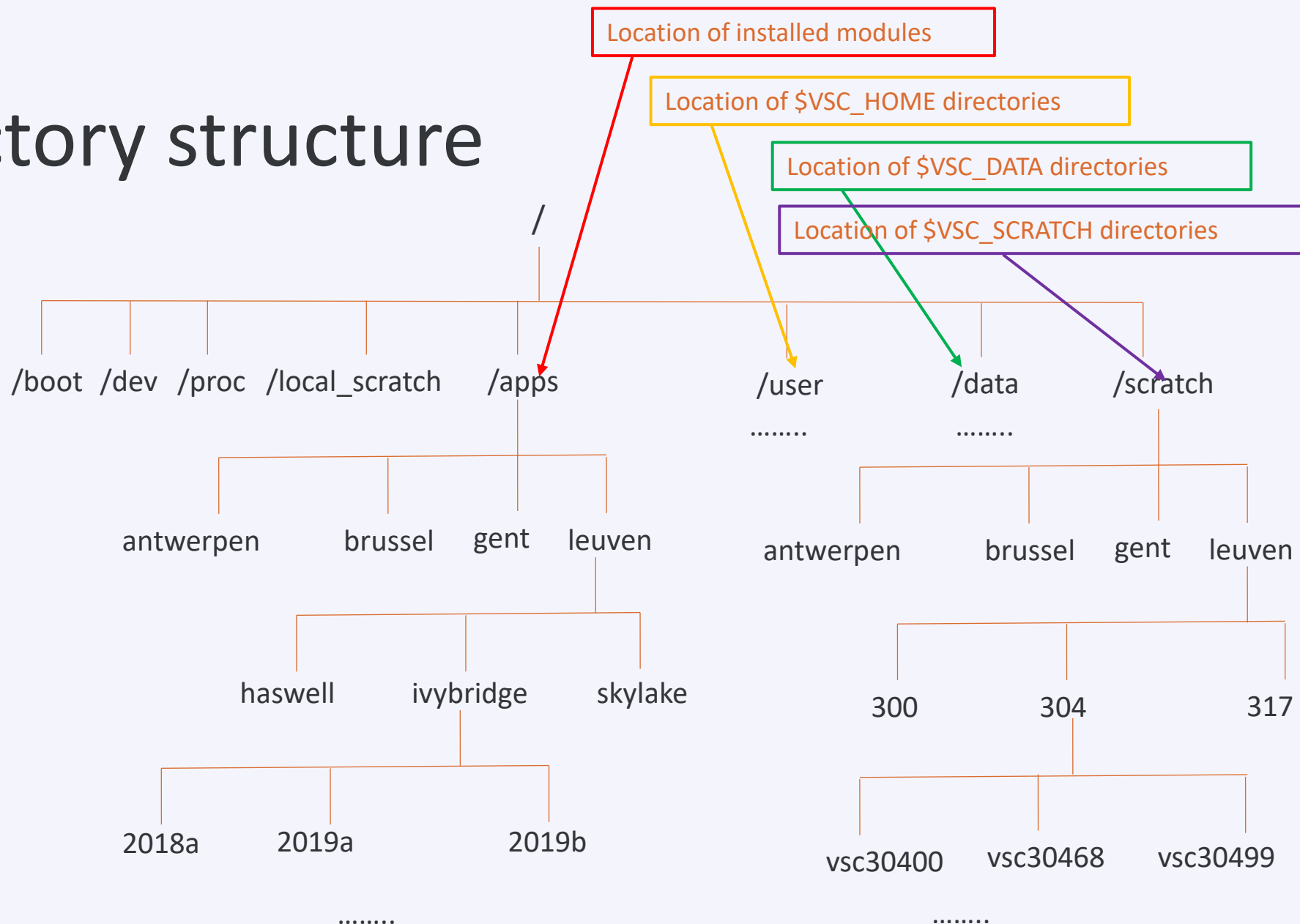
Temporary storage

- Temporary storage on the cluster nodes has a different location compared to regular Linux system.
- `$VSC_SCRATCH_NODE` defines space that is available per node (to be used only during the job execution, need to copy the data as everything will be erased after the job ends).
- Do not use `/tmp` directory on compute node (very limited space ~10GB, once exceeded the system and your job will crash).
- Use `$VSC_SCRATCH_NODE (/local_scratch)` instead (~200GB)

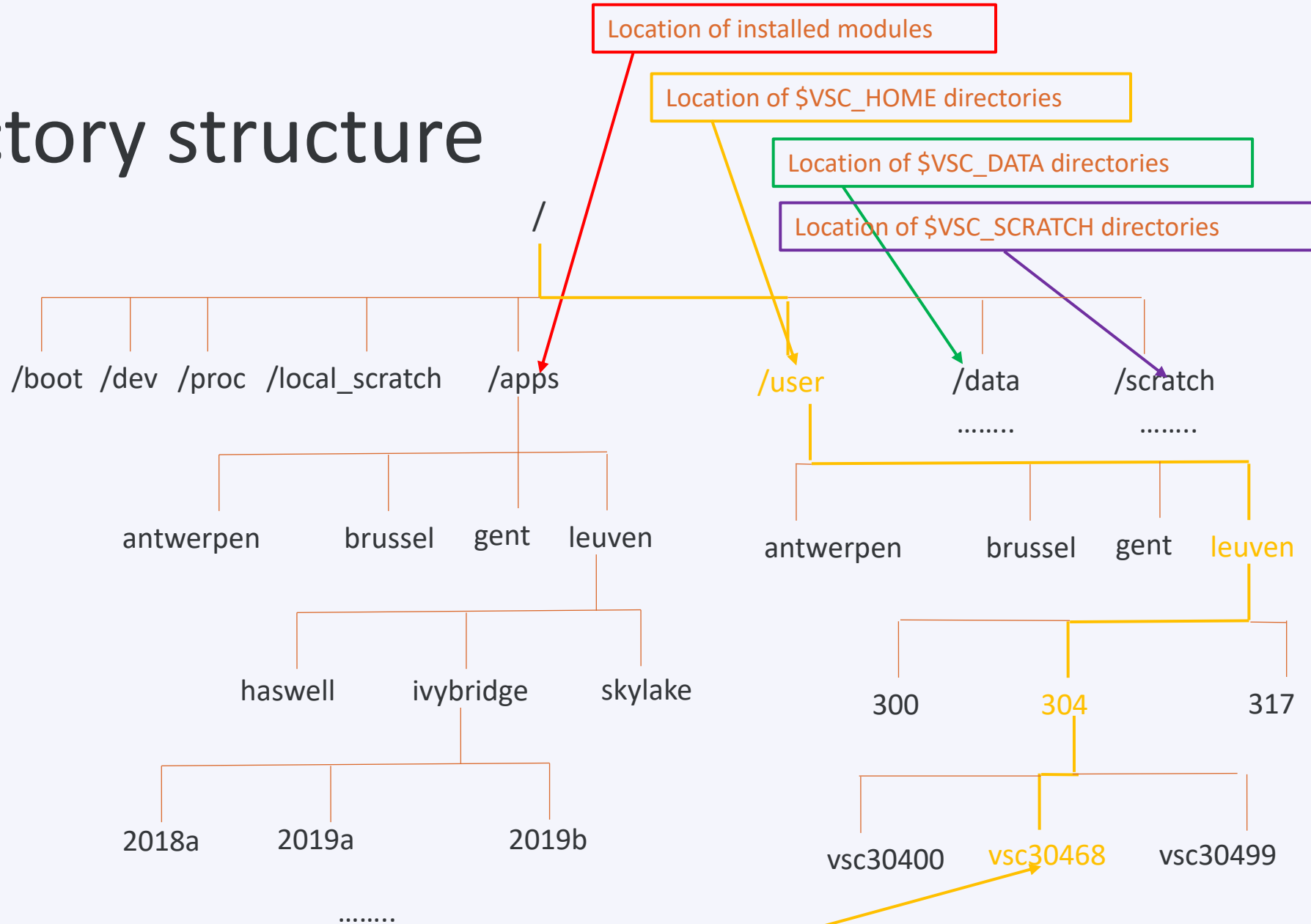
Linux File System



Directory structure

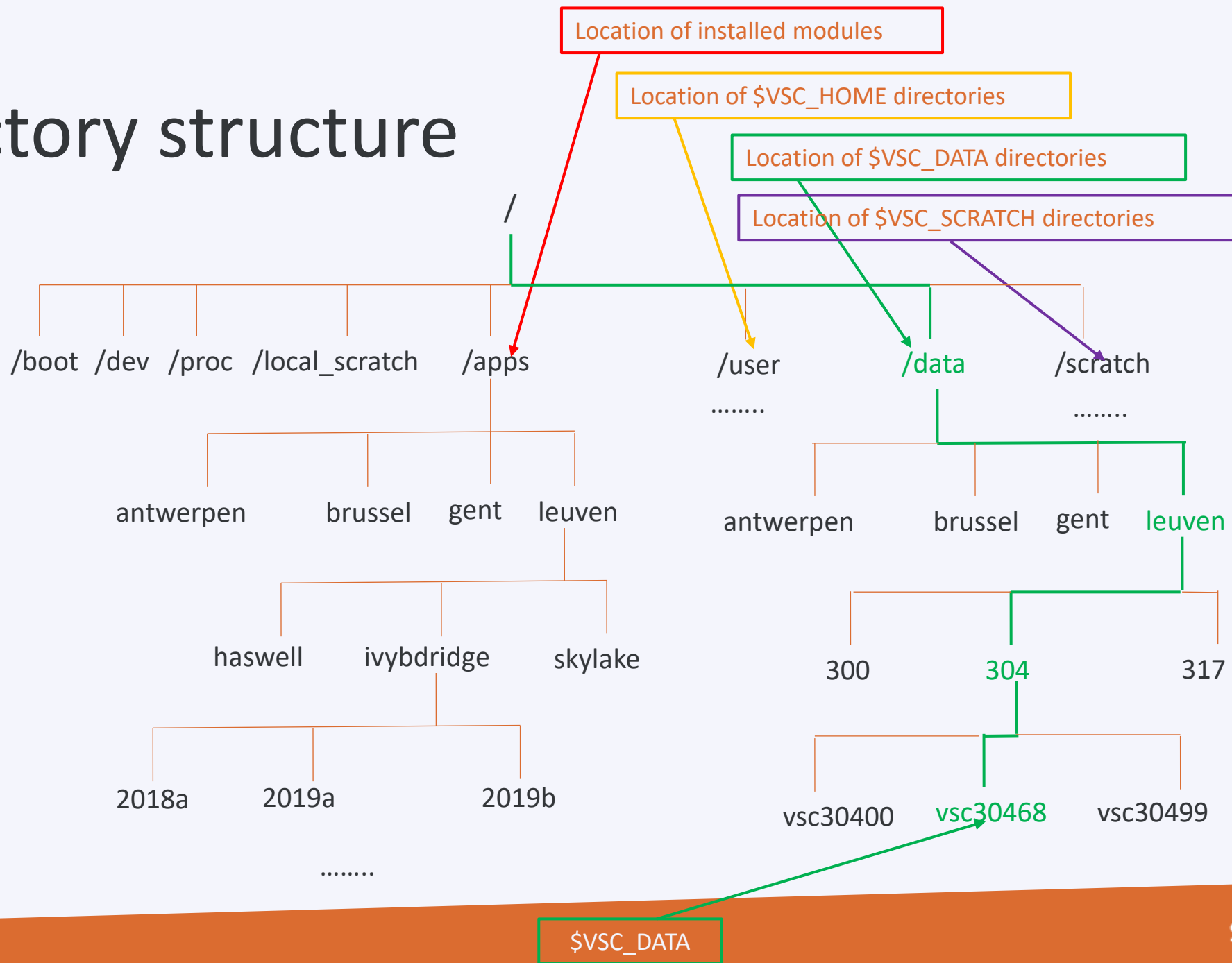


Directory structure

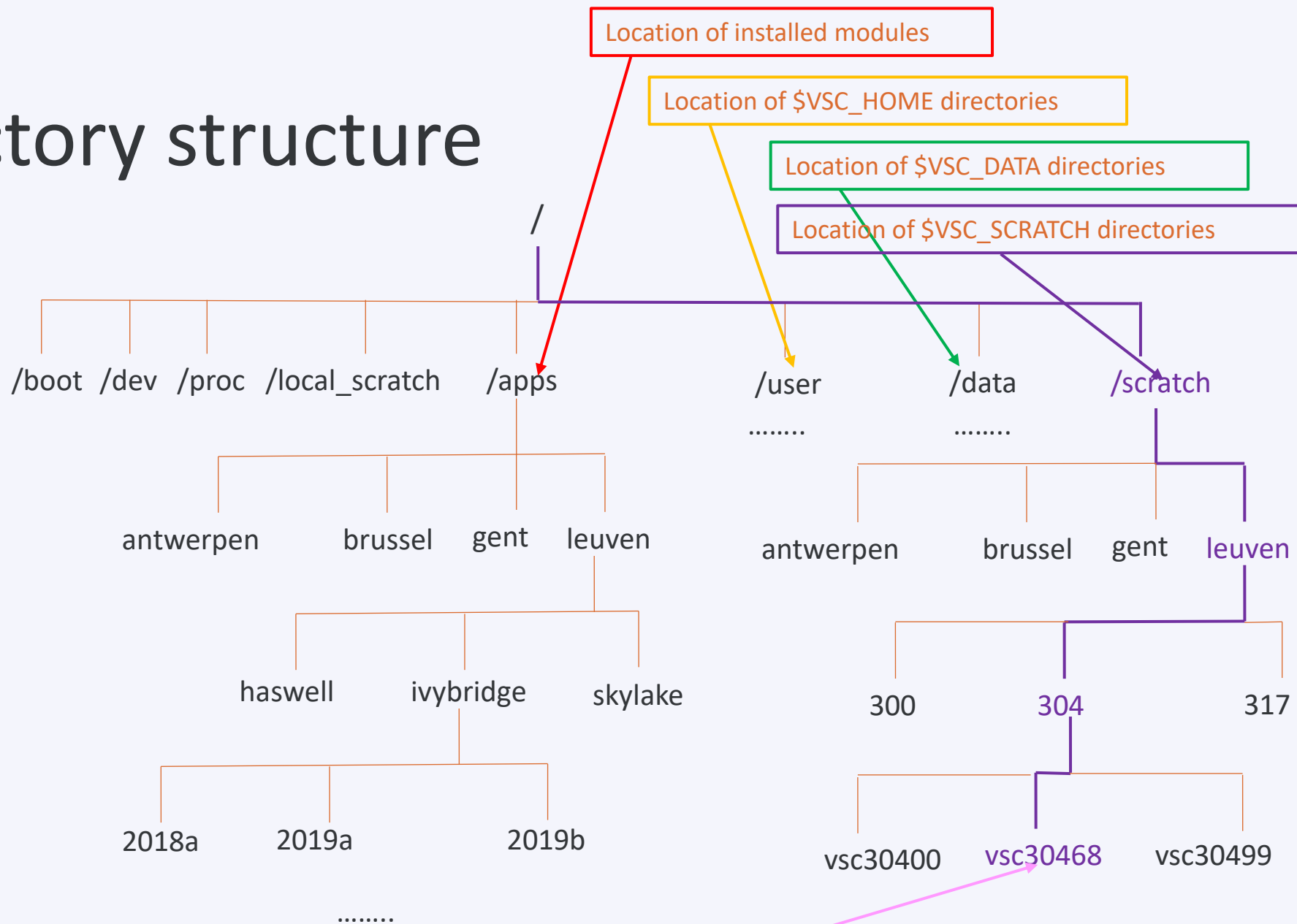


`$VSC_HOME`

Directory structure



Directory structure

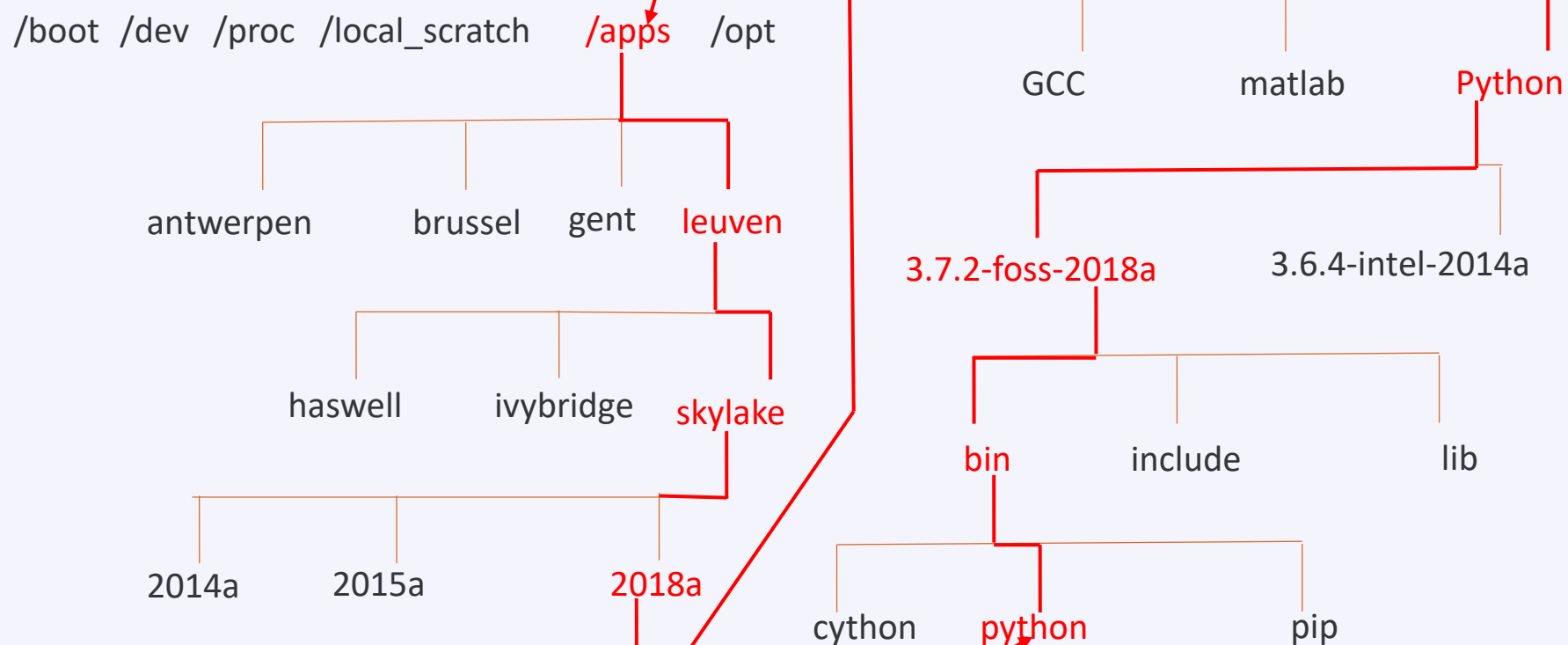


\$VSC_SCRATCH

Directory structure

Path on Genius:

/apps/leuven/skylake/2018a/software/Python/3.7.2-foss-2018a



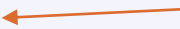
Location of installed modules Genius

Location of python (from module Python/3.7.2-foss-2018a)

Modules

Set the environment to use software packages:

- `$ module available` or `module av R`
 - Lists all installed software packages
- `$ module av |& grep -i python`
 - To show only the modules that have the string 'python' in their name, regardless of the case
- `$ module list`
 - Lists all 'loaded' modules in current session
- `$ module load matlab/R2014a`
 - Adds the 'matlab' command in your PATH
- `$ module load GCC`
 - 'Load' the (default) GCC version – not recommended (cannot be reproduced)
- `$ module unload R/3.1.2-foss-2014a-x11`
 - Removes all only the selected module, other loaded modules – dependencies are still loaded
- `$ module purge`
 - Removes all loaded modules from your environment



You can add extra name or characters for searching available modules

Modules

- A few small tips for HPC intros regarding modules:

- `module -t av python | grep -i -e '^python'`
- `module -r av '^Python'`
- `module -r av '^Python.+foss.+'`

-i -> case insensitive
Works only for availability,
module load is always case
sensitive

- The `-t` option forces terse output, i.e., something that is machine readable, and hence better to pipe through grep.
- The `-r` option allows you to use regular expressions, e.g., `^Python` means that the module name should start with Python, while `^Python.+foss` means that the module name should start with Python and contain Foss as a substring.

Modules

- `$ module swap foss intel`
 - `= module unload foss; module load intel`
- `$ module try-load packageXYZ`
 - try to load a module with no error message if it does not exist
- `$ module keyword word1 word2 ...`
 - Keyword searching tool, searches any help message or whatis description for the word(s) given on the command line
- `$ module help foss`
 - Prints help message from modulefile
- `$ module spider foss`
 - Describes the module

Modules

- **ml** – convenient tool
- `$ ml`
 - = module list
- `$ ml foss`
 - =module load foss
- `$ ml -foss`
 - =module unload foss (not purge!)
- `$ ml show foss`
 - Info about the module
- Possible to create user collections:
 - module save <collection-name>
 - module restore <collection-name>
 - module describe <collection-name>
 - module savelist
 - module disable <collection-name>

More info: http://lmod.readthedocs.io/en/latest/010_user.html

Find the right command

- Executing the right command can be vital for your system. However in Linux there are so many different command lines that they are often hard to remember. So how do you search for the right command you need? The answer is **apropos**:
- ```
$ apropos ownership
```

|                         |                                   |
|-------------------------|-----------------------------------|
| <pre>chgrp (1)</pre>    | - change group ownership          |
| <pre>chgrp (1p)</pre>   | - change the file group ownership |
| <pre>chown (1p)</pre>   | - change the file ownership       |
| <pre>chown (2)</pre>    | - change ownership of a file      |
| <pre>chown32 (2)</pre>  | - change ownership of a file      |
| <pre>fchown (2)</pre>   | - change ownership of a file      |
| <pre>fchown32 (2)</pre> | - change ownership of a file      |
| <pre>.....</pre>        |                                   |

# Monitoring the system:


- `free`
  - Displays the status of RAM and VRAM
  - Mem: refers to RAM
  - Swap: refers to virtual RAM (the swap file)
  - Too little RAM will cause 'thrashing' (constantly moving information from RAM to VRAM)
- `top`
  - Displays all the tasks, but also available CPU and memory in the top bar
- File `/proc/cpuinfo` (`/proc/meminfo`)
  - contains info about procesor/memory, no CPU usage
- GPUs: `nvidia-smi` (`watch "nvidia-smi"`)

# scp

- The scp command allows you to copy files over ssh connections.
- scp examplefile

```
touch test.txt
```

```
scp $HOME/test.txt vsc30468@login.hpc.kuleuven.be:$VSC_DATA/
```



Recognized only on the cluster, not on the remote host

Syntax similar to cp:

scp location-of-the-file-on-one-computer location-of-the-file-on-second-computer

# scp

## Own PC

## VSC cluster

File exists: /home/mag/test.txt

want to copy to the cluster into  
\$VSC\_DATA

```
scp /home/mag/test.txt
vsc30468@login.hpc.kuleuven.be: $VSC_DATA/
```

Reconginzed only on the cluster,  
not on the remote host

```
scp /home/mag/test.txt
vsc30468@login.hpc.kuleuven.be: /data/leuven/30
4/vsc30468
```

Path to the file can be checked  
with e.g. `echo $VSC_DATA` on  
the cluster

# Searching

- A large majority of activity on UNIX systems involve searching for files and information.

- **find** – utility to find files

```
find $VSC_HOME -name "test9*"
```

searches for files with name starting with test9 in  
\$VSC\_HOME directory

- **grep** – great utility, searches for patterns inside files and will return the line, if found

```
grep -H -R test9 $VSC_HOME
```

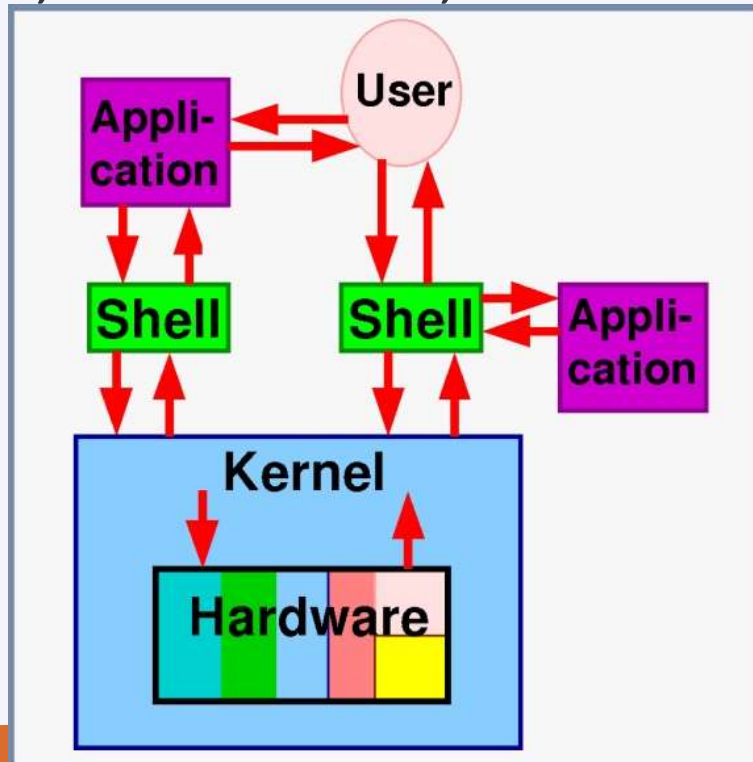
searches for files with test9 in their text in \$VSC\_HOME  
directory

# The Shell revisited: features



# The shell

- Not just an interface to the computer, also a scripting language – allows automation of tasks
- Shells can be scripted: provide all the resources to write complex programs (variables, conditionals, iterations...)



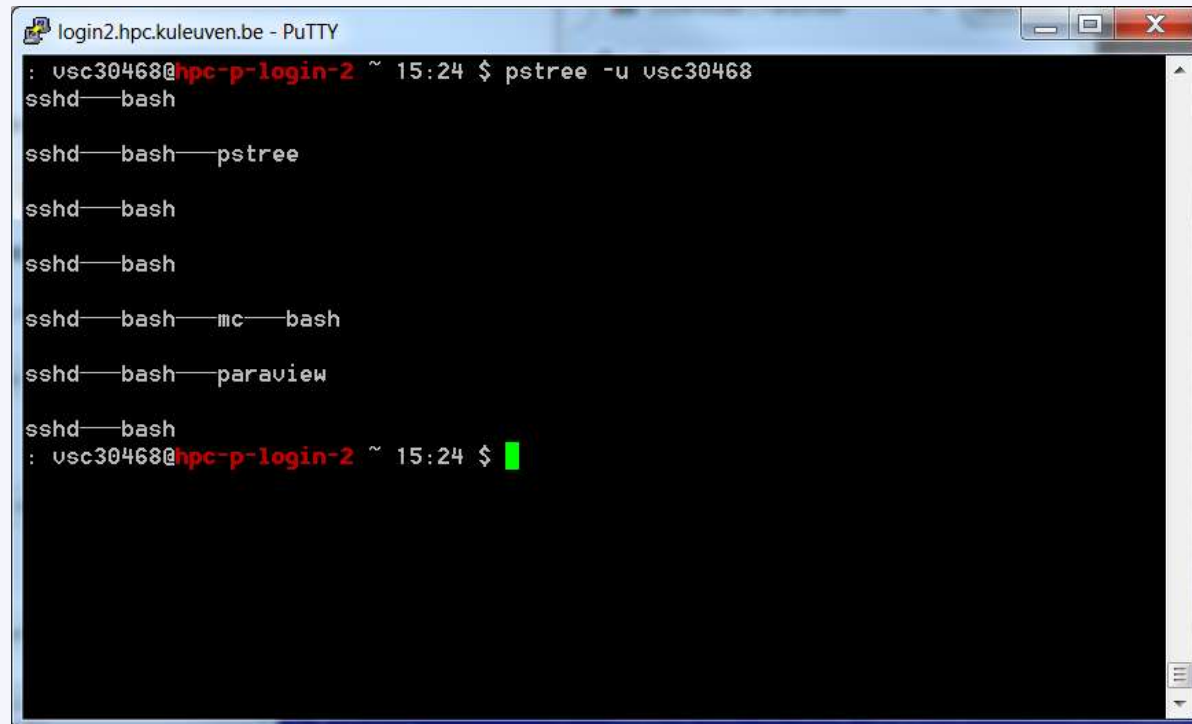
- Upon startup, shell executes commands found in the `~/.rc` file, allowing users to customize their shell.

Source: [opensuse.org](https://opensuse.org)

# The shell

- After login to the cluster or starting a job: a new shell is opened
- Processes originating from each shell can be checked with `ps tree`

- `ps tree` shows only processes on the current node (login1, or login2 or NX or compute node)



```
login2.hpc.kuleuven.be - PuTTY
: usc30468@hpc-p-login-2 ~ 15:24 $ ps tree -u usc30468
sshd--bash
sshd--bash--ps tree
sshd--bash
sshd--bash
sshd--bash
sshd--bash--mc--bash
sshd--bash--paraview
sshd--bash
: usc30468@hpc-p-login-2 ~ 15:24 $
```

# Most popular shells

- There are several types of shells for Linux.
- Check it with  
**\$ echo \$SHELL**

| Shell | Prompt | Name               | Note                                                                                 |
|-------|--------|--------------------|--------------------------------------------------------------------------------------|
| sh    | \$     | Bourne Shell       | Default on some Unix systems                                                         |
| bash  | \$     | Bourne Again Shell | Enhanced replacement for the Bourne shell Default on most Linux and Mac OS X systems |
| csh   | %      | C Shell            | Default on many BSD systems                                                          |
| tcsh  | >      | TC Shell           | Enhanced replacement for the C shell                                                 |
| ksh   | \$     | Korn Shell         | Default on AIX systems                                                               |

# Starting shells

- In practice, users seldom need to start a shell manually. Whenever someone logs in, or opens a terminal, a shell is started automatically.
- You can start a different shell, or another instance of the same shell. Because the shell is "just another" program, new shells can be launched from an existing shell.
- The new shell is referred to as a **subshell** of the original shell. When the subshell is exited, control is returned to the original shell.
- Subshell inherits all variables/context from the parent shell.
- If you quit the subshell, its context will purge.
- The apparent differences between the subshell and the parent shell are minimal, and care must be taken to keep track of which shell you are in.

# Return/Exit Code

- Shell commands are **CASE SENSITIVE!**
- Upon exiting, every command returns an integer to its parent called a return value.
- The shell variable `$?` expands to the return value of previously executed command (e.g. 0 when success).

compare:

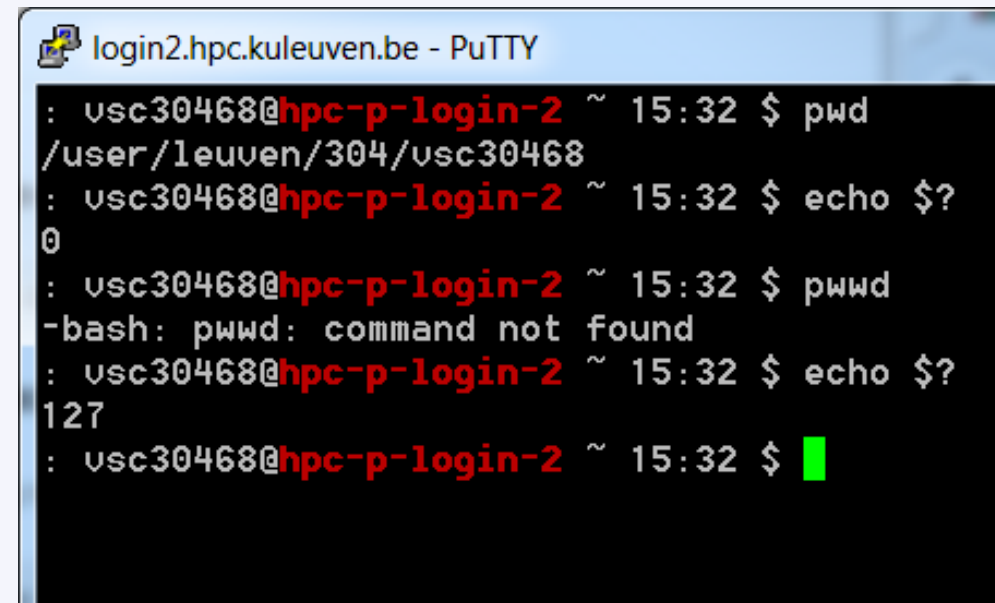
`pwd`

`echo $?`

with

`pwd` (does not exist, mistyped)

`echo $?`



```
login2.hpc.kuleuven.be - PuTTY
: usc30468@hpc-p-login-2 ~ 15:32 $ pwd
/user/leuven/304/usc30468
: usc30468@hpc-p-login-2 ~ 15:32 $ echo $?
0
: usc30468@hpc-p-login-2 ~ 15:32 $ pwd
-bash: pwd: command not found
: usc30468@hpc-p-login-2 ~ 15:32 $ echo $?
127
: usc30468@hpc-p-login-2 ~ 15:32 $
```

# AND &&

- Multiple commands can be separated with a ;  
e.g. `cd $VSC_HOME; pwd`
- **&&** and **||** conditionally separate multiple commands.
- When commands are conditionally joined, the first will always execute. The second command may execute or not, depending on the return value of the first command.
- For example, a user may want to create a directory, and then move a new file into that directory. If the creation of the directory fails, then there is no reason to move the file. The two commands can be coupled as follows:
  - `echo "one two three four five" > numbers.txt;`
  - `mkdir $VSC_DATA/my-dir && mv numbers.txt $VSC_DATA/my-dir`

# OR ||

- Similarly, multiple commands can be combined with `||`.
- In this case, **bash** will execute the second command only if the first command "fails" (has a non zero return value). This is similar to the "or" operator found in programming languages.
- E.g., we attempt to change the permissions on a file. If the command fails, a message to that effect is echoed to the screen.
  - `chmod 600 $VSC_DATA/my-dir/numbers.txt || echo "chmod failed"`
- In the first case, the **chmod** command succeeded, and no message was echoed. In the second case, the **chmod** command failed (because the file didn't exist), and the "chmod failed" message was echoed (in addition to **chmod**'s standard error message).

# Escape character

- ", \$, `, and \ are still interpreted by the shell, even when they're in double quotes.
- The backslash (\) character is used to mark these special characters so that they are not interpreted by the shell, but passed on to the command being run (for example, echo)

- E.g. to output the string: (Assuming that the value of \$X is 5):

A quote is ", backslash is \, backtick is `.

A few spaces are     and dollar is \$. \$X is 5.

**we would have to write:**

```
$ echo "A quote is \", backslash is \\, backtick is \`."
```

A quote is ", backslash is \, backtick is `.

```
$ echo "A few spaces are ; dollar is \$. \$X is ${X}."
```

A few spaces are     ; dollar is \$. \$X is 5.



# Escape character

- `$` is used for interpreting variable which has some value assigned
- You can define a variable locally in the shell, e.g.  
`now=`date``  
and use it later on in your shell/scripts:  
`echo "Now, the date/hour is: ${now}"`
- You can define a variable, and let subshell inherit its value  
`export now=`date``      # in parent shell  
`bash`                      # start the child/sub shell  
`echo "Subshell: time in parent shell was: ${now}"`
- The `export` command defines a variable in the parent and child shells

# Escape character

- When you create a file that contains space in it, e.g. `touch "my file"` it is difficult to use it later
  - How to copy the file (`cp source destination`)
  - -> use escape character so that space is understood as a part of the file and not as a separator in command syntax
  - `cp my\ file myfile`
- Better avoid using “special” characters (`"`, `$`, ```, `\`, ... ) in your filenames!

# Auto-Completion

- Have the shell automatically complete commands or file paths.
- Activated using the **<TAB>** key on most systems
- examples
  - `$ whe<TAB>`
  - `$ whereis`
  - `$ ls -l /etc/en<TAB>`
  - `$ ls -l /etc/environment`
- When more than one match is found, the shell will display all matching results (use **<TAB>** twice)
  - `$ ls -l /etc/host<TAB>`

# Globbering: use wildcard

| Wildcard       | Function                                      |
|----------------|-----------------------------------------------|
| *              | Matches 0 or more characters                  |
| ?              | Matches 1 character                           |
| [abc]          | Matches one of the characters listed          |
| [a-c]          | Matches one character in the range            |
| [!abc]         | Matches any character not listed              |
| [!a-c]         | Matches any character not listed in the range |
| {tacos,nachos} | Matches one word in the list                  |

```
$ ls -l /etc/host*
$ ls -l /etc/hosts.{allow,deny}
$ ls -l /etc/hosts.[!a]*
$ ls -l /etc/host?
```

# quoting

- Double (") quotes can be used:
  - to prevent the shell from interpreting spaces as argument separators,
  - to prevent file name pattern expansion.

```
$echo "Hello World"
Hello World
$echo "You are logged as $USER"
You are logged as vsc30468
$echo *.log
$echo "*.log"
*.log
```

# quoting

- Single quotes bring a similar functionality, but what is between quotes is never substituted

```
$echo 'You are logged as $USER'
You are logged as $USER
```

- Back quotes (`) can be used to call a command within another

```
$cd /lib/modules/`uname -r`; pwd
/lib/modules/2.6.9-1.6_FC2
```

Back quotes can be used within double quotes

```
$echo "You are using Linux `uname -r`"
You are using Linux 2.6.9-1.6_FC2
```

# What was I doing???

- Not to loose your job after closing your laptop:
  - Use NX GUI connection
  - Use command line + tmux
    - Start session: `$ tmux new -s test`
    - Detach session: `Ctrl+b+d` (safe to go)
    - List session: `$ tmux ls`
    - Reattach session: `$ tmux a -t test`
    - Exit screen session (within tmux): `$ exit`

# What was I doing???

## Manage Windows and Session Tabs

|          |                 |
|----------|-----------------|
| Ctrl+B C | Create window   |
| Ctrl+B W | List Windows    |
| Ctrl+B N | Next window     |
| Ctrl+B P | Previous window |
| Ctrl+B F | Find window     |
| Ctrl+B , | Name window     |
| Ctrl+B & | Kill window     |



# What was I doing???

## Panes/splits

Ctrl+B %

Vertical split

Ctrl+B "

Horizontal split

Ctrl+B O

Swap panes

Ctrl+B Q

Show pane numbers

Ctrl+B X

Kill pane

Ctrl+B Arrow  
Keys

Move to pane



# What was I doing???

- Not to loose your job after closing your laptop:
  - Use NX GUI connection
  - Use command line + screen
    - Start session: `$ screen -S test`
    - Detach session: `Ctrl+a+d` (safe to go)
    - List session: `$ screen -ls`
    - Reattach session: `$ screen -r test`
    - Exit screen session (within screen): `$ exit`

# Screen

- Create new window: `ctrl-a c`
- Go to previous/next window: `ctrl-a p/n`
- Go to window by number: `ctrl-a <window-nr>`
- Show current windows, move: `ctrl-a ", <window-nr>`
- Close window: `ctrl-a K`
- Detach screen: `ctrl-a d`
- List current screen sessions: `$ screen -ls`
- Re-attach to session: `$ screen -r <session-id>`
- Kill dead session: `$ screen -wipe`
- Get help: `ctrl-a ?`
- Monitor for activity: `ctrl-a M` (same to stop monitoring)
- Monitor for inactivity: `ctrl-a _` (same to stop monitoring)

# Screen

- Split screen horizontally: ctrl-a S
- Split screen vertically: ctrl-a |
- Go to next screen region: ctrl-a <tab>
- Remove current region: ctrl-a X
- Remove all but current region: ctrl-a Q
- Enter copy mode: ctrl-a [  
• Paste: ctrl-a ]
- Dump window contents to file: ctrl-a h
- Enable logging: ctrl-a H
- Useful .screenrc file that eliminates some of screen's nuisances:
  - # Turn off that annoying start up message
  - startup\_message off
  - # Increase scroll back buffer to a more useful number of lines
  - defscrollback 10000

# Screen - settings

- In your **.bashrc** file

```
case ${TERM} in
 xterm)
 echo "Hello terminal!!!"
 ;;
 screen)
 echo "Hello screen!!!"
 ;;
esac
```

# &

- **&** is a command line operator that instructs the shell to start the specified program **in the background**.
- This allows you to have more than one program running at the same time without having to start multiple terminal sessions.
- Starting a process in background: add **&** at the end of your line:  
**gedit &**  
check with **ps**

# Command history: Arrow Up

- Previously executed commands can be recalled by using the **Up Arrow** key on the keyboard.
- Most Linux distributions remember the last 500 commands by default.
- Display commands that have recently been executed
  - The `history` command displays a user's command line history.
  - You can execute a previous command using `! [NUM]` where NUM is the line number in history you want to recall.
  - The **history** command itself comes at the end of the list. From the command line, the **UP** and **DOWN** arrow keys will quickly traverse this list up and down, while the **LEFT** and **RIGHT** arrow keys will move the cursor to allow the user to edit a given command.

# Command history and sessions

- Not only does the bash shell maintain a command history within a session, but the shell also preserves command histories between sessions. When the bash shell exits, it dumps the current command history into a file called **.bash\_history** in a user's home directory. Upon startup, the shell initializes the command history from the contents of this file.
- What repercussions does this have for multiple interactive shells (owned by the same user) running at the same time? Because the history is only saved to disk as the shell exits, commands executed in one bash process are not available in the command history of a simultaneously running bash process. Also, the last shell to exit will overwrite the histories of any shells that exited previously.



# Command history: Ctrl +R

- This key sequence mimics !cmd in spirit. Text typed after the CTRL+R key sequence is matched against previously typed commands, with the added advantage that matching command lines are viewed immediately as the text is typed.
- You also have the opportunity to edit the recalled line (using the LEFT and RIGHT arrow keys, or other command line editing keystrokes) before executing the command.

# Command history: fc

- The `fc` command allows users to "fix" the previously entered command, by opening up the user's default editor (`vi` by default) with the previously entered command as text. Upon exiting the editor (presumably after somehow editing the command), the new text will be immediately executed. For those proficient in quickly exiting an editor, the command comes in handy.

The image shows three terminal windows side-by-side, illustrating the process of setting up an environment:

- Left window (login1.hpc.kuleuven.be - PuTTY):** Shows the command `module load Python/2.7.6-foss-2014a` being executed.
- Middle window (login1.hpc.kuleuven.be - PuTTY):** Shows the user `vsc30468@hpc-p-login-1` running `module load Python/2.7.6-foss-2014a`, followed by `/usr/bin/modulecmd bash $*`.
- Right window (login1.hpc.kuleuven.be - PuTTY):** Shows the user running `module load Python/2.7.6-foss-2014a`, followed by `/usr/bin/modulecmd bash $*`. It then displays the output of `module li`, listing currently loaded modules such as `mc/4.6.1`, `GCC/4.8.2`, `OpenMPI/1.6.5-GCC-4.8.2`, `gompil/2014a`, `OpenBLAS/0.2.8-gompi-2014a-LAPACK-3.5.0`, `FFTW/3.3.3-gompi-2014a`, `ScaLAPACK/2.0.2-gompi-2014a-OpenBLAS-0.2.8-LAPACK-3.5.0`, `foss/2014a`, `bzip2/1.0.6-foss-2014a`, `zlib/1.2.8-Foss-2014a`, `ncurses/5.9-foss-2014a`, `libreadline/6.3-foss-2014a`, `Tcl/8.6.1-foss-2014a`, `SQLite/3.8.4.1-foss-2014a`, and `Python/2.7.6-foss-2014a`.

# Command history

!**\$**

Repeats the last argument of the last command.

:**h**

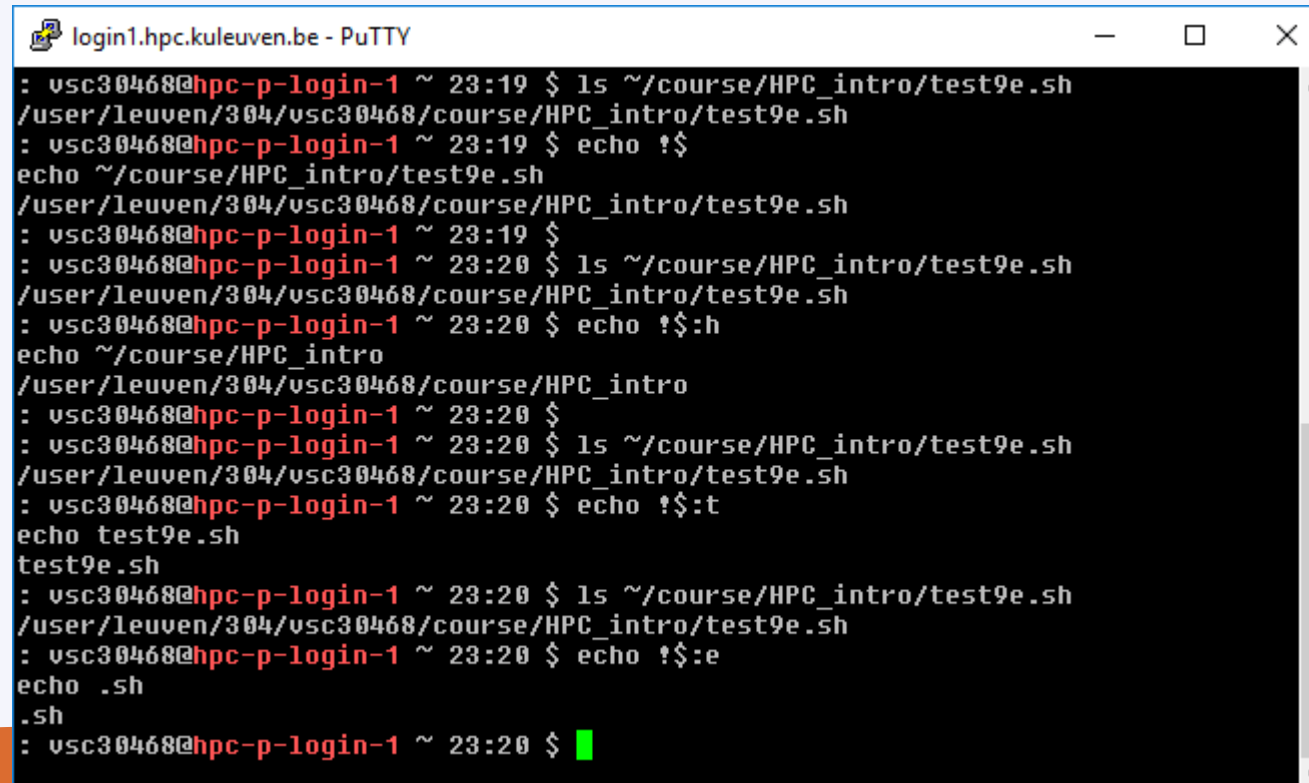
If you put it after a filename, it will change that filename to remove everything up to the folder.

:**t**

Leaves only  
filename

:**e**

Leaves only  
the extension



```
login1.hpc.kuleuven.be - PuTTY
: vsc30468@hpc-p-login-1 ~ 23:19 $ ls ~/course/HPC_intro/test9e.sh
/user/leuven/304/vsc30468/course/HPC_intro/test9e.sh
: vsc30468@hpc-p-login-1 ~ 23:19 $ echo !$
echo ~/course/HPC_intro/test9e.sh
/user/leuven/304/vsc30468/course/HPC_intro/test9e.sh
: vsc30468@hpc-p-login-1 ~ 23:19 $
: vsc30468@hpc-p-login-1 ~ 23:20 $ ls ~/course/HPC_intro/test9e.sh
/user/leuven/304/vsc30468/course/HPC_intro/test9e.sh
: vsc30468@hpc-p-login-1 ~ 23:20 $ echo !$:h
echo ~/course/HPC_intro
/user/leuven/304/vsc30468/course/HPC_intro
: vsc30468@hpc-p-login-1 ~ 23:20 $
: vsc30468@hpc-p-login-1 ~ 23:20 $ ls ~/course/HPC_intro/test9e.sh
/user/leuven/304/vsc30468/course/HPC_intro/test9e.sh
: vsc30468@hpc-p-login-1 ~ 23:20 $ echo !$:t
echo test9e.sh
test9e.sh
: vsc30468@hpc-p-login-1 ~ 23:20 $ ls ~/course/HPC_intro/test9e.sh
/user/leuven/304/vsc30468/course/HPC_intro/test9e.sh
: vsc30468@hpc-p-login-1 ~ 23:20 $ echo !$:e
echo .sh
.sh
: vsc30468@hpc-p-login-1 ~ 23:20 $
```

# List Of Useful Bash Keyboard Shortcuts

- **ALT+B** – Move backward.
- **ALT+F** – Move forward.
- **ALT+T** – Swaps the last two words.
- **ALT+U** – Capitalize all characters in a word after the cursor.
- **ALT+L** – Uncapitalize all characters in a word after the cursor.
- **ALT+.** – Use the last word of the previous command.
- **!!** – Repeats the last command.
- **ESC+t** – Swaps the last two words.
- **CTRL+A** – Quickly move to the beginning of line.
- **CTRL+B** – To move backward one character.
- **CTRL+C** – Stop the currently running command. (Putty and MFA firewall!)

# List Of Useful Bash Keyboard Shortcuts

- **CTRL+D** – Delete one character (backward).
- **CTRL+E** – Move to the end of line.
- **CTRL+F** – Move forward one character.
- **CTRL+H** – Delete the characters before the cursor, same as BACKSPACE.
- **CTRL+J** or **CTRL+M** – Same as ENTER/RETURN key.
- **CTRL+K** – Delete all characters after the cursor.
- **CTRL+L** – Clears the screen and redisplay the line.
- **CTRL+T** – Swaps the last two characters.
- **CTRL+U** – Delete all characters before the cursor (Kills backward from point to the beginning of line).
- **CTRL+W** – Delete the words before the cursor.
- **CTRL+Y** – Retrieves last item that you deleted or cut.
- **CTRL+Z** – Stops the current command.

# Input and Output

- Programs and commands can contain an input and output. These are called 'streams'. UNIX programming is oftentimes stream based.
- STDIN – 'standard input,' or input from the keyboard
- SDTOUT – 'standard output,' or output to the screen
- STDERR – 'standard error,' error output which is sent to the screen.

# File Redirection

- Often we want to save output (stdout) from a program to a file. This can be done with the 'redirection' operator.
  - `myprogram > myfile`
- Similarly, we can **append** the output to a file instead of rewriting it with a double '>>'
  - `myprogram >> myfile`

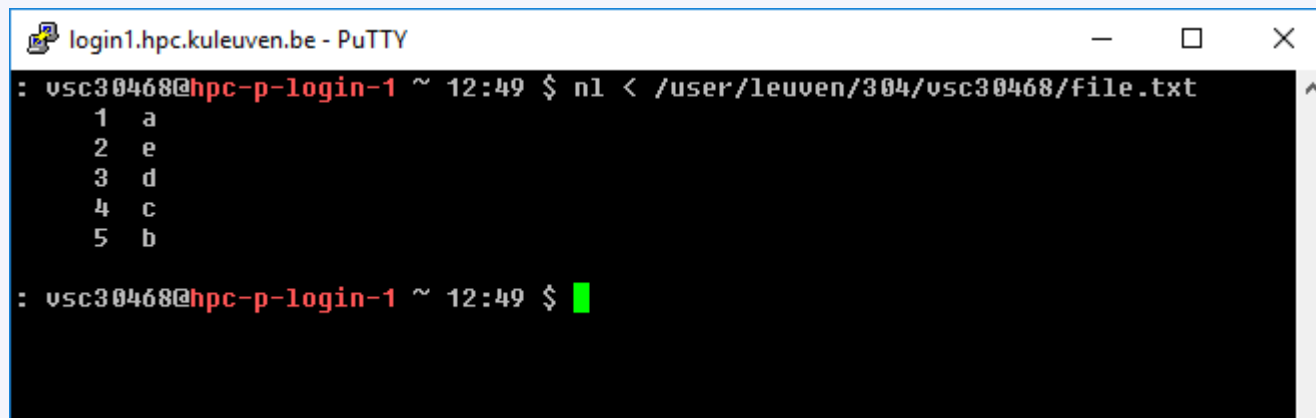
# Redirecting stderr

- Performing a normal redirection will not redirect stderr. In Bash, this can be accomplished with '2>'
  - `command 2> file1`
- Or, one can merge stderr to stdout (most popular) with '2>&1'
  - `command > file 2>&1`



# Input Redirection

- Input can also be given to a command from a file instead of typing it to the screen, using “<” operator
  - `mycommand < programinput`
- Not all commands read standard input (ls, date, who, pwd, cd, ps, ...)



The screenshot shows a PuTTY terminal window titled "login1.hpc.kuleuven.be - PuTTY". The prompt is "usc30468@hpc-p-login-1 ~ 12:49". The user has entered the command "n1 < /user/leuven/304/usc30468/file.txt". The output of the command is displayed as a list of five lines: "1 a", "2 e", "3 d", "4 c", and "5 b". The prompt is now "usc30468@hpc-p-login-1 ~ 12:49 \$" with a green cursor.

```
login1.hpc.kuleuven.be - PuTTY
: usc30468@hpc-p-login-1 ~ 12:49 $ n1 < /user/leuven/304/usc30468/file.txt
1 a
2 e
3 d
4 c
5 b
: usc30468@hpc-p-login-1 ~ 12:49 $
```

# Pipes

- Using a pipe operator ‘|’ commands can be linked together. The pipe will link the standard output from one command to the standard input of another.
- Very helpful for searching files
- e.g. when we want to list the files, but only the ones that contain test in their name:

```
ls -la | grep test
```

# Hands-on 2

# Shell

# Environment variables

- Shells let the user define *variables*. They can be reused in shell commands. By convention, shell variables have lower case names.
- You can also define *environment variables*: variables that are also visible within scripts or executables called from the shell. By convention, environment variables have UPPER CASE names.
- **env**  
Lists all exported environment variables and their value.

# Environment variables

- We can view the environment variables through `set` or `env` commands
- The `set` command will display all the global functions written by the user
- The `env` command displays only the variables and not the functions
- We can reassign values for the variables either temporarily or permanently
  - Temporary
    - Type `export varname=value` at the command prompt
  - Permanent
    - Type `export varname=value` in `.bashrc` in your `$VSC_HOME` directory

# Environment variables

- Control the characteristics of the shell
  - View them with `[set]env`, or `$VARIABLE`
  - Set them with `export`
- Change up your prompt! `export PS1="myNEWprompt: "`
- Modify PATH:  
`export PATH=${PATH}:/home/student/program`
- But these have to be declared every time you use your shell.
- Solution: save them inside `$VSC_HOME/.bashrc`

# Shell variables examples

## Shell variables (bash)

```
projdir=$VSC_HOME/Downloads
ls -la $projdir; cd $projdir
```

## Environment variables (bash)

```
cd $HOME
```

```
export DOC=$HOME/Documents
echo $DOC
```

```
/user/leuven/304/vsc30468/Documents
```

(displays the information if parameter is set)



# Standard environment variables

Used by lots of applications!

**LD\_LIBRARY\_PATH**

Shared library search path

**DISPLAY**

Screen id to display X (graphical) applications on.

**EDITOR**

Default editor (vi, emacs...)

**HOME**

Current user home directory

**HOSTNAME**

Name of the local machine

**MANPATH**

Manual page search path

**PATH**

Command search path

**PRINTER**

Default printer name

**SHELL**

Current shell name

**TERM**

Current terminal type

**USER**

Current user name

# PATH environment variables

e.g. `which` or `whereis` searches in that location

## PATH

Specifies the shell search order for commands

```
/home/abox/bin:/usr/local/bin:/usr/kerberos/bin:/usr/bin:/bin
:/usr/X11R6/bin:/bin:/usr/bin
```

e.g. `whereis` searches in that location

## LD\_LIBRARY\_PATH

Specifies the shared library (binary code libraries shared by applications, like the C library) search order for `ld`

```
/usr/local/lib:/usr/lib:/lib:/usr/X11R6/lib
```

## MANPATH

Specifies the search order for manual pages

e.g. `whereis` searches in that location

```
/usr/local/man:/usr/share/man
```

# Environment variables

- **Paths** (\$PATH, \$LD\_LIBRARY\_PATH, \$MAN\_PATH, \$CPATH, ...) are modified when modules are loaded
- After “module load” env will display a new value:

## Example

```
$> echo $PATH
/user/leuven/307/vsc30745/.tmux/bin:/apps/leuven/bin:/usr/local/bin:/usr/lpp/mmfs/bin:./usr/bin:/usr/sbin:/opt/moab/bin:/opt/mam/bin:/usr/local/bin:/usr/bin:/usr/local/sbin:/usr/sbin:/opt/ibutils/bin
$> module load matlab/R2019a
$> echo $PATH
/apps/leuven/skylake/2018a/software/MATLAB/R2019/bin:/user/leuven/307/vsc30745/.tmux/bin:/apps/leuven/bin:/usr/local/bin:/usr/lpp/mmfs/bin:./usr/bin:/usr/sbin:/opt/moab/bin:/opt/mam/bin:/usr/local/sbin
```

# Do-It-Yourself

## Example

```
$> module purge # start from clean slate
$> env | grep PATH # default PATH(s)
$> which python
$> module load Python/3.6.4-intel-2018a
$> env | grep PATH # PATH(s) are modified
$> which python
```

## Questions

1. Which new directories are now added to \$PATH?
2. Which python was originally used (after login)?
3. Which python is used after `module load`?

# Aliasing

- Alias – Alternate name for a command(s)
- You can be inventive with it, but be careful
- If you log out from bash, your aliases will be purged!
- To define an alias permanently, put it in your `.bashrc`
- E.g.  
Image, your jobs always store the results in your scratch folder.  
So, you want an easy way to copy them to your data folder:

```
alias backup="cp -r $VSC_SCRATCH/results $VSC_DATA/backup"
```

- To disable an alias, do:

```
unalias backup
```

# Alias and Unalias

- `alias newname=oldname`
  - eg. `alias copy=cp`
- Then we can use `copy` in the same way we use `cp` command
  - eg. `copy file1 file2` //copies content of file1 to file2
- To remove alias use `unalias` command
  - `unalias copy`
- After this we cannot use `copy` to perform copying function

# Alias

Shells let you define command *aliases*: shortcuts for commands you use very frequently.

## Examples

```
alias la='ls -la'
```

Useful to always run commands with default arguments.

```
alias rmi='rm -i'
```

Useful to make **rm** always ask for confirmation.

```
alias data='cd /data/leuven/304/vsc30468'
```

Useful to replace very long and frequent commands.

```
alias schck='. /home/mag/env/chck.sh'
```

Useful to set an environment in a quick way

(. is a shell command to execute the content of a shell script).

# which command

Before you run a command, `which` tells you where it is found

```
which ls
```

```
alias ls='ls --color=auto'
 /usr/bin/ls
```

```
which alias
```

```
/usr/bin/alias
```

```
which help
```

```
/usr/bin/which: no help in
(/usr/local/bin:/usr/local/sbin:/usr/bin:/usr/sbin:/bin
:/sbin:/home/mag/.local/bin:/home/mag/bin)
```



# ~/.bashrc file

~/.bashrc

Shell script read each time a bash shell is started (login, or when the job starts on a compute node)

You can use this file to define

- Your default environment variables (PATH, EDITOR...).
- Your aliases.
- Your prompt (see the [bash](#) manual for details).
- A greeting message.

Do NOT put “`module load`” in your `.bashrc`. It creates conflicts

# bash configuration Files

- bash has two different login files.
  - **.bashrc** gets read when you open a local shell on a machine
  - **.bash\_profile** only gets read if and only if you login from a remote machine. Note that **.bash\_profile** itself reads in your **.bashrc** file as well.
- If you want aliases to be executed regardless, then you should put them in the **.bashrc** file.
- On the cluster please edit only **.bashrc** file – in case of problem we can always allow you access thanks to correct **.bash\_profile**

# ~/.bash\_profile

- This is how your ~/.bash\_profile looks like
- Tip: never touch it

~/.bash\_profile

```
File: ~/.bash_profile
Get the aliases and functions
Get whatever is in your
.bashrc config file
if [-f ~/.bashrc]; then
 . ~/.bashrc
fi
```

```
File: .bashrc
Description: A default .bashrc
###Source global defs###
if [-f /etc/bashrc]; then
 . /etc/bashrc
fi
```

```
###set the prompt###
uncomment out only one
this is hostname and time
PS1="\h-(\@): "
this is hostname and
history number
#PS1="\h-(\!)# "
this is hostname and
working directory
#PS1="\h-(\w)# "
this is hostname and
shortened working
directory
#PS1="\h-(\W)# "
```

```
path manipulation
add ~/bin to the path,
cwd as well
PATH="$PATH:$HOME/bin:./"

env variables
make sure that you
change this to your
username
MAIL="/afs/umbc.edu/users/u/s/username/M
ail/inbox"
export PATH
unset USERNAME

User-specific aliases
and functions
alias rm="rm -i"
```

# Flavours of Unix Shells

- Two main flavours of Unix Shells
  - **Bourne** (or Standard Shell): `sh`, `ksh`, `bash`, `zsh`
    - Fast
    - `$` for command prompt
  - **C shell**: `csch`, `tcsh`
    - easier for scripting
    - `%`, `>` for command prompt
- To check shell:
  - `% echo $SHELL` (shell is a pre-defined variable -default)
  - `% echo $shell` (shell that is running)
- To switch shell:
  - `% exec <shellname>`     #e.g., `% exec bash`
  - `$ shellname`

# What shell am I running?

- Use the `echo` command  
E.g., to check your `SHELL` environment variable:

```
mag@localhost ~]$ tcsh
[mag@localhost ~]$ echo $SHELL
/bin/bash
[mag@localhost ~]$ echo $shell
/bin/tcsh
[mag@localhost ~]$
```

- Issue a `ps` command to see all the processes in your current login session

# Customization of a Session

- Each shell supports some customization.
  - User prompt
  - Where to find mail
  - Shortcuts (alias)
- The customization takes place in *startup* files
  - Startup files are read by the shell when it starts up
  - The Startup files can differ for different shell

# Startup files

- **sh,ksh:**

/etc/profile (out-of-the-box login shell settings)  
/etc/profile.local (addtnl. local system settings)  
~/.profile (addtnl. user customized settings)  
~/.kshrc (non-login shell user customization)

- **bash:**

/etc/profile (out-of-the-box login shell settings)  
/etc/bash.bashrc (out-of-box non-login settings)  
/etc/bash.bashrc.local (global non-login settings)  
~/.bash\_profile (login shell user customization)  
~/.bashrc (non-login shell user customization)  
~/.bash\_logout (user exits from interactive login shell)

- **cshtcsh:**

/etc/login (out-of-the-box login shell settings)  
/etc/csh.login (non-login shell customizations)  
/etc/csh.login.local (global non-login settings)  
~/.login: (login shell user customizations)  
~/.cshrc: (non-login shell user customizations)  
~/.cshrc.logout: (non-login shells at logout)  
~/.logout: (read by login shells at logout)



# Customization of a Session - prompt

- **LOGNAME**: contains the user name
- **HOSTNAME**: contains the computer name.
- **RANDOM**: random number generator
- **SECONDS**: seconds from the beginning of the execution
- **PS1**: sequence of characters shown before the prompt
  - \t** hour
  - \d** date
  - \w** current directory
  - \W** last part of the current directory
  - \u** user name
  - \\$** prompt character

# Customization of a Session

- To add colors to the shell prompt check the following command syntax:

```
$ echo '\e[x;ym test \e[m'
```

Where,

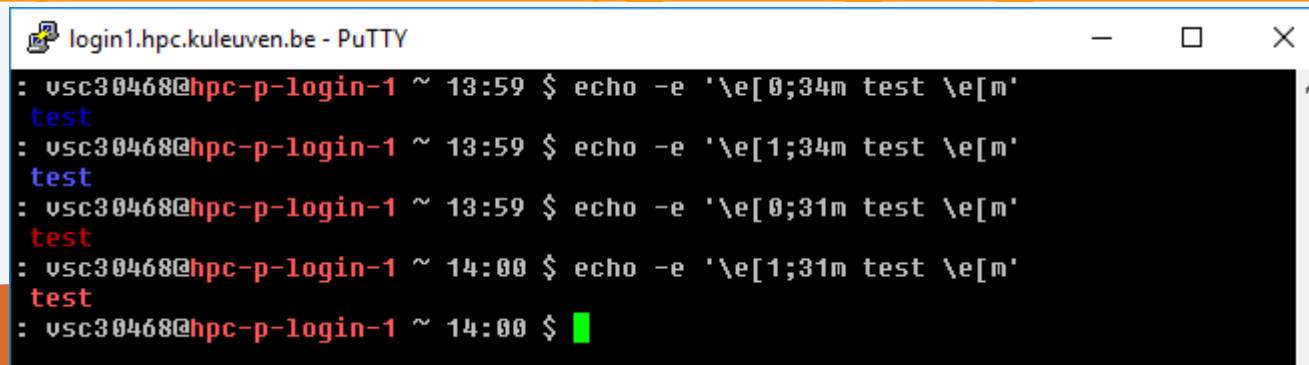
- \e[ : Start color scheme.
- x;y : Color pair to use (x;y)
- test: to be printed
- \e[m : Stop color scheme.

| Color  | Code |
|--------|------|
| Black  | 0;30 |
| Blue   | 0;34 |
| Green  | 0;32 |
| Cyan   | 0;36 |
| Red    | 0;31 |
| Purple | 0;35 |
| Brown  | 0;33 |

Note: You need to replace digit 0 with 1 to get light color version.

- More info about colors e.g. at

[http://misc.flogisoft.com/bash/tip\\_colors\\_and\\_formatting](http://misc.flogisoft.com/bash/tip_colors_and_formatting)

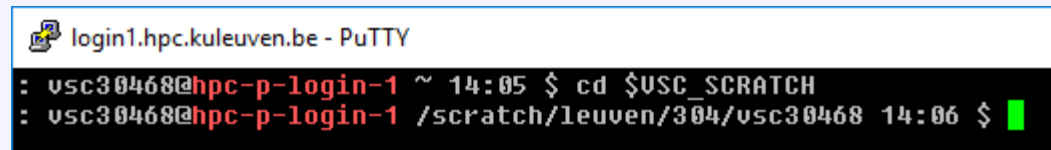


```
login1.hpc.kuleuven.be - PuTTY
: vsc30468@hpc-p-login-1 ~ 13:59 $ echo -e '\e[0;34m test \e[m'
test
: vsc30468@hpc-p-login-1 ~ 13:59 $ echo -e '\e[1;34m test \e[m'
test
: vsc30468@hpc-p-login-1 ~ 13:59 $ echo -e '\e[0;31m test \e[m'
test
: vsc30468@hpc-p-login-1 ~ 14:00 $ echo -e '\e[1;31m test \e[m'
test
: vsc30468@hpc-p-login-1 ~ 14:00 $
```

# Customization of a Session

- Standard PS1:

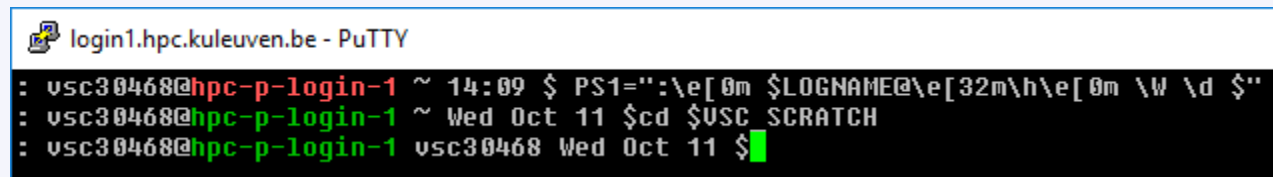
```
\u@\[\e[1;31m\]\h\[\e[0m\] \w `date +%H:%M`
```



```
login1.hpc.kuleuven.be - PuTTY
: vsc30468@hpc-p-login-1 ~ 14:05 $ cd $VSC_SCRATCH
: vsc30468@hpc-p-login-1 /scratch/leuven/304/vsc30468 14:06 $
```

- Change PS1, e.g.

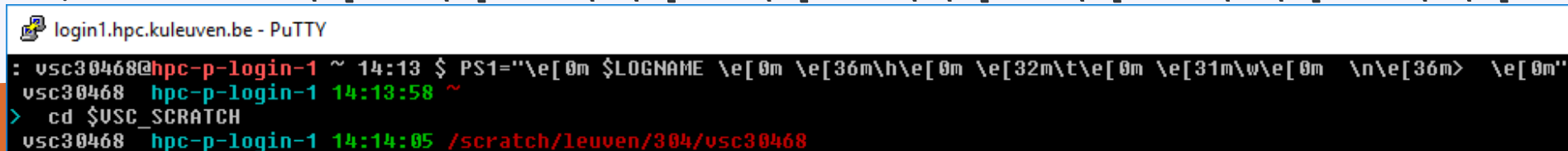
```
PS1=":\e[0m $LOGNAME@\e[32m\h\e[0m \W \d $"
```



```
login1.hpc.kuleuven.be - PuTTY
: vsc30468@hpc-p-login-1 ~ 14:09 $ PS1=":\e[0m $LOGNAME@\e[32m\h\e[0m \W \d $"
: vsc30468@hpc-p-login-1 ~ Wed Oct 11 $cd $VSC_SCRATCH
: vsc30468@hpc-p-login-1 vsc30468 Wed Oct 11 $
```

- Another example:

```
PS1="\e[0m $LOGNAME \e[0m \e[36m\h\e[0m \e[32m\t\e[0m \e[31m\w\e[0m \n\e[36m> \e[0m"
```




```
login1.hpc.kuleuven.be - PuTTY
: vsc30468@hpc-p-login-1 ~ 14:13 $ PS1="\e[0m $LOGNAME \e[0m \e[36m\h\e[0m \e[32m\t\e[0m \e[31m\w\e[0m \n\e[36m> \e[0m"
vsc30468 hpc-p-login-1 14:13:58 ~
> cd $VSC_SCRATCH
vsc30468 hpc-p-login-1 14:14:05 /scratch/leuven/304/vsc30468
```

# Environment Variables

- Use the **env** command to see all environment variables
- **set/export** to see all shell variables
- Set or change environment variables from the command-line:  
new values last only for current login session.

sh/bash/ksh      **set:** NEW\_VARIABLE=newvalue  
                  **append:** OLD\_VARIABLE=\$OLD\_VARIABLEnewvalue  
                  **prepend:** OLD\_VARIABLE=newvalue\$OLD\_VARIABLE  
                  **add:** OLD\_VARIABLE=\${OLD\_VARIABLE}:newvalue  
                  **export** OLD\_VARIABLE

csh/tcsh            **set:** set NEW\_VAR=newvalue  
                  **append:** set OLD\_VAR=(\$OLD\_VAR newvalue)  
                  **prepend:** set OLD\_VAR=(newvalue \$OLD\_VAR)  
  
                  **set:** setenv OLD\_VAR newvalue  
                  **append:** setenv OLD\_VAR \${OLD\_VAR}newvalue  
                  **prepend:** setenv OLD\_VAR newvalue\${OLD\_VAR}



The order decides where system checks for command first (important if you have your own version and there is another version on the cluster)

# Introduction to bash

- The bash shell is one of the many shells that are available to you on the VSC nodes.
- Almost any installation of Linux defaults to the bash shell.
- bash is one of the many GNU.org (<http://www.gnu.org>) projects.
- bash manuals:
  - A comprehensive online manual is provided at <http://www.gnu.org/software/bash/manual/bashref.html>
  - Aliases - <http://www.gnu.org/software/bash/manual/bashref.html#Aliases>
  - Controlling the Prompt - <http://www.gnu.org/software/bash/manual/bashref.html#Controlling-the-Prompt>

# Universal customization

- Universal .bashrc - written to run on all (relevant) clusters:

```
case ${VSC_INSTITUTE_CLUSTER} in
 breniac)
 ulimit -c 500000
 export LD_LIBRARY_PATH="${HOME}/lib:${LD_LIBRARY_PATH}"
 export PATH="${HOME}/bin:${HOME}/sbin:${PATH}"
 export EDITOR="/usr/bin/vim"
 export PS1=': \u@\[\e[1;31m\]\h\[\e[0m\] \w `date +%H:%M` $ '
 source ${HOME}/.autoenv/activate.sh
 ;;
 genius)
 export EDITOR="/usr/bin/vim"
 alias vim="vim -u .vimrc-simple"
 export PS1=': \u@\[\e[1;34m\]\h\[\e[0m\] \w `date +%H:%M` $ '
 ;;
esac
```

# Hands-on 3

# Shell scripts



# Using the Shell

Command Line Interpreter or CLI

To understand scripts let's practice a bit with the CLI.

At the shell prompt try:

```
cd; echo "Hello, World" > test.txt;
cp test.txt test.txt.bak; vi test.txt
```

The above is all on one line.

What happened?

# Using the Shell

In a file

Create a new file and place the some of commands in it:

```
$ cd $VSC_DATA
$ vim newscript.sh
 echo "Hello world" > hello.txt
 cp hello.txt hello.txt.bak
 cat hello.txt hello.txt.bak > new.txt
 cat new.txt
```

# Using the Shell

In a file

Now we can execute those commands in the order in which they appear in the file by doing this.

There are 3 ways to execute a script:

`$> bash newscript`

`$> sh newscript`

`$> . newscript`

In a sub-shell

In the current shell

# Using the Shell

As a shell script

Now we can take the last step and start to create self-contained scripts that run on their own.

We'll need to do two things:

1. Specify the CLI to use, and
2. Make the script executable  
`chmod +x <script_name>`

# The “Shebang”

To specify that a file is to become a shell script you specify the interpreter like this at the very start of the file:

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

- Shebang is a comment line, so practically not executed
- Shebang starts with #!
- Then, shebang gives the path to an executable that will interpret the script
- E.g. other typical shebangs could be:
  - `#!/bin/python`
  - `#!/bin/perl`
  - `#!/bin/csh`

# When Not to Use Scripts?

- Resource-intensive tasks, especially where speed is a factor (sorting, hashing, etc.)
- Procedures involving heavy-duty math operations, especially floating point arithmetic arbitrary precision calculations, or complex numbers
- Cross-platform portability required
- Complex applications, where structured programming is a necessity (need type-checking of variables, function prototypes, etc.)
- Project consists of subcomponents with interlocking dependencies
- Extensive file operations required (Bash is limited to serial file access, and that only in a particularly clumsy and inefficient line-by-line fashion)
- Need native support for multi-dimensional arrays or data structures, such as linked lists or trees
- Need to generate or manipulate graphics or GUIs
- Need direct access to system hardware or port or socket I/O

# What's Next?

Now let's create a very simple shell script. This will simply echo back what you enter on the command line:

```
#!/bin/bash
echo $1
```

Enter this in a file `new.sh`, then do:

```
chmod 755 new.sh
```

To run the script do:

```
./new.sh text
```

# Shell scripts

- Shell scripts are “programs” that are completely uncompiled, but read and executed by the shell line by line.
- Typically end in `.sh`
- Must be executable with `chmod`
- Start with a “shebang” – tells the shell what to use to interpret it. e.g.,
  - `#!/bin/bash` for a bash script.



# Bash vs. C

## Bash

```
• #! /bin/bash

• number=3
• name="bob"
• echo "$name is your
 chosen name, $number
 your chosen number."

• let inc=number+1
• if ["$inc" == "4"]
 then echo "Addition
 works like a charm."
 fi
```

## C

```
• #include <stdio.h>
• #include <cs50.h>

• int number = 3;
• string name = "bob";
• printf("%s is your chosen
 name, %d your chosen
 number.\n", number, name);

• int inc = number++;
• if (inc == 4) {
 printf("Addition
 works like a
 charm.\n");
 }
```

# Bash vs. C

|                 | Bash                                 | C                                                         |
|-----------------|--------------------------------------|-----------------------------------------------------------|
| Language        | interpreted                          | compiled                                                  |
| Variable types  | Everything is string                 | Multiple types;<br>declaration needed                     |
| Variable access | Via \$                               | By name                                                   |
| At runtime      | Uses other Linux programs<br>to work | Uses subroutines &<br>functions from libraries to<br>work |
| Spacing         | Matters a lot                        | Matters much less                                         |
| Line endings    | None                                 | ;                                                         |

# Resources

The on-line *Advanced Bash Scripting Guide*, available at:

<http://www.tldp.org/LDP/abs/html/>

## Languages

### Interpreted

Bash, Perl, Python

### Compiled

C, C++, Fortran

## Tools

- **sed:** Stream EDitor
- **awk:** Pattern scanning & processing
- **bc:** Arbitrary precision calculator
- **tr:** Translate or delete characters
- **grep:** Print lines matching a pattern

# Example: PBS Job Script

PBS scripts do not need to be executable  
– they are submitted to the queue and executed some other way.

```
#!/bin/bash -l
#PBS -l walltime=00:10:00
#PBS -l nodes=1:ppn=36
#PBS -l pmem=5gb
#PBS -N testjob
#PBS -A lp_hpcinfo_training
#PBS -m abe
#PBS -M my.name@kuleuven.be

set -e
module load intel/2018a

cd $PBS_O_WORKDIR
cp /apps/leuven/training/HPC-intro/cpujob.pbs $VSC_SCRATCH
touch output.log
echo I am done
```

Shebang

Resource List

Module load(s)

Move data

Execute commands

# Hands-on 4

# Application development

# Installing applications – home linux

- Automatic way: **yum**
- Yum is an interactive, rpm based, package manager.
- To check the package: `yum search phrase`
- To install `yum install package-name` (root only!)
- To check installed packages: `yum list installed`
- Possibility to install downloaded rpm package: **rpm -i package**

# Manual installations

- Some applications provide binary files – ready to use after unpacking.
- Check the system – different flavours and architectures!



# Compatibility Statement

- **Definition of the OS version**
  - Kernel version (i.e. kernel 3.10.0-1062.1.2.el7.x86\_64)
  - glibc version (i.e. glibc 2.17)
- **Determining the OS Version**
  - Kernel version (`$ uname -r -> 3.10.0-1062.1.2.el7.x86_64`)
  - System distribution (`$ uname -a`)
  - glibc version (`$ ldd --version -> 2.17`)
  - `$ rpm -qa | grep libc -> glibc-2.17`
- **Determining the OS Flavour/release**
  - `$ cat /etc/*-release`

# Manual installations

- Some simple programs will only require compiling (hello world example from HPC intro:  

```
cp -r /apps/leuven/training/HPC_intro $VSC_HOME; cd HPC_intro
module load foss/2018a; mpicc helloworldmpi.c -o hello.exe
mpirun ./hello.exe
```
- Lots of specific (less frequently used) applications will require the whole configuration (configure-make process) and installation process. Usually manual is provided with instructions (README.txt)

# Compiling simple applications

- The compiler used for all Linux systems is GCC  
<http://gcc.gnu.org>
- To compile a single-file application, developed in C :  
`gcc -o test test.c`  
Will generate a `test` binary, from the `test.c` source file
- For C++ :  
`g++ -o test test.cc`
- The `-Wall` option enables more warnings  
To compile sources files to object files and link the application :  
`gcc -c test1.c`  
`gcc -c test2.c`  
`gcc -o test test1.o test2.o`  
gcc automatically calls the linker `ld`

# make

- The compilation process can be automated using GNU `make` tool:  
<http://www.gnu.org/software/make/manual/>
- `make` reads a file called `Makefile` from the current directory, and executes the rules described in this file
- Every rule has a target name, a colon, and a list of dependencies, and the list of commands to generate the target from the dependencies
- When simply running `make`, the default target that is generated is “all”. A target is only re-generated if dependencies have changed
- Every year, we offer `make` training (half a day).  
Check: <https://www.vscentrum.be/training>

# make

- Makefiles are nice, but they don't easily allow easy adaptation to the different build environment and different build options
- More elaborated build systems have been developed  
Autotools (automake, autoconf), based on Makefiles and shell scripts. Even though they are old and a little bit difficult to understand, they are the most popular build system for free software packages.  
CMake, a newer, cleaner build system  
Sconcs and Waf, other build systems based on Python
- The typical steps to compile a autotools based package are:  
`./configure --prefix=/location-of-the-installation)`  
`make`  
`sudo make install (when admin rights necessary)`  
or  
`make install`

# Python and R packages installation

# Installing your own packages using conda

## Installing Miniconda

- Download the Bash script that will install it from conda.io using, e.g., wget:  

```
$ wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh
```
- Once downloaded, run the installation script:  

```
$ bash Miniconda3-latest-Linux-x86_64.sh -b -p $VSC_DATA/miniconda3
```
- Optionally, you can add the path to the Miniconda installation to the PATH environment variable in your .bashrc file. This is convenient, but may lead to conflicts when working with the module system or OS, so make sure that you know what you are doing in either case.  
The line to add to your .bashrc file would be:  

```
export PATH="${VSC_DATA}/miniconda3/bin:${PATH}
```

**May create conflicts for NX login!**

# Installing Python packages using conda

## Creating an environment

- First, ensure that the Miniconda installation is in your PATH environment variable. The following command should return the full path to the conda command:  

```
$ which conda
```
- If the result is blank, or reports that conda can not be found, modify the `PATH` environment variable appropriately by adding miniconda's bin directory to PATH.
- Creating a new conda environment is straightforward:  

```
$ conda create -n science numpy scipy matplotlib
```
- This command creates a new conda environment called science, and installs a number of Python packages.
- This will default to the latest Python 3 version, if you need a specific version, e.g., Python 2.7.x, this can be specified as follows:  

```
$ conda create -n science python=2.7 numpy scipy matplotlib
```



# Installing Python packages using conda

## Working with the environment

- To work with an environment, you have to activate it. This is done with, e.g.,  
`$ source activate science`  
Here, science is the name of the environment you want to work in.

## Install an additional package

- To install an additional package, e.g., `pandas`, first ensure that the environment you want to work in is activated.  
`$ source activate science`
- Next, install the package:  
`$ conda install pandas`  
Note that conda will take care of all dependencies, including non-Python libraries. This ensures that you work in a consistent environment.

# Installing Python packages - alternatives

## Checking for installed packages

- Pip utility will list all packages that are installed for the Python distribution you are using, including those installed by you, i.e., those in your `PYTHONPATH` environment variable.
- Load the module for the Python version you wish to use, e.g.,:  
`$ module load Python/2.7.14-foss-2018a`
- Run pip:  
`$ pip freeze`
- Note that some packages, e.g., `mpi4py`, `h5py`, `pytables`, ..., are available through the module system, and have to be loaded separately. These packages will not be listed by pip unless you loaded the corresponding module.
- If you have any packages installed in `.local` directory, it will always take priority on whatever the Python version used (conda, module, system). That can lead to strange problems, so please avoid using that location.

# Installing Python packages - pip

1. Load the appropriate Python module, i.e., the one you want the python package to be available for:

```
$ module load Python/2.7.14-foss-2018a
```

2. Create a directory to hold the packages you install, the last three directory names are mandatory:

```
$ mkdir -p "${VSC_HOME}/python_lib/lib/python2.7/site-packages/"
```

3. Add that directory to the `PYTHONPATH` environment variable for the current shell to do the installation:

```
$ export PYTHONPATH="${VSC_HOME}/python_lib/lib/python2.7/site-packages/:${PYTHONPATH}"
```

4. Add the following to your `.bashrc` so that Python knows where to look next time you use it:

```
export PYTHONPATH="${VSC_HOME}/python_lib/lib/python2.7/site-packages/:${PYTHONPATH}"
```

5. Install the package, using the `prefix` install option to specify the install path (this would install the sphinx package):

```
$ pip install --user sphinx
```

or

```
$ pip install --install-option="--prefix=${VSC_HOME}/python_lib" sphinx
```

# Installing Python packages – easy\_install

1. Load the appropriate Python module, i.e., the one you want the python package to be available for:

```
$ module load Python/2.7.14-foss-2018a
```

2. Create a directory to hold the packages you install, the last three directory names are mandatory:

```
$ mkdir -p "${VSC_HOME}/python_lib/lib/python2.7/site-packages/"
```

3. Add that directory to the PYTHONPATH environment variable for the current shell to do the installation:

```
$ export PYTHONPATH="${VSC_HOME}/python_lib/lib/python2.7/site-packages/:${PYTHONPATH}"
```

4. Add the following to your .bashrc so that Python knows where to look next time you use it:

```
export PYTHONPATH="${VSC_HOME}/python_lib/lib/python2.7/site-packages/:${PYTHONPATH}"
```

5. Install the package, using the prefix option to specify the install path (this would install the sphinx package):

```
$ easy_install --prefix="${VSC_HOME}/python_lib" sphinx
```

# Installing R packages using conda

## Creating an environment

- First, ensure that the Miniconda installation is in your PATH environment variable. The following command should return the full path to the conda command:  
`$ which conda`
- If the result is blank, or reports that conda can not be found, modify the `PATH` environment variable appropriately by adding miniconda's bin directory to PATH.
- Creating a new conda environment is straightforward:  
`$ conda create -n science -c r r-essentials r-rodnc`  
This command creates a new conda environment called science, and installs essentials and required packages.

Each package separately in a new env – developers  
do not care about versions!

# Installing R packages using conda

## Working with the environment

- To work with an environment, you have to activate it. This is done with, e.g.,  
`$ source activate science`  
Here, science is the name of the environment you want to work in.

## Install an additional package

- To install an additional package, e.g., ``r-ggplot2``, first ensure that the environment you want to work in is activated.  
`$ source activate science`
- Next, install the package:  
`$ conda install -c r r-ggplot2`  
Note that conda will take care of all independencies. This ensures that you work in a consistent environment.

# Installing R packages using conda

## Updating/removing

- Using conda, it is easy to keep your packages up-to-date. Updating a single package (and its dependencies) can be done using:  
`$ conda update r-rodbc`
- Updating all packages in the environment is trivial:  
`$ conda update --all`
- Removing an installed package:  
`$ conda remove r-mass`

## Deactivating an environment

- To deactivate a conda environment, i.e., return the shell to its original state, use the following command  
`$ source deactivate`

# Installing other R packages using conda

- Installing CRAN package:

```
> install.packages('readr', repos='http://cran.us.r-project.org')
```

- Alternative approach:

```
$ conda skeleton cran readr
```

```
$ conda build r-readr
```

```
$ conda install --use-local r-readr
```

Doing that for the first time you need to install conda-build before:

```
$ conda install conda-build
```

- Some packages not available in r-essentials are still available on conda channels, in that case, it's simple:

```
$ conda config --add channels r; conda install r-readxl
```



# Installing R packages – alternatives

1. Load the appropriate R module, i.e., the one you want the package to be available for:

```
$ module load R/3.6.0-foss-2018a-bare
```

2. start R and install the package from there:

```
> install.packages("DEoptim")
```

3. Alternatively you can download the desired package:

```
$ wget cran.r-project.org/src/contrib/Archive/DEoptim/DEoptim_2.0-0.tar.gz
```

And Install the package from the command line:

```
$ R CMD INSTALL DEoptim_2.2-3.tar.gz -l /$VSC_HOME/R/
```

4. These packages might depend on the specific R version, so you may need to reinstall them for the other version.

# Hands-on 5

# Usefull link(s) – tips and tricks:

- <http://gjbex.github.io/training-material/LinuxTools/>
  - bash
  - cdargs
  - grep
  - network
  - screen
  - ssh
  - tmux
  - top
  - vim

# Questions

Helpdesk:

[hpcinfo@kuleuven.be](mailto:hpcinfo@kuleuven.be) or [https://admin.kuleuven.be/icts/HPInfo\\_form/HPC-info-formulier](https://admin.kuleuven.be/icts/HPInfo_form/HPC-info-formulier)

VSC web site:

<http://www.vscentrum.be/>

VSC documentation: <https://docs.vscentrum.be>

VSC agenda: training sessions, events

Systems status page:

<http://status.kuleuven.be/hpc>



*Stay Connected  
to VSC*

**Linked**  <sup>®</sup>



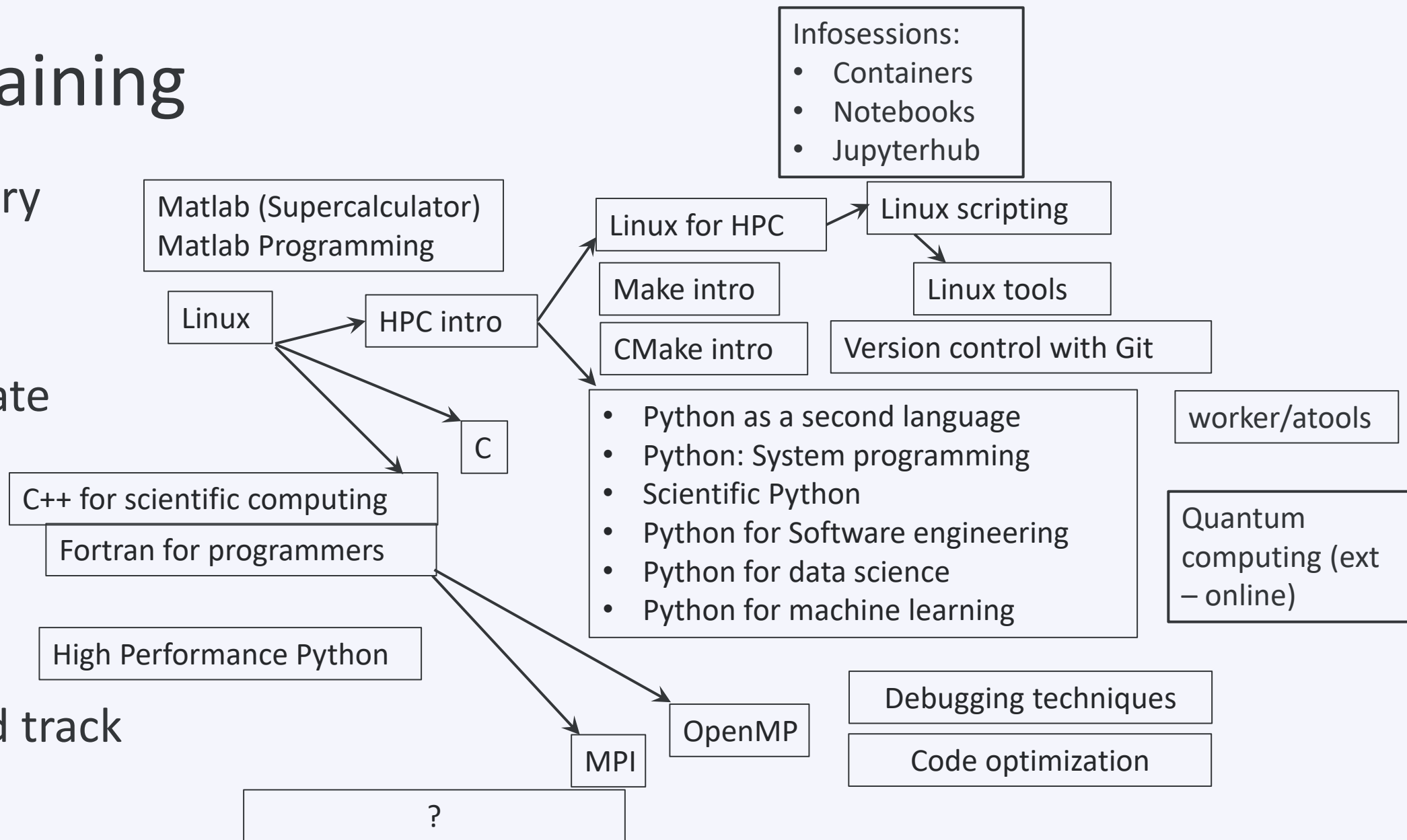
# VSC training

- Introductory

- Intermediate

- Advanced

- Specialized track



PRACE MOOC Defensive programming and debugging and Fortran for Programmers (announced by e-mail)